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Tom Rother

Green's Functions in Classical Physics

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The mill where George Green lived and died in 1841. Today it is a part of the Green's Windmill and Science Centre in Nottingham, UK

Preface

This book is singing the praises of Green's functions. Its concept was formed a couple of years ago, after finishing a consistent Green's function formulation of electromagnetic wave scattering on nonspherical objects. It turned out that such a consistent Green's function formulation provides a sound mathematical basis to discuss the advantages and disadvantages of different numerical approaches which have been developed so far to solve those scattering problems. But I became already acquainted with similar mathematical structures during my early PhD activities in the field of quantum statistics. This long-lasting activity with Green's functions led me to the issue of the conceptual importance of these functions for physics, in general. Unfortunately, even today Green's functions are often considered and discussed only from the point of view of an appropriate mathematical tool for solving differential equations. The works of J. Schwinger and F. Dyson belong to the few exceptions which emphasize the conceptual importance of these functions in quantum statistics and quantum field theory.

Starting from these experiences and first but more philosophical considerations—where the latter are reflected in the prologue of this book—I tried to apply the Green's function formalism to well-known problems of classical physics, some of which are usually solved not by this formalism but other methods. This activity was aimed at convincing myself from the conceptual importance of Green's functions also in classical fields of physics. The present book is the result of this effort. It is written as an introduction for those who want to become more familiar with Green's functions and their importance and usage in classical physics. However, a short outlook regarding the importance of Green's functions in quantum mechanics as well as their calculation by use of the methods discussed in the foregoing chapters is provided in the final chapter of this book. Looking at physics from the point of view formulated in the prologue proved to be very helpful for me when I tried to enter new fields of physics. Maybe the reader will also benefit from this point of view.

Finally, I would like to express my deepest gratitude to my parents Elisabeth and Fritz Rother, to my wife Doreen and to my teacher Prof. Wolf-Dietrich Kraeft for their support in manyfold ways and their continuous interest in my scientific

activities over decades. Special thanks go also to Mr. J. Duff, heritage development officer from the Green's Windmill and Science Centre, Nottingham (UK), for providing me with the cover picture of Green's windmill. I would also like to thank Dr. C. Ascheron, senior editor at Springer Science and Business Media, for his continuous interest and assistance in publishing this book.

Neustrelitz, Germany Tom Rother
Autumn, 2016

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Chapter 1
Prologue

Experience is an individual process. Language is a cultural process of abstraction

1.1 About the "State" of Physics

On the occasion of an international congress of mathematicians that was taking place in Paris in 1900 David Hilbert gave his famous lecture on "mathematical problems". In this lecture he addressed a number of questions, the answers to which he considered to be most important for the further development of mathematics. Problem number 6 is concerned with the mathematical treatment of the axioms of physics. Hilbert himself has considered this problem in detail. In 1924 he published a paper entitled "Grundlagen der Physik" (Engl.: "Foundations of Physics") in the "Mathematische Annalen" (Hilbert 1924). In this paper he proposed a system of axioms that is based on field theoretical considerations. This system of axioms was aimed at overcoming the predominant mechanical point of view on physics at this time. However, the fast development of Quantum Mechanics that passed off in parallel soon led into a total new physics that could neither be explained in terms of particles nor in terms of fields. This new branch of physics came along with new mathematical structures whose epistemological consequences are still under (sometimes quite controversial!) discussions. At this congress Hilbert advocated also a strict axiomatic and self-contained foundation of mathematics—the so-called "Hilbert's program". But this program was soon overthrown by Goedel's incompleteness theorems.

It is especially this last aspect that makes it all the more remarkable that even today a "Theory of Everything" (TOE) enjoys a growing popularity not only in the more popular literature but also among many physicists. How can a TOE be propagated in physics if the much more severe mathematics has already abandoned such an idea? And wouldn't it be much more appropriate to have a common structure of our current physical experience that is open also for new and upcoming experiences? The constant effort for such a common structure is strongly related to the "cultural aspect" not only of physics but of any science. In this context I want the term "cultural aspect" to be understood as the necessity to consolidate the language used to express our experiences in a certain field of science. Only

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this will allow us to effectively exchange and pass on the experiences as well as to integrate new experiences in a satisfactory manner. Regarding physics, this language is essentially a mathematical one. This linguistic aspect of science was nicely expressed already by N. Bohr. In Bohr (1960) he stated that "*physics is to be regarded not so much as the study of something a priori given, but rather as the development of methods of ordering and surveying human experience. In this respect our task must be to account for such experience in a manner independent of individual subjective judgement and therefore objective in the sense that it can be unambiguously communicated in ordinary human language*". And if we assume that gathering experiences in physics is still an open process (a consequence of the—hopefully—never-ending question of "why"?) we are occasionally forced to consolidate our language. Regarding our recent physical experience one may ask if we are in the possession of a common mathematical structure?

If looking at the various physical disciplines one may get the impression that even today we are farther away than ever from such a goal. The different historical roots of different disciplines can considered to be one reason for this situation. That we do not know the linking elements between different disciplines—just think of General Relativity and Quantum Mechanics—may be another reason. To make things worse it must be noted moreover that the degree of mathematization has drastically increased during the last century. Basic physical aspects are sometimes hidden behind the details of complex mathematical structures and solution procedures. And, due to the increasing importance of computer science and the resulting numerical aspects of mathematical solution methods this "concealment effect" has become even more worse. For that very reason and to support the idea of a common structure of our physical experience it is important to clearly distinguish between numerical aspects, aspects of mathematical methods, and the real physical aspects in a certain field of physics. But it seems to me that it is not a common practice to meet this claim. It is moreover increasingly ignored in our daily scientific activity. The huge discrepancy between models discussed in modern cosmology (dark matter, description of the universe seconds after the big bang, ...) and the restricted mathematical capabilities to solve the "simple" physical problem of electromagnetic wave scattering on nonspherical particles is just one example of the situation described above. The latter problem is a problem where I have gathered some experiences over the years. Regarding the former problem it is hard for me to distinguish between wild guess, aspects of mathematical solution methods, and real physical experience. But this could also be my very own problem, of course!

In addition, today's physics faces the following problem: The advent of modern physics can be dated to the time of Galilei or so. He invented the experiment as an essential tool to reveal the laws of nature. In contrast, the ideas of the great Greek philosophers have been developed mostly on the basis of passive observations and logical deductions. Nowadays, physics cannot be imagined without the sometimes complex interplay between experiment and theory. But regarding experiments on the atomic or subatomic scale analyzable data are only generated via several levels of models and with an enormous numerical effort (one may think of the recent LHC experiment at Cern to detect the Higgs particle, for example). Therefore,

caution is advised when we intend to interpret the importance and epistemological consequences of such data. And our recent impossibility to perform experiments on a cosmic scale allots the position of a passive observer to us, even if involuntary. In such situations we are only able to test the consistency and compatibility of these observations with our recent physical experience. Lest I be misunderstood, curiosity, imagination, and speculation are indispensable in our endeavor to put our experimental experience on a firm footing. But we also have to accept the "way through the desert" to meet this target. This means, among other things, that we have to verify the experience gained so far and to consolidate the language we are using to describe this experience at times. New theories, new principles, new notations as well as new explanations should only be introduced according to "Occam's razor". From my point of view, some of the concepts and theories in dispute—especially the dispute regarding epistemological consequences of Quantum Mechanics—suffer from an imprecise terminology. Let us consider two examples to support this point of view. Both of these examples kept me occupied over periods.

The first example concerns the term "velocity" or "momentum". The following statement can frequently be found in textbooks to express an essential difference between classical particle physics and Quantum Mechanics: **It is impossible in Quantum Mechanics to measure position and velocity/momentum at the same time with an (in principle) infinite precision. Position and momentum comply with the uncertainty relation.** Such a statement implies that—in contrast to Quantum Mechanics—this is possible in classical particle physics. I have discussed this aspect frequently with students and colleagues. I usually faced a certain helplessness when I ask about the possibility to measure position and momentum of a classical point mass with an infinite accuracy at a fixed time—even if it is only a matter of an idealized thought experiment. The usual answer is the following: In accordance with the transition from the difference to the derivative, the distance between the two time steps at which the position of the point mass is measured can (at least theoretically) be shortened in a limiting process up to zero to determine the velocity of a point mass at a fixed position. But there are two arguments against this answer. First, the transition from the difference to the derivative makes only sense if the function under debate is known. The first derivative of $x = g/2 \cdot t^2$ with respect to time differs obviously from the first derivative of $x = g/4 \cdot t^2$. Only by temporal successive measurements we are able to find out the correct function, and, therefore, the correct velocity. This becomes already clear if we look at the definition of the uniform motion. To detect a uniform motion we have to measure if the point mass covers equal distances in equal time steps. Second but more important, the above statement contradicts a basic property that we usually assign to a point mass. It is the property that a point mass occupies a certain point in space at a certain time! As a consequence, the motion of a point mass can only be detected if it is found at different times in different positions. It seems therefore more appropriate to consider "velocity/momentum" not as a measurable but a deduced quantity to characterize the state of motion. Really **measurable** in the physics of a classical point mass is—beside mass—only the position at a certain time—provided that we own appropriate standards for "mass", "length", and "time". And, fortunately, we

own such standards! In other words: $x(t)$ contains all the information about a point mass of mass m. All other quantities like velocity, momentum, energy, etc. can be deduced/derived from this "state function". I consider therefore $x(t)$ as the basic **state function of a classical point mass** throughout the second chapter of this book. But it should be emphasized that we have to clarify the relation between the at first abstract "state function" and real measurements already in classical particle physics. Regarding Quantum Mechanics, this point of view raises the following question: What are the smallest time interval between two successive position measurements? And, closely related to that: What are appropriate standards on an atomic and subatomic scale to measure length and time?

The second example is concerned with the two terms "property" and "state" of an object. These two terms are often used synonymously. But would it not be better to clearly differentiate between these two terms since representing two different categories used to structure our physical experience? The term "property" is used to characterize (or, better, to define) a certain physical object or a certain class of physical objects we have already acquired a certain knowledge about. On the other hand, performing a measurement on a certain object aimed at the detection of a certain "state" of this object or a "change of state", and to express this state or this change of state quantitatively by "measure" and "number". However, the property of a defined physical object may represent the state of another physical object. But within a certain object class the properties of an object persist unchanged. For a better understanding let us have a look at the following example from mathematics. In the second chapter of this book, when dealing with the Lippmann-Schwinger equation, we will discuss this aspect again from a physical point of view.

The object "natural even number" may be defined by its two properties of being always positive and divisible by 2. A certain number can be considered to represent the state of this object. But if we consider the object "integer number" both these properties get lost. These properties are now resolved into the states "even number", "odd number", "positive number", and "negative number" which can be assigned to this new object. In mathematics, the necessity to define new objects may be caused by an operation that results in a new state that cannot be assigned to the object to which the operation was applied. Adding two natural even numbers will always produce a new natural even number. Contrary, subtraction can produce negative numbers.

From this point of view it's hard for me to understand the following statement I have found in a textbook about Quantum Mechanics: **In classical physics, the two statements "to possess a property" and "to measure a state" are identical. This does not apply to Quantum Mechanics!** But in both these fields of physics we should actually be able to define the two different objects "classical point mass" and "quantum particle", for example, by their respective properties and possible states. And, finally, procedures must be defined to map these (at first abstract) states (but not the properties!) to measurable quantities. Let me emphasize again: While a certain object may be found in different states its properties remain unchanged. Just as a simple example: We can condense our experimental experience that the "electron" interacts in a certain way with an inhomogeneous magnetic field" into

the property "spin". The two possible values $\pm\hbar/2$ are then the two possible states of this property. The state of this property can be measured in a Stern-Gerlach experiment, for example. That is, we do not measure the property "spin" but the possible states assigned to this property. Therefore I'm convinced that the definition of object classes by corresponding properties and their respective states, and the definition of a procedure to map these states to measurable quantities represent a quite general framework to practice physics. This book is aimed at a corroboration of this point of view.

Based on this point of view let us now turn toward the basic structural elements of physics. We will face these elements again and again in this book.

1.2 Basic Structural Elements of Physics

My negative answer to the above posed question, if we are already in the possession of a common structure of our physical experience, may serve as a justification for this book. However, I do not want to raise the expectation to provide a satisfactory answer to this question. Instead, it is the intention of the book at hand to give thought-provoking impulses for a corresponding discussion of this issue. It is focusing on a special class of functions—the Green's functions. This is due to my belief that these functions represent a basic mathematical tool that is abstract enough to allow a common structure of our experiences gained so far in physics, and that this structure is still open to include upcoming experiences (I have read somewhere that it is an advantage of abstract expressions that, at first, one can imagine nothing but nothing wrong either). In what follows I will try to justify my belief in more detail.

I consider the 8 categories

- **object**
- **property**
- **state**
- **cause/source**
- **effect**
- **interaction**
- **measure**
- **number**

as fundamental in physics. The first 6 categories are not only restricted to rational considerations. In old sagas and in the Greek mythology, for example, the **state** of the object **world** is **caused** by the **effect** of the deities as well as the **interaction** of the deities among each other or with the humans. The deities are described by their divinely **properties**. And is not every history of creation finally an expression of the human want to trace back the state of the world to a certain cause? Contrary, in science we want to avoid such a subjective explanation. This can be achieved with the two additional categories **measure** and **number** with which we can establish

a link to mathematics. If I would be requested to provide a short definition of "physics" (and that is a legitimate request in view of the intention of this book) my answer would be the following:

Physics *refers to a certain part of human activities that tries to express cause and effect relations in specified object classes by* ***measure*** *and* ***number****.* ***Objects*** *are defined by their properties.* ***Effect*** *expresses the fact that a considered object may be observed in a certain* ***state****, or that it changes its* ***state****. The corresponding* ***cause*** *may be a priori given and justified only by our experimental experience. But it may also be traced back to a known* ***interaction*** *between similar or different objects. The former may be called* ***impressed causes/sources****, and the latter may be called* ***induced causes/sources****—to adopt the well-known notation from Electrodynamics. It is an essential goal of our activities in physics to replace impressed sources by induced sources. And the experience that an* ***interaction*** *can be replaced by an equivalent* ***cause/source*** *can be considered as a generalization of the well-known Huygens' principle of optics.*

Even if not exhaustive I consider this answer something like a "least common denominator" since it accounts for the above mentioned categories and emphasizes the very rational nature of physics. According to this understanding of physics these categories are indeed fundamental. Moreover, it is quite remarkable that they can be linked to the Green's function formalism. In other words: I am convinced that using Green's functions will allow us to sharpen our physical language and to make more precise statements about nature. This book is therefore focused on the things in common of different physical disciplines rather than their differences. Now, let us see how the Green's functions come into play.

$$\psi(\alpha) \;=\; \int G(\alpha,\beta)\cdot\rho(\beta)\,d\beta \tag{1.1}$$

is the most important expression in this book we will meet again and again. Depending on the problem being considered it will sometimes be modified appropriately. ψ represents the abstract state of an object. This state is dependent on α. α represents a variable like time or position, or both. $\rho(\beta)$ denotes the corresponding source/cause that depends on the variable β. The Green's function $G(\alpha,\beta)$ is the quantity that characterizes a certain object or a process with different objects involved (an interaction process, for example) and establishes a link between the state ψ and the source ρ. It is an essential objective of this book to demonstrate that different physical experiences can be expressed through the mathematical structure of expression (1.1). Regarding this expression we face the following basic questions:

- We know the state of the object and the Green's function, and we ask for the source that is responsible for a certain state.
- We know the state and the source, and we ask for the Green's function that characterizes the object or the process this object gets involved in.
- We know the Green's function and the source, and we ask for the resulting state.

Only the last question can be answered uniquely. If $\rho(\beta)$ represents an induced source it can be considered as the result of an interaction between objects from the same object class as well as from different object classes, as already mentioned. Scattering of a plane electromagnetic wave with a three-dimensional obstacle—let us say an ideal metallic sphere—is a nice example for the latter situation. Scattering describes the interaction of the two objects "ideal metallic sphere" and "plane electromagnetic wave". As a result of this interaction process we observe a scattered field. This interaction may be formulated in terms of appropriate boundary conditions. But the scattered field may also be considered as the effect of a source (an induced surface current) that exists at the sphere's surface. These different point of views on scattering (as in Quantum Mechanics one could certainly speak of different pictures, the interaction- and the source picture) result in different consequences for the respective mathematical solution methods. This aspect is discussed in Chap. 4 in more detail.

The application of the Green's function formalism implies the necessity to specify the considered objects and their possible states, and to split a physical process consequently into cause and effect relations. It is therefore closely related to experimental physics since the same is—more or less obviously—done in the preparation of any experiment. But this splitting comes along with another advantage. By means of source and effect ladders we are able to connect different theoretical levels. This means that an effect on a lower theoretical level may be replaced by an appropriate source on a higher theoretical level. For example, the description of the collision of two hard spheres can be described best on the level of Newtonian mechanics by employing energy- and momentum conservation and the related boundary conditions. According to our more general understanding of Huygens' principle we can replace these boundary conditions by equivalent sources. Corresponding examples will be considered in detail in the next two chapters. To trace back this collision to a theory on an atomic or subatomic scale, i.e., to a corresponding interaction process between the atomic constituents of both spheres, even if possible, would only be an unnecessary complication. The introduction of phenomenological sources on a higher theoretical level is not the only but one possibility to "scale up" complex interaction processes on a lower theoretical level.

Expression (1.1) can be applied to the measurement process as well. The interaction of the considered object with the measurement devise results in a certain **state** of the latter. This state is related to a certain **measure** and must be mapped to a certain **number** (by calibration, for example). Therefore, two different levels of models must be considered altogether. First, we have to model the relation between the source ρ and the state ψ of the considered object according to (1.1) ($G : \rho \rightarrow \psi$). This process requires the knowledge of the Green's function related to the object. Second, we have to model the mapping of the state ψ of the object to state ψ_M of the measurement devise by use of its related Green's function according to (1.1) ($G_M : \psi \rightarrow \psi_M$). That is, the state ψ of the object is now acting as a source that causes a certain state of the measurement devise via a certain interaction process. Performing a precise measurement requires a precise knowledge of this interaction process as well as of the sources and states involved. Any uncertainty of this

knowledge results in a corresponding uncertainty of the number of a measurement. It is demonstrated in Chap. 5 that certain types of stochastic sources in the physics of classical point masses result already in a mathematical formalism that is only known from Quantum Mechanics, so far.

Regarding the categories **object** and **interaction** I want to add the following remark: Both categories are reflecting an important aspect of our human perception and the way we gain physical experience. Meant is the decomposition of an entity into parts (objects) which are at first considered to exist independently. Only afterwards they are considered to be interrelated among each other by assumed essential interaction processes that have been extracted from our observations. With "assumed" I want to express the fact that the assessment of an interaction process as "essential" is strongly dependent on our level of knowledge. Therefore, if a parameter is assigned to an object, and if this parameter only gains importance in an interaction process, this will have an impact on the importance of this parameter as well as on its number measured in a certain experiment. The determination of the "observable mass" of an electron with the renormalization procedure in Quantum Field Theory is an example of this situation. This procedure—even if sometimes considered as less esthetic—expresses the important principle that there do not exist ideally isolated objects, i.e. objects, that do not interact with their environment. We may compare such a principle with the principle of the impossibility of a perpetual motion machine. This principle makes physics more complex and less accessible to a strict mathematical consideration. But, on the other hand, it is closer to reality. We will come back to this aspect in the next chapter when discussing the Lippmann-Schwinger equation of the motion of a classical point mass in the presence of friction.

To summarize the idea of the discussion so far: I consider the three categories **source**, **effect**, and **interaction** as the trinity of physics. And all these categories are reflected in the Green's function formalism! But even such basic principles as Causality (clearly expressed already by relation (1.1) itself), energy conservation of interaction processes, Reciprocity, etc. can be related to or expressed in a straightforward way by Green's functions. Corresponding examples are frequently discussed in this book.

The following methodological aspect strikes me also as important from a numerical point of view: Using Green's functions will allow us to map complex physical processes to simple graphical structures and to relate these structures to certain mathematical procedures. Feynmann diagrams used in Quantum Field Theory are well-known examples for this mapping. But similar diagrams are also known in Quantum Statistics, in classical Electrodynamics, in Angular Momentum Theory, etc.. In so doing we are able to prepare complex physical processes for a systematic numerical treatment, and, hopefully, to perform numerical calculations even faster. It may be compared to the advantage of introducing matrices to solve algebraic equations, or the advantage that comes along with using complex functions in Electrodynamics. However, this will only be possible if regularly recurring structures are identified that are independent of the object class under

consideration. This can be achieved in some situations with the above mentioned Lippmann-Schwinger equation.

I do not want to conceal that there is a problem with the Green's function in relation (1.1) if eigenvalue problems are considered. But this problem can be solved—at first in a pragmatic way—if replacing the Green's function by an appropriate expansion of Dirac's delta function, and by a restriction to a certain type of sources. I will call this modification the "source picture" of the Fourier series for reasons that will become clear later on in chapters two and three. But I will try to give a more severe mathematical justification of this source picture in Chap. 5 of this book.

At the end of this section I want to reflect shortly about the following aspect which must be taken into account if the importance and epistemological consequences of a new theory is discussed: Even if physics is firmly rooted in mathematics it is primarily based on our experimental experience. And this experience—which is incapable of proof from a stringent mathematical point of view—can be condensed into more or less general principles. These principles are on the top of physics and constitute the essential difference from mathematics. That is, from all possible mathematical structures we have to select those ones that match to these principles. If reading textbooks about conventional Quantum Mechanics, for example, one may get the impression that its laws—especially the Schrödinger equation—cannot be deduced from such a principle. But it was already demonstrated by Schwinger that this equation (and not only this) can be derived from a quantum action principle as Hamilton's equations of motion may be deduced from the action principle in Classical Mechanics. Regarding this subject I highly recommend the book (Schwinger 2001), but especially the Prologue and Schwinger's notes on the Stern-Gerlach experiment therein.

1.3 About Classical Physics and Quantum Mechanics

Even if existing since nearly 100 years, there are still controversial and sometimes mystic discussions regarding the epistemological consequences of Quantum Mechanics. We are obviously able to describe the behaviour of objects on the atomic and subatomic scale in a quite formal mathematical way rather than to align it with our experience from classical physics. In the younger days of Quantum Mechanics those contradictions have been discussed on a purely philosophical level. But since the beginning of the 1980s there exist several experimental results (and the number of corresponding experiments is growing continuously even in our days) which seem to confirm the correctness of the strange behaviour of quantum objects. Two experiments are within the focus of these discussions. These are the double-slit and Bell's experiment. Both experiments are discussed in detail in Chaps. 4 and 5.

Regarding the double-slit experiment Feynman noticed in "The Character of Physical Law" (Feynman 1967): *I will take just this one experiment, which has been designed to contain all of the mystery of Quantum Mechanics, to put you up against*

the paradoxes and mysteries and peculiarities of nature one hundred per cent. Any other situation in Quantum Mechanics, it turns out, can always be explained by saying: You remember the case of the experiment with the two holes? It's the same thing. How does it looks like, and what does it tells us? If shooting quantum objects (photons, electrons, etc.) against a double-slit we can observe a frequency distribution on a screen in the far field behind the double-slit that corresponds to the well-known interference pattern of classical plane wave scattering on a double-slit. This observation is one of our crucial experimental justifications for introducing an abstract probability state concept that allows for a superposition of such states, and, finally, for linking the abstract states to measurable probabilities by calculating the scalar product appropriately. In other words, it is an important experimental justification for the formal mathematical concept behind Quantum Mechanics.

On the other hand, we have Bell's experiment as an essential indication of the alleged "nonlocal character" of Quantum Mechanics, and, strongly related to this, as an evidence of the existence of so-called "entangled states". Bell's experiment has its roots in the basic discussion regarding the completeness of Quantum Mechanics. This discussion was initiated by Einstein, Podolsky and Rosen (EPR) on the one side, and by Bohr on the other side in two famous papers published in 1935 (Einstein et al. 1935; Bohr 1935). In the paper of EPR Quantum Mechanics was accused of being incomplete, and, therefore, that one has to look for hidden parameters to replace it by a complete theory. In his answer, Bohr defended his position of understanding Quantum Mechanics as a complete theory and his insistence on the principle of complementarity. Bohr's position is also known as the "Copenhagen interpretation". But, again, this discussion was purely philosophical until the famous paper of Bell (Bell 1964). He derived therein an inequality (now called Bell's inequality) that allows for an experimental proof of the nonlocal character of Quantum Mechanics as well as the existence of entangled states. But it took again more than one decade until the first experiments with polarization-entangled photons provided us with an indication that Bell's inequality can, indeed, be violated in Quantum Mechanics. These experiments have been performed by A. Aspect and co-workers at the beginning of the 1980s (Aspect et al. 1982). The existence of entangled states is the most essential difference between Quantum Mechanics and classical physics, according to Schrödinger. He wrote in (Schroedinger 1935): *When two systems, of which we know the states by their respective representatives, enter into temporary physical interaction due to known forces between them, and when after a time of mutual influence the systems separate again, then they can no longer be described in the same way as before viz. by endowing each of them with a representative of its own. I would not call that one but rather that characteristic trait of Quantum Mechanics, the one that enforces its entire departure from classical lines of thought. By the interaction the two representatives have become entangled*. Today, Schrödinger's position is well accepted among most of the physicists. And there is little doubt that entangled states belong exclusively to the realm of Quantum Mechanics. Since entangled states did not play any role in conjunction with the double-slit experiment, it seems that we have to add Bell's experiment to the above given statement of Feynman to cover "the whole mystery of Quantum Mechanics".

Chapter 5 of this book provides a critical analysis of this point of view and demonstrates moreover, that well-established and in many experiments well-proven mathematical concepts of Quantum Mechanics can be applied with benefit to certain situations in classical physics as well. But the following general aspects are already to be mentioned at this point:

1. Probabilities are of essential importance in Quantum Mechanics. Even if we are faced with an ideal situation, quantum mechanics allows only probability statements with respect to the experimental outcome. To get a first impression of the probability concept in Quantum Mechanics let us have a rather phenomenological look at the well-known Stern-Gerlach experiment.

   Sending electrons through an inhomogeneous magnetic field results in a deflection of the electrons up or down with respect to a fixed direction. That is, we are operating within a two-dimensional but classical event space. But we are unable to predict whether a single electron will be deflected up or down when traversing the inhomogeneous magnetic field. The only thing we can do is to repeat this experiment many times until we are able to relate a probability to each of these two classical events. Let us assume that the probability is $1/2$ for both these events. The observation of the deflection of electrons when traversing the magnetic field is qualitatively related to the interaction of this field with the property "spin" assigned to every electron. That is, the spin is considered to be a characteristic property (a kind of angular momentum) of electrons. As a result of our experiment the property spin is restricted to have only the two values $s_+ = +\hbar/2$ (related to an upward deflection of the electron) and $s_- = -\hbar/2$ (related to a downward deflection of the electron) with respect to a certain direction. The outcome of a spin measurement in a single event can therefore be predicted only with a probability of $1/2$. This situation is expressed in Quantum Mechanics by introducing the abstract probability state vector

$$| \psi\rangle = \frac{1}{\sqrt{2}} \cdot (| \varphi_1\rangle + | \varphi_2\rangle) \tag{1.2}$$

   in a two-dimensional spin space. It consists of a superposition of the eigenvector

$$| \varphi_1\rangle = (1, 0) \tag{1.3}$$

   related to the eigenvalue $+1$, and the eigenvector

$$| \varphi_2\rangle = (0, 1) \tag{1.4}$$

   related to the eigenvalue -1. Both eigenvalues and eigenvectors are eigenvalues and eigenvectors of Pauli's spin matrix

$$\mathbf{\Sigma_1} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = | \varphi_1\rangle\langle\varphi_1 | - | \varphi_2\rangle\langle\varphi_2 | \tag{1.5}$$

(please, note that $|\alpha\rangle\langle\beta|$ represents the dyadic product of both vectors $|\alpha\rangle$ and $|\beta\rangle$!). Hence, the possible spin values are the eigenvalues of the spin operator

$$\mathbf{S} = \frac{\hbar}{2}\,\boldsymbol{\Sigma}_{\mathbf{1}}\,. \tag{1.6}$$

Equation (1.2) is the complete characterization of the electron with respect to its two possible spin values in the experiment considered above. Calculating the scalar product of the state vector (1.2) with itself (or, better, calculating the corresponding scalar product of the projections of $|\psi\rangle$ onto the two orthogonal subspaces defined by $|\varphi_1\rangle$ and $|\varphi_2\rangle$) will provide us with the probabilities related to each of the two possible spin values. This is how we express quantitatively (i.e., in terms of probabilities) our experimental experience: **Sending single electrons through an inhomogeneous magnetic field will result in a random deflection of the electrons up and down**.

However, probabilities are of less importance in classical physics. They are mostly considered in conjunction with uncertainties of measurements in real experiments, uncertainties in the determination of initial- or boundary conditions, and in conjunction with uncertainties regarding the knowledge of material parameters. But in Chap. 5 we will introduce special stochastic sources and interaction mechanisms to demonstrate the principal importance of probability statements already in classical physics. **Probabilities should therefore be accepted as objectively measurable quantities (e.g. in the sense of an observable empirical probability within a classical event space) not only in Quantum Mechanics but general in physics.**

2. In contrast to the classical physics of a point mass, Quantum Mechanics and classical Electrodynamics are characterized by the fact that both these theories are formulated in terms of abstract and not directly observable states/fields. This necessarily requires a "translation" of the respective states/fields into measurable quantities such as probabilities, currents, energy fluxes, intensities, etc. This conceptual difference results also in an essential difference regarding the description of comparable interaction processes. The different scattering behaviour of particles and fields on a hard sphere and the difference in the probabilities measured in the quantum mechanical Bell's experiment and its classical counterpart are two examples which will be discussed in detail from this point of view. As a result of this discussion, it turns out that the probabilities of the quantum mechanical Bell's experiment may alternatively be obtained from the superposition of two nondisjoint substates which are not entangled! That is, it can be traced back to the same cause we already know from the quantum mechanical double-slit experiment. In so doing, it is shown in Chap. 5 that there is no need to add Bell's experiment to Feynman's quote mentioned before. Moreover (and may be even more important), it is thus demonstrated that entangled states can already be introduced to describe corresponding probability experiments with classical objects.

3. It may be of some advantage to bring eigenvalue problems into a source picture. This is what I already called the "source picture" of the Fourier series in the foregoing section. Regarding Quantum Mechanics, it expresses the fact that a state of a certain object at a former time may be considered as the source of the state of the object at a later time. According to this understanding of eigenvalue problems the solution of the time independent Schrödinger's equation for the hydrogen atom, for example, provides us "only" with the abstract mathematical model of an isolated hydrogen atom and its inner degrees of freedom. Only if applying a certain source to this object, or if imbedding it into a real environment that results in a certain interaction will bring the object "hydrogen atom" to real physical life. Introducing corresponding sources into Quantum Mechanics represents just a little formal change. In textbooks this is often prosaically called the "preparation of an initial state". However, if consequently introducing such a source picture it becomes clear from the very beginning that Causality applies also to Quantum Mechanics. The opposite position, i.e., the abandoning of Causality in Quantum Mechanics is sometimes discussed in the literature.

I hope, on the one hand, that the reader will not be deterred by this lengthy and quite personally formulated Prologue. But, on the other hand, it represents my justification for writing this book and may possibly support the understanding of some of the discussions that can be found in the following chapters. May this book be regarded as a proposal for the discussion of a common mathematical structure of our physical experience, and as a discussion of the importance of Green's functions to achieve this goal. And, at the very end of this Prologue (and being fully aware of the possibility that I by myself have to take a good look in the mirror!) I cannot refrain from making the following remark: Newton's statement *physics, beware of metaphysics* has not lost its importance even in our days!

Chapter 2
Green's Functions of Classical Particles

From some things we have to distance ourself to approach them

The simple harmonic oscillator is of importance in different fields of physics. Beside the advantage of a complete analytical treatment this object can be used with benefit to study the conceptual differences between classical physics and Quantum Mechanics, for example. We will come back to this aspect in the last chapter of this book. However, the simple harmonic oscillator is considered in this chapter exclusively from the well-known position of classical physics. Among other things, we will derive the related Green's function. This will enable us to corroborate some of the aspects addressed from a more general position in the Prologue with first examples. The Green's function of the simple harmonic oscillator contains as a limiting case the Green's function of a point mass that moves forceless, on an inclined plane, or that undergoes a free fall. In a next step we consider the Green's function of the damped harmonic oscillator and study its behaviour if an impressed periodic source is applied. The Green's function of the damped harmonic oscillator contains the Green's function of the simple harmonic oscillator and the Green's function related to the motion of a point mass in the presence of friction as limiting cases.

After looking at these simple physical situations we turn toward the so-called "Lippmann-Schwinger equation" and its iterative solution. In so doing, it is demonstrated that the Green's functions of the forceless point mass and the simple harmonic oscillator can be used to get a first approximation of the Green's functions related to the motion of a point mass in the presence of a weak friction, and to the weakly damped harmonic oscillator. The Green's function of the forceless point mass in combination with the Lippmann-Schwinger equation is used moreover to determine the Green's function of the simple harmonic oscillator. The discussion of the "observable mass" in the context of the motion of a point mass in the presence of friction will allow us to illustrate a basic aspect behind the renormalization procedure in Quantum Field Theory already at this point.

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All the Green's functions are derived again but on a more systematic way in a separate section. The important Kramers-Kronig relation, that holds for the Fourier transform of the Green's function of the damped harmonic oscillator, is considered in the last part of this section.

The subsequent section deals with the temporal boundary value problem of a simple harmonic oscillator and its description in terms of "inner states of freedom" of a corresponding "super oscillator". The "source picture" of the Fourier series, that was already mentioned in the Prologue, is introduced and discussed in this context.

The next section starts with the description of a few simple interaction processes by use of the Green's function formalism. This is followed by solving the more complex problems of particle scattering on a rigid sphere and the Kepler problem. Both these problems are solved by employing the Green's function of the simple harmonic oscillator in polar coordinates. With these two examples we intend to build already in this chapter a bridge to the problem of plane wave scattering on a sphere that will be discussed in detail in Chap. 4.

2.1 The Simple Harmonic Oscillator

2.1.1 Classical Consideration

The Lagrangian

$$L(x, \dot{x}) \;=\; \frac{1}{2} m \dot{x}^2 \;-\; \frac{1}{2} k\, x^2 \tag{2.1}$$

is used as a starting point for our treatment of the simple harmonic oscillator. m represents the mass, and k denotes the spring constant. Applying Hamilton's action principle we get the corresponding Euler-Lagrange equation, and, finally, the equation of motion of the "state function" $x(t)$. According to Hamilton's action principle the first variation δW of the action W must vanish. The action itself is expressed by the definite integral

$$W \;=\; \int_{t_1}^{t_2} L(x, \dot{x})\, dt \;. \tag{2.2}$$

The boundary values $x(t_1)$ and $x(t_2)$ are assumed to be known, and, therefore, kept fixed in the variation procedure. The resulting Euler-Lagrange equation reads

$$\frac{\partial L}{\partial x} \;-\; \frac{d}{dt}\, \frac{\partial L}{\partial \dot{x}} \;=\; 0 \;. \tag{2.3}$$

Applying this equation to the Lagrangian (2.1) yields the well-known equation of motion of the simple harmonic oscillator:

$$m\,\frac{d^2x(t)}{dt^2} \;+\; k\,x(t) \;=\; 0\;. \tag{2.4}$$

This equation can be rewritten into

$$\frac{d^2x(t)}{dt^2} \;+\; \omega^2\,x(t) \;=\; 0\;, \tag{2.5}$$

where ω^2 is given by

$$\omega^2 \;=\; \frac{k}{m}\;. \tag{2.6}$$

$$x(t) \;=\; A\cdot\cos\omega t \;+\; B\cdot\sin\omega t \tag{2.7}$$

is its general periodic solution. $x(t)$ allows for a complete description of the behaviour of the simple harmonic oscillator once the amplitudes A and B are known.

These amplitudes are usually calculated from the initial values

$$x(t_1 = 0) \;=\; x_1 \tag{2.8}$$

and

$$\left[\frac{dx(t)}{dt}\right]_{t_1=0} = v_1\;, \tag{2.9}$$

i.e., the position and velocity at the initial time $t_1 = 0$. We can choose any other time as the initial time, of course. But in what follows, let us use w.l.o.g. $t_1 = 0$ as the initial time. Then

$$x(t) \;=\; x_1\cdot\cos\omega t \;+\; \frac{v_1}{\omega}\cdot\sin\omega t\;. \tag{2.10}$$

The two limiting cases

- $v_1 = 0\,;\; x_1 \neq 0$
- $v_1 \neq 0\,;\; x_1 = 0$

result in particularly simple expressions for the motion of the simple harmonic oscillator.

All this is well-known and need no further explanation. However, according to the action principle it seems to be more appropriate to fix the position at two different times, and to calculate the amplitudes A and B from these two boundary conditions. In a corresponding experiment we would have to measure the position of the oscillator at two different times, or, equivalently, the two times the oscillator will take up two predefined positions within one period. According to the problem with the measurement of the velocity at a fixed time and a fixed position that was posed in the first section of the Prologue the usage of the boundary values $x(t_1) = x_1$ and $x(t_2) = x_2$ would fit much better into the experimental situation. Then

$$A = \frac{x_1 \sin \omega t_2 - x_2 \sin \omega t_1}{\sin \omega (t_2 - t_1)} \tag{2.11}$$

and

$$B = \frac{x_2 \cos \omega t_1 - x_1 \cos \omega t_2}{\sin \omega (t_2 - t_1)} \,. \tag{2.12}$$

Measurements at times $\omega(t_2 - t_1) = n\pi\,,\ n = 0, 1, 2, \cdots$ should obviously be avoided. This problem seems meaningless if using the initial position and the initial velocity, as discussed at the beginning. But the problem has only been shifted since this initial velocity must be determined at some point from position measurements at two different times. Inserting (2.11) and (2.12) into (2.7) yields

$$x(t) = \frac{x_1 \cdot \sin \omega (t_2 - t) + x_2 \cdot \sin \omega (t - t_1)}{\sin \omega (t_2 - t_1)} \tag{2.13}$$

as the solution of the simple harmonic oscillator if we have measured its position at two different times. A possible definition of an initial velocity may be obtained by comparing (2.7) and (2.12) with (2.10): **The "initial velocity" $\mathbf{v_1}$ is the assumed velocity at $\mathbf{t = 0}$ that results in the two positions $\mathbf{x_1}$ and $\mathbf{x_2}$ at the later times $\mathbf{t_1 \geq t}$ and $\mathbf{t_2 > t_1}$, i.e.,**

$$v_1 := \omega \cdot \frac{x_2 \cos \omega t_1 - x_1 \cos \omega t_2}{\sin \omega (t_2 - t_1)} \,. \tag{2.14}$$

This is something like a "non-differential" definition of an initial velocity based on position measurements at two different times. If $t_1 = t = 0$ and the rest position $x_1 = 0$ is used as the starting point (2.14) becomes simply

$$v_1 = \frac{\omega \cdot x_2}{\sin \omega t_2} \,. \tag{2.15}$$

In what follows, the initial velocity is considered as a parameter of an elastic collision that acts at a certain time on the oscillator at rest—thus resulting in a change of its state of motion. That ω is independent of the initial values is another

interesting, although well-known property of the simple harmonic oscillator. This allows for the determination of the mass m once the spring constant k and ω are known, for example. But, now, let us consider the simple harmonic oscillator from the point of view of Green's functions.

2.1.2 *Green's Function, Green's Theorem, Causality, and Reciprocity*

Using the elastic collision between two point masses at time $t = 0$ is only one possibility to accomplish an initial velocity. However, let us disregard the specific realization of an initial velocity in what follows. It is considered only as a somehow given, impressed source for the observed motion of the harmonic oscillator. That is, it is assumed that without any such source the oscillator would simply rest at $x = 0$. In other words: There is no smoke without a fire. Instead, we intend to express the state of motion $x(t)$ of the oscillator by relation

$$x(t) = \int_0^{t^+} G(t, t') \cdot \rho(t')\, dt' \tag{2.16}$$

once the source $\rho(t)$ is given. $G(t, t')$ is the Green's function we are looking for. It relates the given source $\rho(t')$ to the observed effect $x(t)$ at observation time $t > t'$. The upper index of integration t^+ shall indicate that the time integration must be performed up to $t + \epsilon$ with ϵ representing an arbitrary small but positive real number. This is necessary to take the integral property of the Dirac's delta function and Causality into account, as we will see shortly. The Green's function itself is a function that depends only on the observation time t, and on the time t' the source is acting on the oscillator. Unless otherwise specified, t' in $G(t, t')$ will always denote the source time and t the observation time, in this order.

Causality in this context expresses our (not only) physical experience that an effect can never be observed before its cause. Regarding the Green's function we therefore require the fulfillment of the two additional conditions

$$G(t, t') = 0\,; \quad t < t' \tag{2.17}$$

and

$$\frac{\partial G(t, t')}{\partial t} = 0\,; \quad t < t'\,. \tag{2.18}$$

To derive expression (2.16) we start from the Lagrangian

$$L(x, \dot{x}, \rho) = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2 + \rho(t) \cdot x \tag{2.19}$$

that contains the impressed source $\rho(t)$ linearly in x (and only such linear problems are of our interest throughout this book). From the Euler-Lagrange equation (2.3) we thus get in a straightforward way the following inhomogeneous equation of motion:

$$m \cdot \frac{d^2x(t)}{dt^2} + k \cdot x(t) = \rho(t) \,. \tag{2.20}$$

The equation

$$m \cdot \frac{\partial^2 G(t,t')}{\partial t^2} + k \cdot G(t,t') = \delta(t-t') \tag{2.21}$$

is assumed to hold for the corresponding Green's function. That is, the inhomogeneity in Eq. (2.20) is replaced by an elementary source at the initial time t'. Since any real source may be expressed by a superposition of several elementary sources the effect of any linear problem in the presence of a real source can also be described by a superposition of all the effects that result from each elementary source. This is the actual meaning of the integral relation (2.16).

Green's theorem is one of the important mathematical tools we will apply again and again in this book. Regarding the time dependent problems considered in this chapter it is simply given by

$$\begin{aligned} \int_{t_1}^{t_2} \left[\Psi(t) \cdot \frac{d^2\Phi(t)}{dt^2} - \Phi(t) \cdot \frac{d^2\Psi(t)}{dt^2} \right] dt = \\ \int_{t_1}^{t_2} \frac{d}{dt} \left[\Psi(t) \cdot \frac{d\Phi(t)}{dt} - \Phi(t) \cdot \frac{d\Psi(t)}{dt} \right] dt = \\ \left[\Psi(t) \cdot \frac{d\Phi(t)}{dt} - \Phi(t) \cdot \frac{d\Psi(t)}{dt} \right]_{t_1}^{t_2} . \end{aligned} \tag{2.22}$$

$\Psi(t)$ and $\Phi(t)$ are any two continuous functions of time. In Chap. 3, when dealing with classical fields, Green's theorem becomes a little bit more complicate since we have to take surface- as well as volume integrals additionally into account. However, some of the corresponding aspects can already be discussed at this place in a more simple way.

One of these aspects is concerned with a property that can be derived from Green's theorem and the requirement of causality. It is called **Reciprocity**. Regarding all the temporal problems considered in this chapter Reciprocity characterizes the behaviour of the Green's function if interchanging observation- and source time. It is expressed by the identity

$$G(t,t') = G(-t',-t) \tag{2.23}$$

(please, note that on the right-hand side of this identity $-t$ and $-t'$ are now the source- and observation times, in this order). Equation (2.23) is intuitively understandable since $t > t'$ on the left-hand side must become $-t' > -t$ on the right-hand side, due to the requirement of Causality. To prove identity (2.23) we start from the two equations

$$\frac{\partial^2 G(t,t')}{\partial t^2} + \omega^2 G(t,t') = \delta(t-t') \tag{2.24}$$

and

$$\frac{\partial^2 G(-t,-t'')}{\partial t^2} + \omega^2 G(-t,-t'') = \delta(t-t'') \,, \tag{2.25}$$

where we have chosen $m = 1$ for simplicity. Both of these equations are reversible with respect to time reversal. Next, we consider the integral

$$\int_0^{t''+} \left[G(t,t') \cdot \frac{\partial^2 G(-t,-t'')}{\partial t^2} - G(-t,-t'') \cdot \frac{\partial^2 G(t,t')}{\partial t^2} \right] dt \tag{2.26}$$

of Green's theorem. Using (2.24), (2.25), and the identity

$$\begin{aligned} G(t,t') \cdot \frac{\partial^2 G(-t,-t'')}{\partial t^2} - G(-t,-t'') \cdot \frac{\partial^2 G(t,t')}{\partial t^2} = \\ \frac{\partial}{\partial t} \left[G(t,t') \cdot \frac{\partial G(-t,-t'')}{\partial t} - G(-t,-t'') \cdot \frac{\partial G(t,t')}{\partial t} \right] \end{aligned} \tag{2.27}$$

we get

$$\begin{aligned} G(t'',t') - G(-t',-t'') = \\ \left[G(t,t') \cdot \frac{\partial G(-t,-t'')}{\partial t} - G(-t,-t'') \cdot \frac{\partial G(t,t')}{\partial t} \right]_{t=0}^{t=t''+} . \end{aligned} \tag{2.28}$$

The expression in the square brackets on the right-hand side becomes identical zero, due to the requirement of Causality (see also Fig. 2.1). Thus we have confirmed the expression (2.23) of Reciprocity. We will come back to this derivation when

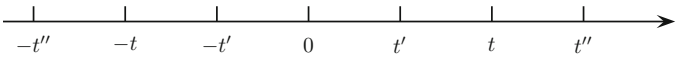

Fig. 2.1 Time bar with the different observation and source times used in the derivation of the Reciprocity property. t' represents the source time and t'' the observation time on the positive time axis. In contrast, $-t''$ represents the source time and $-t'$ the observation time on the negative time axis

dealing with the damped harmonic oscillator. Reciprocity may then be expressed more generally by using the adjoint Green's function since reversibility with respect to time reversal does not holds for this object.

If replacing the first equation of motion (2.24) of the Green's function by equation (2.20) in the above given derivation we get

$$x(t'') \;=\; \int_0^{t''+} G(t'',t)\cdot\rho(t)\,dt \;- \\ \left[x(t)\cdot\frac{\partial G(-t,-t'')}{\partial t} \;-\; G(-t,-t'')\cdot\frac{\partial x(t)}{\partial t}\right]_{t=0}^{t=t''+} \tag{2.29}$$

as an expression for the solution of the simple harmonic oscillator. Taking again Causality into account and assuming homogeneous boundary conditions for both quantities $x(t)$ and $dx(t)/dt$ at the lower boundary $t = 0$ we end up with representation (2.16). All we need to do is to replace t by t' and t'' by t. Our call for homogeneous conditions at $t = 0$ seems to contradict the fact that a unique solution of the equation of motion requires a known initial position and a known initial momentum, both related to inhomogeneous boundary conditions. But we will see later on in Sect. 2.1.5 that these initial values can be replaced by appropriate sources used in relation (2.16). We will face the equivalence between inhomogeneous boundary conditions and sources frequently in this book.

Now, let us consider relation (2.16) again but from a somewhat different point of view. Starting from the assumption that only equation (2.21) of the Green's function is given we may ask for the equation of motion of $x(t)$ that must hold to coincide with relation (2.16) for a given source $\rho(t)$. To this end, let us introduce the inverse $G^{-1}(t,t')$ of the Green's function $G(t,t')$ by the definition

$$\int_0^{t+} G^{-1}(t,\bar{t})\cdot G(\bar{t},t')\,d\bar{t} \;:=\; \delta(t-t')\;. \tag{2.30}$$

Comparing this definition with (2.21) we thus get

$$G^{-1}(t,t') \;=\; \left(m\cdot\frac{\partial^2}{\partial t^2} \;+\; k\right)\delta(t-t')\;. \tag{2.31}$$

It is straightforward to prove the correctness of this expression by insertion into (2.30), and by taking the definition

$$\int_{-\infty}^{\infty} f(x)\cdot\delta(x-x')\;dx \;:=\; f(x') \tag{2.32}$$

of Dirac's delta function into account. Please, note that one consequence of this definition is $[1/x]$ as the unit of measure of Dirac's delta function. Next, let us multiply relation (2.16) by $G^{-1}(t'', t)$ and integrate from $t = 0$ to $t = t''^{+}$ afterwards,

$$\int_0^{t''^{+}} G^{-1}(t'', t) \cdot x(t)\, dt = \int_0^{t''^{+}} G^{-1}(t'', t) \cdot G(t, t') \cdot \rho(t')\, dt'\, dt\,. \tag{2.33}$$

If we revert to (2.31), and if we finally replace t'' by t we end up with (2.20) as the equation of motion of $x(t)$. This derivation avoids the usage of Green's theorem. On the other hand, we have lost control over the boundary- or initial conditions. But this is not really a disadvantage since we intend to replace these conditions by corresponding impressed or induced sources, as already mentioned above. The Lagrangian

$$L(G, \dot{G}, \delta) = \frac{1}{2} m\, \dot{G}^2(t, t') - \frac{1}{2} k\, G^2(t, t') + \delta(t - t') \cdot G(t, t') \tag{2.34}$$

can be considered in this context as the generating function of the equation of motion of the Green's function in the presence of the external but elementary source $\delta(t - t')$. In so doing we have to replace $\partial L/\partial x$ and $\partial L/\partial \dot{x}$ in the Euler-Lagrange equation (2.3) by $\partial L/\partial G$ and $\partial L/\partial \dot{G}$. Then, (2.20) represents the corresponding equation of motion of any function $x(t)$ that meets relation (2.16) with $\rho(t)$ representing a given source.

There exists an alternative way to define the equation of motion of the Green's function from a Lagrangian without the elementary source that should be mentioned here. Instead of (2.34) we can choose

$$\tilde{L}(G, \dot{G}) = L(G, \dot{G}) \cdot H(t - t') \tag{2.35}$$

with $L(G, \dot{G})$ according to

$$L(G, \dot{G}) = \frac{1}{2} m\, \dot{G}^2(t, t') - \frac{1}{2} k\, G^2(t, t')\,, \tag{2.36}$$

i.e., without Dirac's delta function as an external source. $H(t - t')$ denotes the Heaviside function defined by

$$H(t - t') := \begin{cases} 1 & ;\ t - t' > 0 \\ 0 & ;\ t - t' < 0 \end{cases}\,. \tag{2.37}$$

Its first derivative with respect to time t yields Dirac's delta function $\delta(t - t')$. This function ensures that nothing of physical relevance happens before the source is acting on the oscillator. Using this Lagrangian in the Euler-Lagrange equation (2.3)

we thus get

$$\frac{\partial L}{\partial G} - \frac{d}{dt}\frac{\partial L}{\partial \dot{G}} = \left(\frac{\partial L}{\partial \dot{G}}\right)_{t=t'} \cdot \delta(t-t') \; . \tag{2.38}$$

With the definition of

$$\left(\frac{\partial L}{\partial \dot{G}}\right)_{t=t'} := -1 \tag{2.39}$$

as an elementary momentum acting at time t' we have

$$\frac{\partial L}{\partial G} - \frac{d}{dt}\frac{\partial L}{\partial \dot{G}} = -\delta(t-t') \; . \tag{2.40}$$

Inserting (2.36) provides again the equation of motion (2.21) of the Green's function.

We are now in the possession of a quite interesting relation between the Green's function and the solution $x(t)$ of the state of motion. But, unfortunately, we don't know the Green's function itself. As long as an explicite expression of the Green's function is not known (2.16) represents only a formal relation. The solution of the differential equation (2.21) by taking the additional condition

$$\lim_{\epsilon \to 0} G(t = t' + \epsilon, t') = 0 \tag{2.41}$$

into account is therefore our objective in what follows.

2.1.3 Determination of the Green's Function by Trying

Equation (2.21) is a quite simple differential equation with sine- and cosine functions as the two linearly independent solutions of the homogeneous equation. We are therefore able to determine $G(t, t')$ by "skillful trying". The initial time is again set to $t' = 0$ for simplicity. To consider an arbitrary initial time t' we simply have to replace t by $t - t'$ in the final result. Because of the additional condition (2.41) only the sine function will be shortlisted. If multiplying this function by the Heaviside function $H(t)$ we are already in agreement with Causality.

$$G(t, 0) = A \cdot \sin \omega t \cdot H(t) \tag{2.42}$$

is therefore a reasonable *ansatz* for the Greensfunction of Eq. (2.21). The so far unknown coefficient "*A*" can be determined as follows: We insert (2.42) into (2.21) and take into account that

$$\frac{d\delta(t)}{dt} \;=\; -\,\frac{1}{t}\cdot\delta(t) \tag{2.43}$$

holds for the first derivative of Dirac's delta function. This is a consequence of the definition

$$\int_{-\infty}^{\infty} f(x)\cdot\frac{d\delta(x)}{dx}\,dx \;:=\; -\left[\frac{df(x)}{dx}\right]_{x=0} \tag{2.44}$$

of the derivative of Dirac's delta function. Thus we get

$$\frac{\partial G(t,0)}{\partial t} \;=\; A\cdot\omega\cdot\cos\omega t\cdot H(t) \;+\; A\cdot\sin\omega t\cdot\delta(t) \tag{2.45}$$

for the first derivative, and

$$\begin{aligned}\frac{\partial^2 G(t,0)}{\partial t^2} \;&=\; -\,m\,\omega^2\cdot A\cdot\sin\omega t\cdot H(t) \;+ \\ &2\,m\,\omega\cdot A\cdot\cos\omega t\cdot\delta(t) \;-\; m\cdot A\cdot\frac{\sin\omega t}{t}\cdot\delta(t)\end{aligned} \tag{2.46}$$

for the second derivative of the Green's function. Applying these two derivatives in Eq. (2.21) gives

$$\begin{aligned}m\cdot\frac{\partial^2 G(t,0)}{\partial t^2} \;+\; k\cdot G(t,0) \;&=\; A\cdot\sin\omega t\cdot H(t)\cdot\left[k \;-\; m\,\omega^2\right] \;+ \\ &\delta(t)\cdot A\cdot m\cdot\left[2\,\omega\,\cos\omega t \;-\; \frac{\sin\omega t}{t}\right].\end{aligned} \tag{2.47}$$

The first term on the right-hand side becomes identical zero because of (2.6). "A" can be determined from the second term on the right-hand side since the expression $A\cdot m\cdot\left[2\,\omega\,\cos\omega t \;-\; \frac{\sin\omega t}{t}\right]$ must provide 1 if t tends to zero. Applying L'Hospital's rule gives

$$A \;=\; \frac{1}{m\,\omega}\,. \tag{2.48}$$

The Green's function of the simple harmonic oscillator reads therefore

$$G(t,0) \;=\; \frac{\sin\omega t}{m\,\omega}\cdot H(t)\;, \tag{2.49}$$

or, if we consider an arbitrary initial time t',

$$G(t,t') \;=\; \frac{\sin\omega(t-t')}{m\,\omega}\cdot H(t-t')\;. \tag{2.50}$$

The integration of the equation of motion (2.21) by an infinitesimal region across the source time provides another possibility to determine "A". This provides

$$\left[\frac{\partial G(t,0)}{\partial t}\right]_{t=-\epsilon}^{t=+\epsilon} \;+\; \omega^2\cdot\int_{-\epsilon}^{+\epsilon} G(t,0)\,dt \;=\; \frac{1}{m}\;. \tag{2.51}$$

From (2.17) and (2.41) it follows that the integral expression on the left-hand side is identical zero, giving

$$\left[\frac{\partial G(t,0)}{\partial t}\right]_{t=-\epsilon}^{t=+\epsilon} \;=\; \frac{1}{m}\;. \tag{2.52}$$

Then, from (2.45) and if taking $[\sin\omega t\cdot\delta(t)]_{t=0}=0$ into account, (2.48) follows in a straightforward way. But we see moreover that the first derivative of the Green's function $m\cdot G(t,t')$ with respect to the observation time t is discontinous by an amount of 1 at the source time t'! It should be also noted at this point that the somewhat shirtsleeve treatment of Dirac's delta function as an ordinary function will be practiced frequently throughout the book and is well-known to physicists, much to the annoyance of the mathematicians.

Interestingly, in some textbooks I have found the expression

$$G(t,t') \;=\; \frac{\sin\omega|t-t'|}{2\,m\,\omega} \tag{2.53}$$

instead of (2.50) for the Green's function of the simple harmonic oscillator. This is also a solution of the equation of motion (2.21), as one can convince oneself by taking the weak derivative

$$\frac{d|t|}{dt} \;=\; H(t)\;-\;H(-t) \tag{2.54}$$

of the absolute value function into account. Its second derivative produces the factor $1/2$ in (2.53). But on the other hand we have to state that this solution does not agree with identity (2.23), and, therefore, not with the requirement of Causality. That is, interchanging source and observation time that way should provide zero, as we have already discussed. The relation between Causality and the time structure of the Green's function becomes even more obvious if it is derived by the mathematically better founded Fourier transform method.

2.1.4 Determination of the Green's Function by Applying the Fourier Transform Method

The Fourier transform $F(\bar{\omega})$ of the function $f(t)$ is defined according to

$$F(\bar{\omega}) := \int_{-\infty}^{\infty} f(t) \cdot e^{-i\bar{\omega}t}\, dt\,. \tag{2.55}$$

The inversion formula reads

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\bar{\omega}) \cdot e^{i\bar{\omega}t}\, d\bar{\omega}\,. \tag{2.56}$$

The Fourier transform of the derivative of $f(t)$ with respect to t is given by the multiplication of the Fourier transform $F(\bar{\omega})$ by $i\bar{\omega}$. Furthermore, Dirac's delta function may be expressed by

$$\delta(t - t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\bar{\omega}(t-t')}\, d\bar{\omega}\,. \tag{2.57}$$

The application to the equation of motion

$$\frac{\partial^2 G(t,t')}{\partial t^2} + \omega^2 \cdot G(t,t') = \frac{1}{m} \cdot \delta(t - t') \tag{2.58}$$

provides therefore the algebraic equation

$$G(\bar{\omega}, t') = \frac{1}{m} \cdot \frac{e^{-i\bar{\omega}t'}}{\omega^2 - \bar{\omega}^2} \tag{2.59}$$

for the Fourier transform of the Green's function. To move the zero points of the denominator away from the real axis into the upper complex $\bar{\omega}$-plane we add the expression $i\epsilon\,\bar{\omega}$. ϵ therein represents again a small but positive real quantity that will be set to zero at the end of the analysis. With

$$\kappa^2 = \omega^2 + i\epsilon\,\bar{\omega} \tag{2.60}$$

and the inversion formula (2.56) we may thus write

$$\begin{aligned} G(t,t') &= -\frac{1}{2\pi m} \int_{-\infty}^{\infty} \frac{e^{i\bar{\omega}(t-t')}}{\bar{\omega}^2 - \kappa^2}\, d\bar{\omega} = \\ &\quad -\frac{1}{2\pi m} \int_{-\infty}^{\infty} \frac{e^{i\bar{\omega}(t-t')}}{(\bar{\omega} - \kappa_1) \cdot (\bar{\omega} - \kappa_2)}\, d\bar{\omega} \end{aligned} \tag{2.61}$$

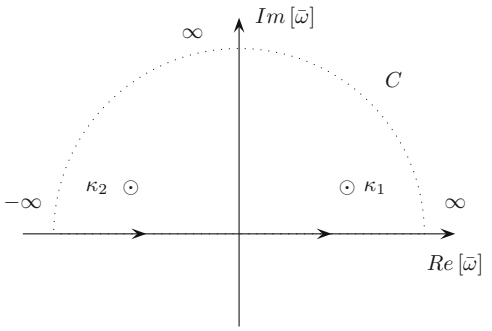

Fig. 2.2 Path of integration in the upper complex $\bar{\omega}$-plane and positions of the zero points of the denominator

for the Green's function in its original time domain. The zero points of the denominator are given by (see also Fig. 2.2)

$$\kappa_1 = \sqrt{\omega^2 - \frac{\epsilon^2}{4}} + i\frac{\epsilon}{2} \tag{2.62}$$

$$\kappa_2 = -\sqrt{\omega^2 - \frac{\epsilon^2}{4}} + i\frac{\epsilon}{2}\,. \tag{2.63}$$

The contribution of the upper semicircle ($Im[\bar{\omega}] \to +\infty$) disappears so that

$$\oint_C d\bar{\omega}\ \cdots\ = \int_{-\infty}^{\infty} d\bar{\omega}\ \cdots \tag{2.64}$$

holds. From the two simple poles $\kappa_{1/2}$ and the application of the residual theorem we obtain

$$\int_{-\infty}^{\infty} \frac{e^{i\bar{\omega}(t-t')}}{(\bar{\omega} - \kappa_1)\cdot(\bar{\omega} - \kappa_2)}\, d\bar{\omega} = 2\pi i \cdot \left[\frac{e^{i\omega(t-t')}}{2\omega} - \frac{e^{-i\omega(t-t')}}{2\omega}\right] \tag{2.65}$$

in the limit $\epsilon \to 0$. From Euler's formula we get finally

$$G(t,t') = \frac{\sin\omega(t-t')}{m\,\omega}\,. \tag{2.66}$$

If $t - t' < 0$ would have been chosen, then we would have to close the integration path in the lower complex $\bar{\omega}$-plane. Then the contribution of the lower semicircle $Im[\bar{\omega}] \to -\infty$ would disappear. But since there are no singularities in the lower complex $\bar{\omega}$-plane we would get zero for the remaining integral along the real $\bar{\omega}$-axis. That is, the special choice of $+i\epsilon\bar{\omega}$ in (2.60) allowed us to derive an expression for the Green's function that is in agreement with Causality. To avoid a nonzero expression for the Green's function in the time domain if $t < t'$ we have to multiply the solution (2.66) by the Heaviside function $H(t - t')$. Thus we end up again with (2.50).

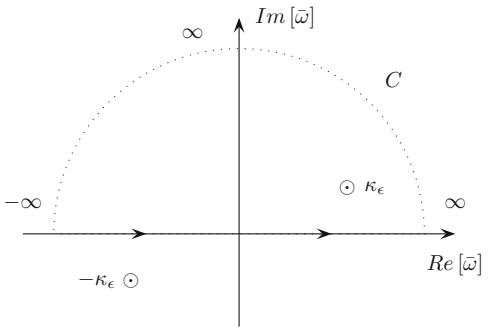

Fig. 2.3 Path of integration in the upper complex $\bar{\omega}$-plane and positions of the zero points of the denominator related to the Fourier transform of Eq. (2.67)

There exist another way to move the singularities of the Fourier transform of the Green's function away from the real axis. We will consider this possibility already at this place since it is also of some importance in Quantum Field Theory to describe particles and antiparticles in conjunction with the Klein-Gordon- and Feynman propagator, for example. Moreover, it emphasizes again the interplay between the temporal boundary conditions based on our physical experience of Causality and the solution of the underlying equation of motion we are looking for. Instead of (2.21) we are now considering the modified equation

$$\frac{\partial^2 G_{\epsilon_+}(t,t')}{\partial t^2} + \left[\omega^2 + i\,\epsilon\right] \cdot G_{\epsilon_+}(t,t') = \frac{1}{m} \cdot \delta(t-t') \,. \tag{2.67}$$

ϵ is again a small but positive real quantity that will be finally set to zero. The two simple poles in the inversion formula (2.61) are now approximately given by (see Fig. 2.3)

$$\pm\left[\omega + i\,\frac{\epsilon}{2\,\omega}\right] = \pm\,\kappa_\epsilon \,. \tag{2.68}$$

The region of integration that results from the requirement of Causality is again the upper complex $\bar{\omega}$-plane. There we have the single pole $+\kappa_\epsilon$ that yields

$$G^{+}_{\epsilon_+}(t,t') = -\frac{i}{2\,m\,\omega} \cdot e^{i\,\omega\,(t-t')} \tag{2.69}$$

for the Green's function in the time domain. The upper "+-sign" shall indicate that it results from the pole $+\kappa_\epsilon$. Multiplying this result by the Heaviside function provides

$$G^{+}_{\epsilon_+}(t,t') = -\frac{i}{2\,m\,\omega} \cdot e^{i\,\omega\,(t-t')} \cdot H(t-t') \,. \tag{2.70}$$

But this solution is identical with the expression that results from the first term on the right-hand side of (2.65), and, therefore, is only half of the truth. This can simply

be proven by inserting (2.70) into Eq. (2.21). Taking identity

$$f(t) \cdot \delta(t) \; = f(0) \cdot \delta(t) \tag{2.71}$$

and relation (2.43) into account, and applying L'Hospital's rule to the term that contains the derivation with respect to time of Dirac's delta function gives

$$\frac{\partial^2 G^+_{\epsilon_+}(t,t')}{\partial t^2} \; + \; \omega^2 \cdot G^+_{\epsilon_+}(t,t') \; = \; \frac{1}{2} \cdot \delta(t-t') \; . \tag{2.72}$$

On the other hand, integration in the lower $\bar{\omega}$-plane with the single pole $-\kappa_\epsilon$ provides

$$G^-_{\epsilon_+}(t,t') \; = \; \frac{i}{2\,m\,\omega} \cdot e^{-i\,\omega\,(t-t')} \cdot H(t'-t) \; . \tag{2.73}$$

Inserting this expression again into Eq. (2.21) yields the other half of the solution

$$\frac{\partial^2 G^-_{\epsilon_+}(t,t')}{\partial t^2} \; + \; \omega^2 \cdot G^-_{\epsilon_+}(t,t') \; = \; -\frac{1}{2} \cdot \delta(t-t') \; , \tag{2.74}$$

i.e.,

$$G_{\epsilon_+}(t,t') \; = \; G^+_{\epsilon_+}(t,t') \; - \; G^-_{\epsilon_+}(t,t') \; = \; -\frac{i}{2m\omega} \cdot e^{i\,\omega\,|t-t'|} \tag{2.75}$$

is indeed a possible solution of the equation of motion of the Green's function of the simple harmonic oscillator. But, unfortunately, this Green's function is not in agreement with our physical experience of Causality and Reciprocity since it is nonzero if we have $t < t'$, and since it is symmetric if interchanging source- and observation time. On the other hand, in Quantum Field Theory Green's functions of the type $G^-_{\epsilon_+}(t,t')$ are used to describe the motion of antiparticles "backwards in time" as it is sometimes called in the literature. And, surprisingly, this is in agreement with corresponding scattering experiments. But let us come back to the simple harmonic oscillator. The missing part of the "classical" solution may be obtained from the equation

$$\frac{\partial^2 G^+_{\epsilon_-}(t,t')}{\partial t^2} \; + \; \left[\omega^2 \; - \; i\,\epsilon\right] \cdot G^+_{\epsilon_-}(t,t') \; = \; \frac{1}{m} \cdot \delta(t-t') \; . \tag{2.76}$$

The only singularity in the upper complex plane that contributes to the solution we are looking for is now located in the second quadrant. The corresponding part of the Green's function is then given by

$$G^+_{\epsilon_-}(t,t') \; = \; \frac{i}{2\,m\,\omega} \cdot e^{-i\,\omega\,(t-t')} \cdot H(t-t') \; . \tag{2.77}$$

Substituting this expression in the equation of motion (2.21) provides

$$\frac{\partial^2 G_{\epsilon_-}^{+}(t,t')}{\partial t^2} + \omega^2 \cdot G_{\epsilon_-}(t,t') = \frac{1}{2} \cdot \delta(t-t') \,. \tag{2.78}$$

The sum of $G_{\epsilon_+}^{+}(t,t')$ and $G_{\epsilon_-}^{+}(t,t')$ is again identical with (2.50).

2.1.5 *First Examples of Simple Sources*

After the successful determination of the Green's function of the simple harmonic oscillator we are now asking for first examples of sources to see the integral relation (2.16) in action. As already discussed in the Prologue, we will generally classify the sources into induced and impressed sources according to the terminology used in Electrodynamics. Induced sources are sources which can be traced back to the interaction of the considered object with other objects from the same or other object spaces. Replacing such an interaction by a corresponding source was our more general understanding of Huygens' principle. A quite simple example of an impressed source represents the reflection of a point mass from an ideal elastic wall. It will be discussed in detail later on in this chapter. The light pressure on a rigid sphere—a problem that was solved in 1909 by Debye by use of Mie's theory of light scattering is another example of an induced source that results from the interaction between objects of different object spaces. On the other hand, impressed sources are a priori given sources which act in such a way on the considered object that the caused effect coincides with our experimental experience. That's the justification for using this source. The motion of a point mass on an inclined plane and its free fall caused by the gravitational force is an example of such an impressed source that will also be discussed in detail in what follows. A theoretical description of this gravitational source is given on the deeper level of General Relativity. But this is outside the scope of this book. Other examples of impressed sources are known from macroscopic Electrodynamics. This is a continuum theory of the fields generated by appropriate sources. A description of the nature of these sources requires a microscopic theory of charges and currents. A similar situation is also known from Continuum Mechanics if the material parameters are determined from corresponding macroscopic experiments rather than from an underlying microscopic theory. According to this understanding the following sources are considered to be impressed.

The two limiting cases subsequent to Eq. (2.10) result from the two sources

$$\rho(t') = m \cdot x_1 \cdot \frac{d\delta(t')}{dt'} \tag{2.79}$$

and

$$\rho(t') \;=\; m \cdot v_1 \cdot \delta(t') \;=\; p_1 \cdot \delta(t') \;. \tag{2.80}$$

Regarding the first source we have to consider (2.44). p_1 in the second source represents the initial momentum. If adding both sources

$$\rho(t') \;=\; p_1 \cdot \delta(t') \;+\; m \cdot x_1 \cdot \frac{d\delta(t')}{dt'} \tag{2.81}$$

we thus get from (2.16) the state of motion (2.10) for a given initial position and momentum, as known from the classical treatment. The attentive reader would actually have to raise a protest at this point! The representation (2.16) of the state of motion was derived in Sect. 2.1.2 by assuming homogeneous initial conditions. In other words: Eq. (2.20) and the requirement of homogeneous initial conditions seem to be in conflict with the sources (2.79) and (2.80) since the expression within the square brackets in (2.29) is nonzero for inhomogeneous initial conditions. But it is exactly this term that is generated by the source (2.81). Based on relation (2.16) and by use of the sources (2.79)–(2.81) we are therefore able to provide the state of motion of the simple harmonic oscillator with definite initial values. However, it should be mentioned that in the literature representation (2.16) is often restricted to sources which are in agreement with homogeneous initial conditions. That is, Eq. (2.16) is considered to provide only a special solution of the inhomogeneous equation. The general solution of the homogeneous equation is added afterwards, and the total solution is fitted to potentially given inhomogeneous initial conditions. But it was the main goal of this section to demonstrate that a definite initial state may also result from relation (2.16) and corresponding sources.

The periodic external excitation with frequency $\tilde{\omega}$ of the simple harmonic oscillator given by the source

$$\rho(t') \;=\; p_1 \cdot \omega \cdot \cos \tilde{\omega} t' \tag{2.82}$$

is also of some interest. $\tilde{\omega}$ may differ from the frequency ω of the oscillator, in general. Note also that the frequency ω of the oscillator was incorporated into this source for dimensional reasons. Let us further assume that this source will act on the oscillator up to the observation time t. From (2.16) and (2.50) we thus get

$$x(t) \;=\; \frac{p_1}{m} \cdot \int_0^t \sin \omega(t - t') \cdot \cos \tilde{\omega} t' \; dt' \;. \tag{2.83}$$

Evaluation of the integral provides the final solution

$$x(t) \;=\; \frac{p_1}{m} \cdot \frac{\omega}{(\omega^2 - \tilde{\omega}^2)} \cdot (\cos \tilde{\omega} t - \cos \omega t) \;. \tag{2.84}$$

for the state of motion as one can convince oneself in a straightforward way by inserting this expression and the source (2.82) into (2.20). And, if $t = 0$ is considered, we see that homogeneous initial conditions hold for this solution. Inhomogeneous initial conditions can be considered by adding the sources (2.79)–(2.82) appropriately. An example of this situation is the Kepler problem we consider in detail later on in this chapter. Moreover, if the external frequency and the frequency of the oscillator become identical (i.e., if we have $\tilde{\omega} = \omega$)

$$x(t) = \frac{p_1}{2m} \cdot t \cdot \sin \omega t \tag{2.85}$$

follows from L'Hospital's rule. The amplitude is linearly increasing with time, and if t tends to infinity the system is linearly running into the resonance catastrophe.

2.2 The Damped Harmonic Oscillator

The damped harmonic oscillator provides the opportunity to introduce the "adjoint problem" or rather the corresponding adjoint Green's function. Beside the conservative force of the simple harmonic oscillator a nonconservative and velocity dependent force $Q = -\beta \cdot \dot{x}$ must additionally be considered. This force cannot be derived from a potential. It is used as an inhomogeneity on the right-hand side of the Euler-Lagrange equation (2.3). This equation results from a generalized Hamilton principle where only the kinetic energy is varied. The corresponding equations of motion are then given by

$$m \cdot \frac{d^2x(t)}{dt^2} + \beta \cdot \frac{dx(t)}{dt} + k \cdot x(t) = \rho(t) \tag{2.86}$$

and

$$m \cdot \frac{\partial^2 G(t,t')}{\partial t^2} + \beta \cdot \frac{\partial G(t,t')}{\partial t} + k \cdot G(t,t') = \delta(t-t') \,. \tag{2.87}$$

To represent the solution again in the form of relation (2.16) the equation of motion

$$m \cdot \frac{\partial^2 \tilde{G}(t,t')}{\partial t^2} - \beta \cdot \frac{\partial \tilde{G}(t,t')}{\partial t} + k \cdot \tilde{G}(t,t') = \delta(t-t') \tag{2.88}$$

of the adjoint Green's function $\tilde{G}$ is needed. It differs in the negative friction term from (2.87). The relation between these two Grenn's functions is therefore given by

$$\tilde{G}(t,t') = G(-t,-t') \tag{2.89}$$

if (2.88) and (2.87) are compared. To derive the Reciprocity relation we start from the integral

$$\int_0^{t''+} \left[G(t,t') \cdot \frac{\partial^2 G(-t,-t'')}{\partial t^2} \; - \; G(-t,-t'') \cdot \frac{\partial^2 G(t,t')}{\partial t^2} \right] dt \; . \tag{2.90}$$

Taking the equations of motion into account gives

$$\begin{aligned} & G(t'',t') \; - \; G(-t',-t'') \; = \\ \beta \cdot & \int_0^{t''+} \left[G(t,t') \cdot \frac{\partial G(-t,-t'')}{\partial t} \; + \; G(-t,-t'') \cdot \frac{\partial G(t,t')}{\partial t} \right] dt \; + \\ & \left[G(t,t') \cdot \frac{\partial G(-t,-t'')}{\partial t} \; - \; G(-t,-t'') \cdot \frac{\partial G(t,t')}{\partial t} \right]_{t=0}^{t=t''+} \; . \end{aligned} \tag{2.91}$$

Please, note that m was set to unity for simplicity. Due to Causality and the assumed homogeneous initial conditions the last term on the right-hand side becomes identical zero. It remains the expression

$$\begin{aligned} & G(t'',t') \; - \; G(-t',-t'') \; = \\ \beta \cdot & \int_0^{t''+} \left[G(t,t') \cdot \frac{\partial G(-t,-t'')}{\partial t} \; + \; G(-t,-t'') \cdot \frac{\partial G(t,t')}{\partial t} \right] dt \; . \end{aligned} \tag{2.92}$$

Integration by parts of

$$\begin{aligned} \int_0^{t''+} G(t,t') \cdot \frac{\partial G(-t,-t'')}{\partial t} dt \; = \; & \left[G(t,t') \cdot G(-t,-t'') \right]_{t=0}^{t=t''+} \; - \\ & \int_0^{t''+} G(-t,-t'') \cdot \frac{\partial G(t,t')}{\partial t} dt \end{aligned} \tag{2.93}$$

causes the remaining integral term in (2.92) to disappear. Thus we end up again with (2.23). However, this cancellation would not have happened if in (2.90) the original equation of motion (2.87) of the Green's function with the positive friction term had been used instead of the adjoint equation (2.88). Because of (2.89) the Reciprocity relation may also be expressed in a more symmetric form by use of the adjoint Green's function according to

$$\tilde{G}(t',t'') \; = \; G(t'',t') \, . \tag{2.94}$$

Exercise: Derive relation (2.16). Note, that we can proceed in exactly the same way described above. In (2.90) we simply have to replace the equation of

motion (2.87) of the Green's function $G(t, t')$ by the corresponding equation of motion (2.86) of the state of the damped harmonic oscillator.

2.2.1 *Determination of the Green's Function by Applying the Fourier Transform Method*

The Fourier transform of equation (2.87) of the Green's function is again given by expression (2.59) with the denominator modified by (2.60). But due to the additional friction term κ is now given by

$$\kappa^2 = \omega^2 + i2\gamma\bar{\omega} , \tag{2.95}$$

in contrast to the former expression (2.60). The damping parameter

$$\gamma = \frac{\beta}{2m} \tag{2.96}$$

is moreover introduced. The two simple poles

$$\kappa_1 = \sqrt{\omega^2 - \gamma^2} + i\gamma \tag{2.97}$$

and

$$\kappa_2 = -\sqrt{\omega^2 - \gamma^2} + i\gamma \tag{2.98}$$

must now been considered in the inversion formula (2.61). In dependence on the damping parameter γ we have to distinguish three different situations. $0 < \gamma < \omega$ represents an underdamped oscillator. The simple poles are located in the first and second quadrant of the complex $\bar{\omega}$-plane. $\gamma = \omega$ (then we have $\kappa_1 = \kappa_2$!) results in a single pole of second order that is located on the positive imaginary $\bar{\omega}$-axis. This describes the critically damped oscillator. For the overdamped oscillator $\gamma > \omega$ holds. Now there are two simple poles on the imaginary $\bar{\omega}$-axis. Applying the residual theorem we thus get the three expressions

- $0 < \gamma < \omega$:

$$G(t, t') = \frac{e^{-\gamma\,(t-t')}}{m} \cdot \frac{\sin\left[\sqrt{\omega^2 - \gamma^2} \cdot (t - t')\right]}{\sqrt{\omega^2 - \gamma^2}} \cdot H(t - t') \tag{2.99}$$

- $\gamma = \omega$:

$$G(t, t') = \frac{e^{-\gamma\,(t-t')}}{m} \cdot (t - t') \cdot H(t - t') \tag{2.100}$$

- $\gamma > \omega$:

$$G(t,t') \;=\; \frac{e^{-\gamma\,(t-t')}}{m}\cdot\frac{\sinh\left[\sqrt{\gamma^2\,-\,\omega^2}\cdot(t-t')\right]}{\sqrt{\gamma^2\,-\,\omega^2}}\cdot H(t-t') \tag{2.101}$$

for the respective Green's function. With the sources discussed in Sect. 2.1.5 we get from relation (2.16) the known results for the state of motion of the damped harmonic oscillator if inhomogeneous initial conditions are given (see Morse and Ingard (1986), for example). Regarding the underdamped oscillator we observe not only a decaying amplitude in time but also a shift to a lower frequency compared to the simple harmonic oscillator. The simple harmonic oscillator, on the other hand, appears as a limiting case of the damped harmonic oscillator if γ tends to zero. And, according to (2.94), the corresponding adjoint Green's functions result from interchanging t and t' in (2.99)–(2.101).

2.2.2 The Periodically Excited Damped Harmonic Oscillator

If the periodic source

$$\rho(t') \;=\; C\cdot e^{-i\tilde{\omega}t'} \tag{2.102}$$

with an arbitrary constant C is acting on a damped harmonic oscillator, then the oscillator will follow this external excitation after a certain setting time. Its behaviour may be described in this case by

$$x(t) \;=\; x_0(\tilde{\omega})\cdot e^{-i\tilde{\omega}t}\;, \tag{2.103}$$

where $x_0(\tilde{\omega})$ represents an in general complex-valued amplitude. That is, there will be in general a phase shift between the external excitation and the caused periodic motion of the damped harmonic oscillator. If the external source was switched on at time $t' = -\infty$ we may assume that the oscillator can be found in steady state for every observation time $t > 0$. By use of its Green's function we are now going to derive an explicite expression of the complex-valued amplitude function of the steady state motion of the damped harmonic oscillator. For this purpose we employ once again the Fourier transform of the equation of motion of the corresponding Green's function. It reads

$$G(\bar{\omega},t') \;=\; \frac{1}{m}\cdot\chi(\bar{\omega})\cdot e^{-i\bar{\omega}t'}\;, \tag{2.104}$$

where

$$\chi(\bar{\omega}) \;=\; \left[\omega^2 \,-\, \bar{\omega}^2 \,+\, i2\gamma\bar{\omega}\right]^{-1} \tag{2.105}$$

(please, note that we have to discriminate between the angular frequency $\tilde{\omega}$ of the external periodic excitation and the variable $\bar{\omega}$ of the Fourier transform). According to (2.56) we have on the other hand

$$G(t,t') \;=\; \frac{1}{2\pi}\int_{-\infty}^{\infty} G(\bar{\omega},t')\cdot e^{i\bar{\omega}t}\,d\bar{\omega}\,. \tag{2.106}$$

Thus we get from (2.16), (2.102), and (2.104)

$$x(t) \;=\; \frac{C}{2\,m\,\pi}\cdot\int_{-\infty}^{\infty}\int_{-\infty}^{t}\chi(\bar{\omega})\cdot e^{-it'(\bar{\omega}+\tilde{\omega})}\cdot e^{i\bar{\omega}t}\,dt'\,d\bar{\omega} \tag{2.107}$$

as an expression for the state of motion. The integration with respect to t' provides Dirac's delta function $\delta(\bar{\omega}+\tilde{\omega})$. This results in

$$x(t) \;=\; \tilde{C}\cdot\chi(-\tilde{\omega})\cdot e^{-i\tilde{\omega}t}\,, \tag{2.108}$$

where $\tilde{C} = C/2\pi m$. The complex-valued amplitude function reads therefore

$$x_0(\tilde{\omega}) \;=\; \tilde{C}\cdot\chi(-\tilde{\omega}) \;=\; \tilde{C}\cdot\left[\omega^2 \,-\, \tilde{\omega}^2 \,-\, i2\gamma\tilde{\omega}\right]^{-1}\,. \tag{2.109}$$

Exercise: Show that the same result follows from Eqs. (2.16), (2.99), and (2.102). If taking $t' = -\infty$ as the lower integration limit the integration with respect to t' can be performed in a straightforward way.

Expression (2.109) can moreover be split into real and imaginary parts according to

$$x_0(\tilde{\omega}) \;=\; x_0'(\tilde{\omega}) \,+\, i\cdot x_0''(\tilde{\omega})\,, \tag{2.110}$$

where

$$x_0'(\tilde{\omega}) \;=\; \frac{\tilde{C}\cdot(\omega^2 \,-\, \tilde{\omega}^2)}{(\omega^2 \,-\, \tilde{\omega}^2)^2 \,+\, 4\,\gamma^2\,\tilde{\omega}^2} \tag{2.111}$$

and

$$x_0''(\tilde{\omega}) \;=\; \frac{2\,\gamma\,\tilde{\omega}\,\tilde{C}}{(\omega^2 \,-\, \tilde{\omega}^2)^2 \,+\, 4\,\gamma^2\,\tilde{\omega}^2}\,. \tag{2.112}$$

In the limiting case of a vanishing damping constant γ the imaginary part becomes identical with Dirac's delta function, i.e.,

$$x_0''(\tilde{\omega}) = \tilde{C} \cdot \pi \cdot \delta(\omega^2 - \tilde{\omega}^2) \,. \tag{2.113}$$

This follows from

$$\lim_{\epsilon \to 0} \frac{\epsilon}{(\omega^2 - \tilde{\omega}^2)^2 + \epsilon^2} = \pi \, \delta(\omega^2 - \tilde{\omega}^2) \tag{2.114}$$

as one of the existing representations of this function. The two limiting cases of an angular frequency $\tilde{\omega}$ of the external excitation that is much higher or much lower than the oscillators own frequency ω are also of some interest. Then we have

- $\tilde{\omega} >> \omega$:

$$x_0'(\tilde{\omega}) = -\frac{\tilde{C}}{\tilde{\omega}^2} \tag{2.115}$$

$$x_0''(\tilde{\omega}) = \frac{2\,\tilde{C}\,\gamma}{\tilde{\omega}^3} \tag{2.116}$$

- $\tilde{\omega} << \omega$:

$$x_0'(\tilde{\omega}) = \frac{\tilde{C}}{\omega^2} = \text{const.} \tag{2.117}$$

$$x_0''(\tilde{\omega}) = \frac{2\,\tilde{C}\,\gamma\,\tilde{\omega}}{\omega^4} \,. \tag{2.118}$$

The imaginary part is always a positive real number in both of these limiting cases. This is a consequence of the positive sign in the exponent of the external excitation (2.102). A negative sign in the exponent would result in an always negative real number of the imaginary part. The complex-valued amplitude function plays a major role for the modeling of material properties with and without absorption. This is of importance if we intend to describe the propagation of microwaves in dielectric media or in light scattering analysis, for example, where the imaginary part is used to consider the loss of energy.

The real and imaginary parts (2.111) and (2.112) are not independent of each other. They comply with the so-called "Kramers-Kronig relations"

$$x_0'(\tilde{\omega}) = \frac{2}{\pi} \cdot \text{pv} \int_0^\infty \frac{\Omega \cdot x_0''(\Omega)}{\Omega^2 - \tilde{\omega}^2} \, d\Omega \tag{2.119}$$

$$x_0''(\tilde{\omega}) = -\frac{2\,\tilde{\omega}}{\pi} \cdot \text{pv} \int_0^\infty \frac{x_0'(\Omega)}{\Omega^2 - \tilde{\omega}^2} \, d\Omega \,. \tag{2.120}$$

"pv" in front of the integral denotes Cauchy's principal value integration. The derivation of the Kramers-Kronig relations will be discussed in detail in Sect. 2.5.3. However, the proof of relation (2.119) in the limiting case of a vanishing damping constant is straightforward. It follows from the imaginary part (2.113) and relation

$$\delta(\omega^2 - \omega_n^2) \;=\; \frac{1}{2\,\omega_n} \cdot [\delta(\omega - \omega_n) \;+\; \delta(\omega + \omega_n)] \tag{2.121}$$

—another relation that holds for Dirac's delta function. The reverse proof that we get Dirac's delta function for the imaginary part $x_0''(\tilde{\omega})$ if using $x_0'(\tilde{\omega})$ for a vanishing damping in (2.120) and after integration—albeit more elaborate—is also possible. And, finally, we may state that the behaviour of the amplitude function in the time domain can be related to the imaginary part $x_0''(\tilde{\omega})$. If the imaginary part is given by Dirac's delta function, then the amplitude function becomes independent of time. On the other hand, the amplitude function becomes damped in time and in dependence on the parameter γ if the imaginary part takes the shape of a Lorentzian profile, as known from spectroscopy.

2.3 Basic Motions of a Point Mass

Some basic motions of a point mass are limiting cases of the simple- and damped harmonic oscillator. The forceless motion, the motion on the inclined plane (including free fall), and the motion in the presence of friction are the situations we intend to consider in what follows. Looking at such simple examples is again aimed at a more detailed corroboration of some of the positions formulated in the Prologue. But we will also resort to some of these examples when discussing basic interaction processes and their characterization with respect to energy conservation by use of the Green's function formalism.

We go back to the Green's function (2.50) of the simple harmonic oscillator and consider the limiting case $\omega = 0$. Applying L'Hospital's rule this gives the simple expression

$$G(t, t') \;=\; \frac{(t - t')}{m} \cdot H(t - t') \tag{2.122}$$

for the Green's function of a forceless point mass. Its uniform motion with the constant velocity v_1 follows in a straightforward way from our basic relation (2.16) and the source (2.80) (a primary impact with momentum $p_1 = m \cdot v_1$). Thus we get

$$x(t) \;=\; v_1 \cdot t\,. \tag{2.123}$$

But we can also use (2.122) to describe the frictionless motion of a point mass on an inclined plane including the free fall. The corresponding source that has to be

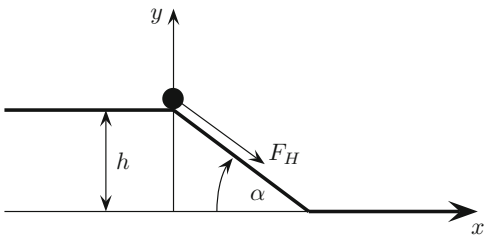

Fig. 2.4 Geometry of the inclined plane

used in (2.16) reads

$$\rho(t') \;=\; F_H(t') \;=\; m \cdot g \cdot \sin\alpha \cdot H(t') \tag{2.124}$$

(see Fig. 2.4). According to this source the gravitational force is switched on at the initial time $t' = 0$ (in so doing, we have to arrange beforehand that the point mass was positioned at a higher level—on top of the Leaning Tower of Pisa, for example). It is then acting on the point mass up to the observation time t. $\alpha = \pi/2$ corresponds to the free fall. The distance s (we have $y(t) = h - s(t) \cdot \sin\alpha$, where $s(0) = 0$) the point mass covers on the inclined plane up to the observation time t is then given by

$$s(t) \;=\; g\,\sin\alpha \cdot \int_0^{t^+} (t - t')\,dt' \;=\; \frac{g}{2}\,t^2 \cdot \sin\alpha\ . \tag{2.125}$$

The well-known result of the free fall follows from $\alpha = \pi/2$.

The equation of motion of a point mass in the presence of friction may be obtained by canceling the linear term in (2.86),

$$\frac{d^2x(t)}{dt^2} \;+\; 2\,\gamma\,\frac{dx(t)}{dt} \;=\; \frac{1}{m} \cdot \rho(t)\ . \tag{2.126}$$

From (2.101) and with $\omega = 0$ we get on the other hand

$$G(t,t') \;=\; \frac{e^{-\gamma\,(t-t')}}{m} \cdot \frac{\sinh[\gamma \cdot (t-t')]}{\gamma} \cdot H(t-t') \;= \\ \frac{1}{2\,\gamma\,m} \cdot \left[1 \;-\; e^{-2\gamma(t-t')}\right] \cdot H(t-t') \tag{2.127}$$

for the corresponding Green's function. Applying the source

$$\rho(t') \;=\; 2\,\gamma\,m \cdot v_1 \cdot H(t')\ , \tag{2.128}$$

in (2.16) results in the state of motion

$$x(t) \;=\; v_1 \cdot t \;-\; \frac{v_1}{2\,\gamma} \cdot \left(1 \;-\; e^{-2\gamma t}\right) \;. \tag{2.129}$$

For larger observation times the state of motion becomes simply

$$x(t) \;=\; v_1 \cdot \left(t \;-\; \frac{1}{2\,\gamma}\right) \;. \tag{2.130}$$

$1/2\gamma$ is a characteristic time constant of this motion that depends on the coefficient γ of the friction. But (2.129) demonstrates once again the aspect that the initial velocity at $t \;=\; 0$ is identical zero, as required in the process of the derivation of relation (2.16) by use of Green's theorem (see also the discussion subsequent to Eq. (2.29)).

2.4 Lippmann-Schwinger Equation

The Lippmann-Schwinger equation plays an important role in Quantum Mechanics where it is used as a starting point to derive iterative solutions for scattering problems, for example. This section is aimed at the demonstration that this equation can be introduced and applied with benefit already in classical physics. Among others, it will allow us to derive expressions for the Green's functions we have considered so far by starting from the solution of a more simple situation. Our first example is concerned with the motion of a point mass in the presence of friction that was considered right now.

$$\frac{\partial^2 G_0(t,t')}{\partial t^2} \;=\; \frac{1}{m} \cdot \delta(t-t') \tag{2.131}$$

is the equation for the Green's function of the unperturbed problem without any friction. It is assumed that we are already in the possession of its solution (2.122). On the other hand,

$$\frac{\partial^2 G(-t,-t'')}{\partial t^2} \;-\; 2\gamma \cdot \frac{\partial G(-t,-t'')}{\partial t} \;=\; \frac{1}{m} \cdot \delta(t-t'') \tag{2.132}$$

is the adjoint equation of the problem in the presence of friction we intend to solve. To derive the Lippmann-Schwinger equation we proceed along the same track used to derive the Reciprocity relation (2.23), or (2.94) as appropriate, that holds for the damped harmonic oscillator. In so doing, we start from the integral

$$\int_0^{t''+} \left[G_0(t,t') \cdot \frac{\partial^2 G(-t,-t'')}{\partial t^2} \;-\; G(-t,-t'') \cdot \frac{\partial^2 G_0(t,t')}{\partial t^2} \right] dt \;. \tag{2.133}$$

Because of the additional friction term $2\gamma\,\partial G(-t,-t'')/\partial t$ in (2.132), and by use of the Reciprocity relation (2.23) this integral gives

$$G(t'',t') \;=\; G_0(t'',t') \;+\; 2\,\gamma\,m\int_{t'}^{t''+} G_0(t,t')\cdot\frac{\partial G(t'',t)}{\partial t}\,dt\;. \tag{2.134}$$

The lower and upper integration limit are a consequence of the product $H(t-t')\cdot H(t''-t)$ of the Heaviside functions. Equation (2.134) is already the Lippmann-Schwinger equation we are looking for. The first term on the right-hand side represents the known Green's function of the frictionless problem. On the other hand, the Green's function (2.127) of the problem with friction has been obtained from the Green's function (2.101) of the overdamped harmonic oscillator if ω was set to zero. A straightforward calculation (if (2.43), (2.71) as well as L'Hospital's rule is taken into account!) shows that (2.127) obeys both the Lippmann-Schwinger equation (2.134) and the equation of motion (2.132) but with a positive sign in the friction term instead of the negative sign of its adjoint. It is therefore interesting to see if this analytical solution can also be obtained from the iterative solution of the Lippmann-Schwinger equation. For this purpose, let us replace the exponential function in Eq. (2.127) by the first 4 terms of its Taylor expansion. This reads

$$G(t,t') \;=\; \frac{1}{m}\cdot\left[(t-t') \;-\; \gamma\,(t-t')^2 \;+\; \frac{2}{3}\,\gamma^2\,(t-t')^3 \;-\; \cdots\right]\cdot H(t-t')\;. \tag{2.135}$$

The first iteration of the Lippmann-Schwinger equation (2.134) provides on the other hand

$$G^{(1)}(t,t') \;=\; G_0(t,t') \;+\; 2\,\gamma\,m\int_{t'}^{t+} G_0(\bar{t},t')\cdot\frac{\partial G_0(t,\bar{t})}{\partial \bar{t}}\,d\bar{t}\;. \tag{2.136}$$

Applying G_0 according to (2.122) gives

$$G^{(1)}(t,t') \;=\; \frac{1}{m}\cdot\left[(t-t') \;-\; \gamma\,(t-t')^2\right]\cdot H(t-t')\;. \tag{2.137}$$

Next, let us replace the unknown Green's function $G(t,t')$ on the right-hand side of (2.134) by this first iteration. This provides the second iteration

$$G^{(2)}(t,t') \;=\; \frac{1}{m}\cdot\left[(t-t') \;-\; \gamma\,(t-t')^2 \;+\; \frac{2}{3}\,\gamma^2\,(t-t')^3\right]\cdot H(t-t')\;, \tag{2.138}$$

and so on. This iteration process actually reflects the Taylor expansion of the exponential function $exp[-2\gamma(t-t')]$ so that we will finally arrive at the analytical solution (2.127). Now, if choosing (2.80) as the source acting on the point

mass (2.16) and the Green's function according to (2.136) yields

$$x^{(1)}(t) \;=\; v_1 \cdot t \;-\; v_1 \cdot \gamma \cdot t^2 \tag{2.139}$$

as a first iteration of the state of motion, and so on. If we are primarily interested in an iterative solution of the state of motion rather than its corresponding Green's function we can derive (2.139) in a more direct way that emphasizes the advantage of the source concept. For this purpose let us rewrite (2.126) into

$$\frac{d^2x(t)}{dt^2} \;=\; \frac{1}{m} \cdot \rho(t) \;-\; 2\,\gamma\,\frac{dx(t)}{dt} \;=\; \tilde{\rho}(t)\;. \tag{2.140}$$

Then, from (2.16) and the source $\tilde{\rho}(t)$

$$x(t) \;=\; \frac{1}{m} \cdot \int_0^{t^+} G_0(t,t') \cdot \rho(t')dt' \;-\; 2\,\gamma \cdot \int_0^{t^+} G_0(t,t') \cdot \frac{dx(t')}{dt'}dt' \tag{2.141}$$

follows. The first term on the right-hand side provides the already known expression $x^{(0)}(t) = v_1 \cdot t$ of the uniform motion. Inserting this expression into the second term on the right-hand side we end up again with (2.139) as a first iteration of the state of motion, and so on. In so doing we avoid the precalculation of the Green's function. However, since we are primarily interested in the Green's function to characterize the object under consideration we prefer to apply the Lippmann-Schwinger equation to this function.

We can proceed in the same way to get an iterative solution for the Green's function of the underdamped harmonic oscillator. In this case the Green's function

$$\frac{\partial^2 G_0(t,t')}{\partial t^2} \;+\; \omega^2\, G_0(t,t') \;=\; \frac{1}{m} \cdot \delta(t-t') \tag{2.142}$$

of the simple harmonic oscillator is used as the unperturbed problem. It represents again the first term on the right-hand side of (2.134).

$$\frac{\partial^2 G(-t,-t'')}{\partial t^2} \;-\; 2\gamma \cdot \frac{\partial G(-t,-t'')}{\partial t} \;+\; \omega^2\, G(-t,-t'') \;=\; \frac{1}{m} \cdot \delta(t-t'') \tag{2.143}$$

is the corresponding adjoint equation. From (2.50) and noting that

$$\frac{\partial G_0(t'',t)}{\partial t} \;=\; -\,\frac{\cos\omega(t''-t)}{m} \cdot H(t''-t) \;+\; \frac{\sin\omega(t''-t)}{m\,\omega} \cdot \delta(t''-t) \tag{2.144}$$

holds we get

$$G^{(1)}(t'',t') \;=\; G_0(t'',t') \;+\; 2\,\gamma\,m \int_{t'}^{t''+} G_0(t,t') \cdot \frac{\partial G_0(t'',t)}{\partial t}\,dt \;=$$

$$G_0(t'',t') \;-\; \frac{2\,\gamma}{m\,\omega} \cdot \int_{t'}^{t''} \sin\omega(t-t') \cdot \cos\omega(t''-t)\,dt\;. \qquad (2.145)$$

A tedious but straightforward evaluation of the integral gives finally

$$G^{(1)}(t'',t') \;=\; G_0(t'',t') \;-\; \gamma \cdot (t''-t') \cdot G_0(t'',t') \qquad (2.146)$$

as the first iteration of the Lippmann-Schwinger equation for the Green's function of the damped harmonic oscillator. But the same expression can be obtained from (2.99) if replacing again the exponential function $exp[-\gamma\,(t''-t')]$ by the first two terms of its Taylor expansion, and by neglecting γ in the sine function as well as in the denominator. Using this first iteration in (2.16) makes therefore only sense if there is a very weak damping (a very small γ), or if the difference $(t''-t')$ between observation- and source time is small enough. The next higher iteration may be obtained if we use the first iteration instead of $G(t'',t)$ under the integral on the right-hand side of (2.134), i.e. from

$$G^{(2)}(t'',t') \;=\; G_0(t'',t') \;+\; 2\,\gamma\,m \int_{t'}^{t''+} G_0(t,t') \cdot \frac{\partial G^{(1)}(t'',t)}{\partial t}\,dt\;, \qquad (2.147)$$

and so on. But it should be emphasized at this point that the iteration procedure, if applied to the damped harmonic oscillator, does not provide the shift to a lower frequency at any step of iteration. It contains only the initial frequency of the simple harmonic oscillator.

The simple harmonic oscillator has been considered as the unperturbed problem and the friction term as the actual perturbation, so far. But the Green's function (2.50) of the simple harmonic oscillator may be also derived by the iteration procedure from the Green's function of the forceless point mass, as we will demonstrate now. In this case, the Green's function (2.122) represents the solution of the unperturbed problem (2.131). It is assumed to be given. Equation (2.142), on the other hand, is the equation we intend to solve. Since this latter problem is self-adjoint we start from the Lippmann-Schwinger equation

$$G(t'',t') \;=\; G_0(t'',t') \;-\; \omega^2\,m \int_{t'}^{t''+} G_0(t,t') \cdot G(t'',t)\,dt\;, \qquad (2.148)$$

with $G_0(t'', t')$ according to (2.122). But (2.122) agrees already with the first expansion term of (2.50) if expanding the sine function into a Taylor series. The first iteration

$$G^{(1)}(t'', t') \;=\; G_0(t'', t') \;-\; \omega^2\, m \int_{t'}^{t''+} G_0(t, t') \cdot G_0(t'', t)\, dt \tag{2.149}$$

reproduces the second term of this Taylor series, and so on. That is, the iterative solution of the Lippmann-Schwinger equation (2.148) reproduces again the Taylor expansion of the Green's function (2.50).

This is the way the Lippmann-Schwinger equations can be used to gain iterative solutions of more complex linear problems. The usefulness of these solutions are mainly dependent on the definition and solvability of the unperturbed problem, of course. Moreover, many nonlinear equations of interest in physics are still linear in their second derivatives. Therefore, to gain iterative solutions on the basis of corresponding Lippmann-Schwinger equations also in this nonlinear situation seems to be a feasible approach. Wouldn't it be a nice homework for the reader to proof this idea by applying it to the anharmonic oscillator? But there is another aspect that can be discussed in the context of the iterative solutions derived so far in this section. There is an analogy to the renormalization procedure known from Quantum Electrodynamics if applied to the mass of an electron, for example. In the Prologue we shortly touched the point of view that in reality one can never find an isolated object that is free of any interaction with its environment. The renormalization procedure takes this situation into account by introducing an "observable mass". Regarding the above considered example of the motion of a point mass in the presence of friction we can discuss the situation as follows: The "mass" is a characteristic property of a point mass, of course. If we intend to derive the mass solely on the detection of its state of motion we face the problem that, if it is the uniform motion without any friction given by $x_0(t) = v_0 \cdot t$, then there is no dependence on the "mass". The same happens obviously for the free fall. Only if taking an interaction with its environment into account—as it is done with the Stokes' friction term—the mass appears in the resulting state of motion. Let us assume that the Stokes friction parameter β is known. Then, from (2.16) and (2.127) (i.e., if we measure the position at a certain observation time $t > 0$ in a corresponding experiment) we get the state of motion of the point mass. This state of motion and if taking relation $\gamma = \beta/2m$ into account allows us to deduce its mass. In this special situation we are fortunately in the possession of a closed analytical expression of the Green's function, and, if assuming an initial momentum according to (2.80) as the acting source, of the resulting state of motion. The mass that is deduced from this state of motion is therefore also completely known. However, if we do not know this analytical solution we can try to approach it by the above described iteration procedure of the Lippmann-Schwinger equation. This results in a corresponding iteration of the mass that comes along with the hope that every higher iteration will represent a better approach of the true mass. But in contrast to Quantum Theory, there is no singularity problem with this mass that must be solved.

This example was just mentioned to demonstrate the importance of the interaction of the considered object with its environment, and, as a consequence of this interaction, that it could make sense to distinguish between a true- and observable mass already in this classical situation.

It should be finally mentioned that the Lippmann-Schwinger equation in Quantum Theory is often represented in a somewhat different form. By use of definition (2.44) we may write instead of (2.134)

$$G(t,t') \;=\; G_0(t,t') \;+ \\ m \cdot \int_{t'}^{t^+} G_0(\bar{t},t') \cdot \Sigma(\bar{t},\tilde{t}) \cdot G(t,\tilde{t})\, d\tilde{t}\, d\bar{t}\;. \tag{2.150}$$

$\Sigma(\bar{t},\tilde{t})$ therein denotes the so-called "self-energy operator"

$$\Sigma(t,t') \;=\; 2\,\gamma \cdot \frac{\partial \delta(t-t')}{\partial t'}\;. \tag{2.151}$$

In a shorter operator notation (2.150) reads

$$\mathbf{G}(t,t') \;=\; \mathbf{G_0}(t,t') \;+\; m \cdot \mathbf{G_0}(\bar{t},t') \odot \mathbf{\Sigma}(\bar{t},\tilde{t}) \odot \mathbf{G}(t,\tilde{t})\;, \tag{2.152}$$

where we have to integrate over all time variables which appear twice. Regarding the examples considered in this section this "self-energy" represents a loss of energy caused by the state of motion of the point mass in the presence of the phenomenologically introduced friction. We will come back to this operator in the following section.

2.5 Two Systematic Ways to Derive Green's Functions

We have already become acquainted with some Green's functions as well as with their usage to solve simple initial value problems for classical point masses. This was accomplished by using the integral relation (2.16) as a pivotal mediator between cause and effect. And we have just now discussed the Lippmann-Schwinger equation that can be used as a starting point to gain iterative solutions for the corresponding Green's functions. Relation (2.16) was first derived by employing Green's theorem, the requirement of Causality, and by assuming that the underlying equation of motion of the Green's function is identical with the corresponding equation of the state of motion $x(t)$ of the point mass but with its inhomogeneity on the right-hand side (its source/cause) replaced by Dirac's delta function $\delta(t-t')$ (a unit source). In Sect. 2.1.2 we have alternatively discussed that one can consider the equation of motion of the Green's function and relation (2.16) to be given, and that the corresponding equation of the state of motion $x(t)$ follows if the inverse G^{-1}

of the Green's function is introduced appropriately. Now, before dealing with the Green's functions themselves, we will look at this interplay between the equations of motion and relation (2.16) from a third point of view. For this purpose let us consider the more general problem

$$\hat{\mathbf{L}}\, x(t) \;=\; \rho(t) \tag{2.153}$$

with the linear operator $\hat{\mathbf{L}}$ given by

$$\hat{\mathbf{L}} \;=\; \frac{d^2}{dt^2} \;+\; a_1 \frac{d}{dt} \;+\; a_2 \;. \tag{2.154}$$

Relation (2.16) is again used as an *ansatz* that fits to the requirement of Causality. The importance of this relation is justified afterwards by its agreement with our physical experience. Then, if using (2.16) in (2.153), the equation of motion

$$\hat{\mathbf{L}}\, G(t,t') \;=\; \delta(t-t') \tag{2.155}$$

for the Green's function follows immediately if taking the definition of Dirac's delta function (2.32) into account.

The Fourier transform method together with the residual theorem was the most systematic way to derive the Green's function we have considered so far. In the first part of this section we are now going to show that the method discussed in Sect. 2.1.3 in conjunction with the Green's function of the simple harmonic oscillator may be put on a more sound and systematic mathematical footing that is closely related to what is known from solving ordinary differential equations. Let us call it therefore the "classical method" to determine the Green's functions. By using Cauchy's integral formula we may define a complex-valued Dirac's delta function that relates this method to the residual theorem. The Kramers-Kronig relation we have already discussed in the context of the damped harmonic oscillator in the presence of a periodic excitation is finally discussed.

2.5.1 Classical Method to Determine the Green's Functions

For reasons of clarity, let us write down again the four linear equations which of our interest in this section. These are the equation

$$\frac{\partial^2 G(t,t')}{\partial t^2} \;=\; \frac{1}{m} \cdot \delta(t-t') \tag{2.156}$$

of a point mass without friction, the equation

$$\frac{\partial^2 G(t,t')}{\partial t^2} + \omega^2 \cdot G(t,t') = \frac{1}{m} \cdot \delta(t-t') \tag{2.157}$$

of the simple harmonic oscillator, the equation

$$\frac{\partial^2 G(t,t')}{\partial t^2} + 2\,\gamma \cdot \frac{\partial G(t,t')}{\partial t} = \frac{1}{m} \cdot \delta(t-t') \tag{2.158}$$

of a point mass with friction, and, finally, the equation

$$\frac{\partial^2 G(t,t')}{\partial t^2} + 2\,\gamma \cdot \frac{\partial G(t,t')}{\partial t} + \omega^2 \cdot G(t,t') = \frac{1}{m} \cdot \delta(t-t')\,. \tag{2.159}$$

of the damped harmonic oscillator. In what follows $m = 1$ is again chosen for simplicity. The final result must be multiplied by $1/m$ to take the dependence on the mass into account. We are looking for solutions that are in accordance with the requirement of Causality

$$G(t,t') = 0, \quad \text{if } t < t' \tag{2.160}$$

as well as with the condition

$$\lim_{\epsilon \to 0} G(t'+\epsilon, t') = 0\,. \tag{2.161}$$

That all these Green's functions are only dependent on the temporal difference $t-t'$ is an experience we have gathered in the foregoing considerations. This holds not only for the complete analytical solutions but also for all the iterative solutions of the Lippmann-Schwinger equation. But also without this previous knowledge and due to the linearity of the problems one may assume such a time dependence. Therefore, introducing the new variable $\tau = t - t'$ we may write

$$\frac{d^2 G(\tau)}{d\tau^2} = \delta(\tau) \tag{2.162}$$

$$\frac{d^2 G(\tau)}{d\tau^2} + \omega^2 \cdot G(\tau) = \delta(\tau) \tag{2.163}$$

$$\frac{d^2 G(\tau)}{d\tau^2} + 2\,\gamma \cdot \frac{dG(\tau)}{d\tau} = \delta(\tau) \tag{2.164}$$

$$\frac{d^2 G(\tau)}{d\tau^2} + 2\,\gamma \cdot \frac{dG(\tau)}{d\tau} + \omega^2 \cdot G(\tau) = \delta(\tau)\,. \tag{2.165}$$

Now, if using

$$G(\tau) \;=\; F(\tau)\cdot H(\tau)\;, \tag{2.166}$$

as an appropriate *ansatz* for the Green's function, the requirement of Causality is already satisfied. It remains the determination of the function $F(\tau)$. For this purpose we have to insert (2.166) into the corresponding equation. Let us start with the most simple situation (2.162).

Taking the first derivative of the Heaviside function and Dirac's delta function into account we thus get

$$\frac{d^2F(\tau)}{d\tau^2}\cdot H(\tau) \;+\; \left[2\cdot\frac{dF(\tau)}{d\tau} \;-\; \frac{F(\tau)}{\tau}\right]\cdot\delta(\tau) \;=\; \delta(\tau)\;. \tag{2.167}$$

Next, let us consider function $F(\tau)$ to represent the general solution of the corresponding homogeneous differential equation

$$\frac{d^2F(\tau)}{d\tau^2} \;=\; 0\;. \tag{2.168}$$

This solution is obviously given by

$$F(\tau) \;=\; C_1\cdot\tau \;+\; C_2 \tag{2.169}$$

with so far unknown coefficients C_1 and C_2. But from condition

$$F(\tau) \;=\; 0 \quad \text{if} \quad \tau = 0 \tag{2.170}$$

it follows that

$$C_2 \;=\; 0\;. \tag{2.171}$$

The remaining constant C_1 can be determined by integration of equation (2.167) with respect to τ or by applying identity (2.71). This gives

$$2\cdot\left[\frac{dF(\tau)}{d\tau}\right]_{\tau=0} \;-\; \left[\frac{F(\tau)}{\tau}\right]_{\tau=0} \;=\; 1\;. \tag{2.172}$$

Because of (2.170) L'Hospital's rule can be applied to the second term on the left-hand side thus providing the condition

$$\left[\frac{dF(\tau)}{d\tau}\right]_{\tau=0} \;=\; 1\;. \tag{2.173}$$

This generates indeed a solution of equation (2.167) with constant C_1 given by

$$C_1 = 1 . \tag{2.174}$$

The Green's function reads therefore

$$G(\tau) = \tau \cdot H(\tau) \tag{2.175}$$

or

$$G(t, t') = (t - t') \cdot H(t - t') . \tag{2.176}$$

It is exactly this approach we will call the "classical method" in this book. Now, let us see if this method—looking for the general solution of the corresponding homogeneous equation for the function $F(\tau)$ of *ansatz* (2.166) and determination of the unknown constants from the two conditions

$$F(\tau = 0) = 0 \tag{2.177}$$

and (2.173)—will also succeed in solving the other problems.

$$\frac{d^2F(\tau)}{d\tau^2} + \omega^2 \cdot F(\tau) = 0 \tag{2.178}$$

is the homogeneous equation of $F(\tau)$ related to (2.163). Using the exponential expression

$$F(\tau) = e^{i\lambda\tau} \tag{2.179}$$

as an appropriate *ansatz* results in the characteristic equation

$$\omega^2 - \lambda^2 = 0 \tag{2.180}$$

to determine the parameter λ. We thus get the two values $\lambda_1 = \omega$ and $\lambda_2 = -\omega$.

$$F(\tau) = C_1 \cdot e^{i\omega\tau} + C_2 \cdot e^{-i\omega\tau} \tag{2.181}$$

is the corresponding general solution of (2.178). The unknown coefficients are calculated from (2.177) and (2.173). The result is

$$C_1 = -C_2 \tag{2.182}$$

$$C_2 = \frac{i}{2\,\omega} . \tag{2.183}$$

We note with satisfaction that we end up with the correct expression for the Green's function of the simple harmonic oscillator (see Eq. (2.49) but with $m = 1$!) if using the Euler representation of the sine function.

Regarding the Green's function for the point mass with friction we can proceed in the same way. The corresponding characteristic equation is now given by

$$\lambda^2 - i\,2\,\gamma\,\lambda = 0\,. \tag{2.184}$$

The general solution of the homogeneous equation reads therefore

$$F(\tau) = C_1 + C_2 \cdot e^{-2\gamma\tau}\,. \tag{2.185}$$

The expressions

$$C_1 = -\,C_2 \tag{2.186}$$

$$C_2 = -\,\frac{1}{2\,\gamma} \tag{2.187}$$

are the results of conditions (2.177) and (2.173). Looking at (2.127) we see that our "classical method" produces again the correct result for the Green's function of a point mass in the presence of friction.

$$\lambda^2 - i\,2\,\gamma\,\lambda - \omega^2 = 0 \tag{2.188}$$

is the characteristic equation related to the damped harmonic oscillator. It follows that

$$F(\tau) = e^{-\gamma\tau} \cdot \left[C_1 \cdot e^{i\sqrt{\omega^2-\gamma^2}\cdot\tau} + C_2 \cdot e^{-i\sqrt{\omega^2-\gamma^2}\cdot\tau} \right] \tag{2.189}$$

is the general solution if $\gamma < \omega$ is considered. From (2.177) and (2.173) we get

$$C_1 = -\,C_2 \tag{2.190}$$

$$C_2 = \frac{i}{2\,\sqrt{\omega^2 - \gamma^2}}\,. \tag{2.191}$$

This results again in the correct Green's function (2.99). The same procedure can be applied with success to the other two cases $\gamma = \omega$ and $\gamma > \omega$.

Using the examples of the simple and damped harmonic oscillator we will now discuss an aspect of the "classical method" that has its analogy in Quantum Field Theory. We will slightly touch on this issue in the final chapter of this book. It is concerned with the question of how to solve the corresponding equation of motion by reducing it to the solution of only an ordinary differential equation of first order.

For this purpose, let us consider the operator

$$\hat{\mathbf{L}}_{\mathbf{1}} = \frac{d}{d\tau} - i \cdot \Omega \,, \tag{2.192}$$

where

$$\Omega = \Omega_r + i \cdot \Omega_i \quad ; \; \Omega_r \,, \, \Omega_i \geq 0 \tag{2.193}$$

represents a complex-valued quantity, in general. The general solution of the equation

$$\hat{\mathbf{L}}_{\mathbf{1}} \, F_1(\tau) = 0 \tag{2.194}$$

is obviously given by

$$F_1(\tau) = C_1 \cdot e^{i \, \Omega \, \tau} \,. \tag{2.195}$$

Combination with the conjugate-complex operator

$$\hat{\mathbf{L}}_{\mathbf{1}}^{*} = \frac{d}{d\tau} + i \cdot \Omega^{*} \tag{2.196}$$

provides

$$\hat{\mathbf{L}}_{\mathbf{1}}^{*} \, \hat{\mathbf{L}}_{\mathbf{1}} \, F(\tau) = \hat{\mathbf{L}} \, F(\tau) = \frac{d^2 F(\tau)}{d\tau^2} + 2 \, \Omega_i \, \frac{dF(\tau)}{d\tau} + \left(\Omega_r^2 + \Omega_i^2 \right) F(\tau) \,. \tag{2.197}$$

On the other hand we may state that equation

$$\hat{\mathbf{L}} \, F(\tau) = 0 \tag{2.198}$$

corresponds

- with the equation of the simple harmonic oscillator if

$$\Omega_r = \omega_0 \; ; \; \Omega_i = 0 \tag{2.199}$$

- with the equation of the damped harmonic oscillator if

$$\Omega_r = \sqrt{\omega_0^2 - \gamma^2} \; ; \; \Omega_i = \gamma \,. \tag{2.200}$$

The solution $F(\tau)$ of (2.198) is then given by the combination

$$F(\tau) = -\frac{i}{2 \, \Omega_r} \cdot \left[F_1(\tau) - F_1^{*}(\tau) \right] \tag{2.201}$$

if taking again the two additional conditions (2.173) and (2.177) into account. $F_1^*(\tau)$ represents the solution of the conjugate-complex equation of (2.194), i.e., of

$$\hat{\mathbf{L}}_1^* F_1^*(\tau) = 0 \,. \tag{2.202}$$

Its general solution is

$$F_1^*(\tau) = C_2 \cdot e^{-i\Omega^* \tau} \,. \tag{2.203}$$

The damped harmonic oscillator is again characterized by the nonzero imaginary part Ω_i and a shift to a lower eigenfrequency Ω_r. We will see later on in this book that the "classical method" can be applied with benefit to derive the Green's functions of other problems. However, to find an appropriate *ansatz* for the Green's function (as accomplished with (2.166) for the above discussed examples!) is the important initial step of this method. But such an *ansatz* can often be deduced intuitively from the considered physical situation.

Next, we ask for the relation between the Green's function

$$G(\tau) = \frac{\sin \omega\tau}{\omega} \cdot H(\tau) \tag{2.204}$$

of the equation

$$\left(\frac{d^2}{dt^2} + \omega^2\right) G(\tau) = \delta(\tau) \tag{2.205}$$

of the simple harmonic oscillator and the so far unknown Green's function $\bar{G}(\tau)$ of the first order equation

$$\left(\frac{d}{dt} + i\omega\right) \bar{G}(\tau) = \delta(\tau) \,. \tag{2.206}$$

This equation corresponds with equation (2.202) but with an inhomogeneity given by $\delta(\tau)$. Looking at (2.197) we may write instead of (2.205)

$$\left(\frac{d}{dt} + i\omega\right)\left(\frac{d}{dt} - i\omega\right) G(\tau) = \delta(\tau) \,. \tag{2.207}$$

The solution of (2.206) can therefore be calculated from the Green's function (2.204) by using the relation

$$\bar{G}(\tau) = \left(\frac{d}{dt} - i\omega\right) G(\tau) \,. \tag{2.208}$$

Taking (2.71) into account we thus get

$$\bar{G}(\tau) \;=\; e^{-i\omega\tau}\cdot H(\tau)\;. \tag{2.209}$$

In Chap. 6 we will derive a relation between the Green's function of the Klein-Gordon—and Dirac equation that is similar to (2.208).

Finally, let us come back to the Green's function (2.75) we derived already in Sect. 2.1.4 by employing the Fourier transform method. This Green's function was not in agreement with our additional requirements of Causality and Reciprocity. Since a similar situation is known in Quantum Mechanics in conjunction with the Klein-Gordon equation, for example, it may well be of interest to see how this Green's function can be derived by using the "classical method". To this end, we simply have to replace *ansatz* (2.166) by

$$G(\tau) \;=\; F^{+}(\tau)\cdot H(\tau) \;-\; F^{-}(\tau)\cdot H(-\tau)\;. \tag{2.210}$$

Then, instead of the two conditions (2.173) and (2.177), we now end up with the two conditions

$$\left\{\frac{d[F^{+}(\tau)+F^{-}(\tau)]}{d\tau}\right\}_{\tau=0} \;=\; 1 \tag{2.211}$$

and

$$F^{+}(\tau=0) \;+\; F^{-}(\tau=0) \;=\; 0 \tag{2.212}$$

to determine the unknown coefficients of the two linear independent solutions

$$F^{+}(\tau) \;=\; C_1\cdot e^{i\omega\tau} \tag{2.213}$$

and

$$F^{-}(\tau) \;=\; C_2\cdot e^{-i\omega\tau} \tag{2.214}$$

of the corresponding homogeneous equations of the simple harmonic oscillator. These coefficients are again given by (2.182) and (2.183). The final result reads therefore

$$G(\tau) \;=\; -\frac{i}{2\omega}\cdot\left[e^{i\omega\tau}\cdot H(\tau) \;+\; e^{-i\omega\tau}\cdot H(-\tau)\right] \tag{2.215}$$

which is identical with the result (2.75) derived in Sect. 2.1.4.

2.5.2 *Alternative Formulation by Using Cauchy's Integral Formula*

The inversion formula

$$G(\tau) = \int_{-\infty}^{\infty} G(\bar{\omega}) \cdot e^{\,i\bar{\omega}\tau} \, \frac{d\bar{\omega}}{2\,\pi} \tag{2.216}$$

as well as the Fourier transforms

$$G(\bar{\omega}) = -\frac{1}{\bar{\omega}^2} \tag{2.217}$$

$$G(\bar{\omega}) = -\frac{1}{\bar{\omega}^2 - \omega^2} \tag{2.218}$$

$$G(\bar{\omega}) = -\frac{1}{\bar{\omega}^2 - i2\gamma\bar{\omega}} \tag{2.219}$$

$$G(\bar{\omega}) = -\frac{1}{\bar{\omega}^2 - \omega^2 - i2\gamma\bar{\omega}} \tag{2.220}$$

of the Green's functions related to Eqs. (2.162)–(2.165) are principally involved in the discussion regarding the relation between the "classical"—and Fourier transform method. At first, let us consider the three cases (2.218)–(2.220). The zeroes of the characteristic equations used before to find the general solution $F(\tau)$ of the corresponding homogeneous equations within the "classical method" are obviously identical with the poles of the above given Fourier transforms. And also the exponential *ansatz* (2.179) has its counterpart in the expression $e^{\,i\bar{\omega}\tau}$ of the inversion formula. Since there are only two simple poles $\bar{\omega}_1$ and $\bar{\omega}_2$ located somewhere in the complex $\bar{\omega}$-plane we may write

$$G(\bar{\omega}) \cdot e^{\,i\bar{\omega}\tau} = -\frac{e^{\,i\bar{\omega}\tau}}{(\bar{\omega} - \bar{\omega}_1) \cdot (\bar{\omega} - \bar{\omega}_2)} \,, \tag{2.221}$$

where

$$\begin{aligned} \bar{\omega}_1 &= \omega \\ \bar{\omega}_2 &= -\omega \,, \end{aligned} \tag{2.222}$$

$$\begin{aligned} \bar{\omega}_1 &= i2\gamma \\ \bar{\omega}_2 &= 0 \,, \end{aligned} \tag{2.223}$$

or

$$\bar{\omega}_1 = i\gamma + \sqrt{\omega^2 - \gamma^2}$$
$$\bar{\omega}_2 = i\gamma - \sqrt{\omega^2 - \gamma^2} \tag{2.224}$$

must be used to agree with (2.218)–(2.220), respectively. The poles (2.222) and (2.223) are limiting cases of the poles (2.224) if $\gamma \to 0$ and $\omega \to 0$. Cauchy's integral formula for any analytical and complex-valued function $f(\bar{\omega})$ in a region Γ is given by

$$\oint_\Gamma \frac{f(\bar{\omega})}{(\bar{\omega} - \bar{\omega}_0)} \frac{d\bar{\omega}}{2\,\pi\,i} = f(\bar{\omega}_0)\,. \tag{2.225}$$

With the definition

$$\oint_\Gamma f(\bar{\omega}) \cdot \delta_c(\bar{\omega} - \bar{\omega}_0) \frac{d\bar{\omega}}{2\,\pi} := f(\bar{\omega}_0) \tag{2.226}$$

of a complex-valued Dirac's delta function we get therefore

$$\delta_c(\bar{\omega} - \bar{\omega}_0) = \frac{1}{2\pi i} \cdot \frac{1}{(\bar{\omega} - \bar{\omega}_0)} \tag{2.227}$$

(see Stumpf und Schuler (1973), Johansson et al. (2012), for example). For the three cases of our interest we may therefore write instead of (2.216)

$$G(\tau) = \frac{-i}{(\bar{\omega}_1 - \bar{\omega}_2)} \cdot \int_{-\infty}^{\infty} e^{\,i\bar{\omega}\tau} \cdot [\delta_c(\bar{\omega} - \bar{\omega}_1) - \delta_c(\bar{\omega} - \bar{\omega}_2)]\; d\bar{\omega}\,. \tag{2.228}$$

The paths Γ_1 and Γ_2 of integration are chosen such that only the contribution $\int_{-\infty}^{\infty} \cdots d\bar{\omega}/2\pi$ remains from integral (2.225) (see also Fig. 2.5). Since the section along the positive imaginary axis is traversed twice but with opposite sign it does not

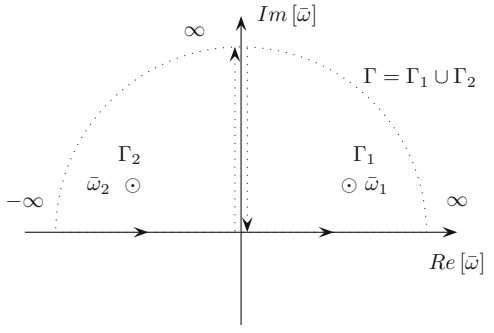

Fig. 2.5 Path of integration in the upper complex $\bar{\omega}$-plane if using Cauchy's integral formula

contribute to the integral. That is, we may replace the two quarter circles at infinity in the upper half-plane by a semi-circle). This gives the general solution

$$G(\tau) \;=\; \frac{-\,i}{(\bar{\omega}_1 - \bar{\omega}_2)} \cdot \left[C_1 \cdot e^{\,i\bar{\omega}_1 \tau} \;-\; C_2 \cdot e^{\,i\bar{\omega}_2 \tau} \right] . \tag{2.229}$$

The unknown coefficients C_1 and C_2 are now calculated from the additional conditions

$$G(\tau = 0) = 0 \tag{2.230}$$

$$\left[\frac{dG(\tau)}{d\tau} \right]_{\tau=0} = 1 \, . \tag{2.231}$$

This results in $C_1 = C_2 = 1$ for the three cases (2.218)–(2.220) under consideration. It is again straightforward to show that one gets the well-known expressions for the corresponding Green's functions if taking the zeroes (2.222), (2.223), and (2.224) in (2.229) into account, and if multiplying the result by the Heaviside function $H(\tau)$.

The Fourier transform of the Green's function has been obtained from the respective equation of motion, so far. But it can also be derived from the integral representation

$$G(\bar{\omega}) \;=\; \int_{-\infty}^{\infty} G(\tau) \cdot e^{-i\bar{\omega}\tau} \, d\tau \tag{2.232}$$

once the Green's function $G(\tau)$ in the time domain is known. Let us demonstrate this by deriving the Fourier transform (2.220) of the underdamped oscillator (if m is set to unity). The corresponding Green's function in the time domain reads

$$G(\tau) \;=\; e^{-\gamma\,\tau} \cdot \frac{\sin(\tilde{\omega} \cdot \tau)}{\tilde{\omega}} \cdot H(\tau) \, , \tag{2.233}$$

where $\tilde{\omega}^2 = \omega^2 - \gamma^2$. Using the Euler representation of the sine function (2.232) provides

$$G(\bar{\omega}) \;=\; -\,\frac{i}{2\tilde{\omega}} \left[\int_0^{\infty} e^{-i\tau(\bar{\omega}-\tilde{\omega}-i\gamma)} \, d\tau \;-\; \int_0^{\infty} e^{-i\tau(\bar{\omega}+\tilde{\omega}-i\gamma)} \, d\tau \right] . \tag{2.234}$$

If we consider these integrals to represent the Fourier transforms of Dirac's delta functions with complex-valued arguments we have

$$G(\bar{\omega}) \;=\; -\,\frac{i}{2\tilde{\omega}} \left[\delta_c(\bar{\omega} - \tilde{\omega} - i\gamma) \;-\; \delta_c(\bar{\omega} + \tilde{\omega} - i\gamma) \right] . \tag{2.235}$$

Applying (2.227) provides (2.220).

Exercise: Show that the same procedure can be applied to derive the Green's function of the critically damped and overdamped oscillator.

It should be also mentioned that the above described procedure may be generalized to linear differential equations of order n. If the Fourier transform has n simple poles, then the general solution for the Green's function reads

$$G(\tau) \;=\; -\,i\cdot\sum_{l=1}^{n} C_l\cdot\frac{e^{\,i\bar{\omega}_l\tau}}{\prod_{k=1,k\neq l}^{n}(\bar{\omega}_l-\bar{\omega}_k)}\;. \tag{2.236}$$

The unknown coefficients C_l are calculated from n additional conditions derived along the same way described in Sect. 2.5.1. The pivotal aspect of the above method is therefore the determination of the poles of the Fourier transform. But I want to emphasize once again that these poles are identical with the zeroes of the characteristic equation that results from the classical *ansatz* in terms of exponential functions to solve the corresponding homogeneous differential equation.

Now, let us see how we can solve case (2.217). Since the Fourier transform has a double pole at $\bar{\omega}=0$ we have to apply Cauchy's integral formula

$$\oint_{\Gamma}\frac{f(\bar{\omega})}{(\bar{\omega}-\bar{\omega}_0)^2}\,\frac{d\bar{\omega}}{2\,\pi}\;=\;i\cdot\left[\frac{df(\bar{\omega})}{d\bar{\omega}}\right]_{\bar{\omega}=\bar{\omega}_0}\;. \tag{2.237}$$

We then get from (2.217) and the inversion formula

$$G(\tau)\;=\;-\,i\,C_0\cdot\left[\frac{de^{\,i\bar{\omega}\tau}}{d\bar{\omega}}\right]_{\bar{\omega}=0}\;=\;C_0\cdot\tau\;. \tag{2.238}$$

$C_0 = 1$ follows from condition (2.231). This is again the known result for the Green's function if multiplied by the Heaviside function. Relation (2.237) may be used moreover to define the first derivative of Dirac's delta function with complex arguments.

Let us finally look once again at the 4 problems considered above but from the point of view of the self-energy operator. This quantity was introduced at the end of Sect. 2.4 that was concerned with the Lippmann-Schwinger equation. Starting from (2.150) the equation of motions (2.156)–(2.159) may be rewritten as follows:

$$\frac{\partial^2 G(t,t')}{\partial t^2}\;+\;\int_{t'}^{t^+}\Sigma(t,\bar{t})\cdot G(\bar{t},t')\,d\bar{t}\;=\;\frac{1}{m}\cdot\delta(t-t')\;. \tag{2.239}$$

$$\Sigma_o(t,t')\;=\;0 \tag{2.240}$$

$$\Sigma_O(t,t')\;=\;\omega^2\cdot\delta(t'-t) \tag{2.241}$$

$$\Sigma_R(t,t')\;=\;2\,\gamma\cdot\frac{\partial\delta(t-t')}{\partial t'} \tag{2.242}$$

are the possible expressions for the self-energy operator entering Eq. (2.239). Σ_o is the characteristic expression of the free point mass. Σ_O is the self-energy operator that is related to the simple harmonic oscillator, and Σ_R characterizes the presence of friction. These expressions can be combined appropriately. The damped harmonic oscillator, for example, is then represented by Eq. (2.239) and

$$\Sigma(t,\bar{t}) \;=\; \Sigma_R(t,\bar{t}) \;+\; \Sigma_O(t,\bar{t})\;. \tag{2.243}$$

According to the convolution theorem the Fourier transform of Eq. (2.239) gives

$$G(\bar{\omega},t') \;=\; -\frac{1}{m}\cdot\frac{e^{-i\bar{\omega}t'}}{\bar{\omega}^2 \;-\; \Sigma(\bar{\omega})}\;, \tag{2.244}$$

where

$$\Sigma_o(\bar{\omega}) = 0 \tag{2.245}$$

$$\Sigma_O(\bar{\omega}) = \omega^2 \tag{2.246}$$

$$\Sigma_R(\bar{\omega}) = i\,2\,\gamma\,\bar{\omega} \tag{2.247}$$

(please, note that the last expression is a consequence of the definition (2.44) of the first derivative of Dirac's delta function). We reached at a point where we can mathematically sharpen our more philosophical considerations in the Prologue regarding the definition of the basic category **objects** by their respective **properties** (see Sect. 1.2). Equation (2.244) together with a specific expression for the self-energy operator may be considered with some justification as an abstract mathematical definition of a specific object in the Fourier transform domain. This object—after it is transformed back into the time domain, and after a source is specified—is then be brought to "physical life" with our pivotal relation (2.16) (i.e., it is transferred into a certain **state** that has to be related by an appropriate procedure to a measurable quantity). But there is another possibility of interpretation. We may characterize an ideal and isolated object—that is an object without any interaction with its environment—by a real-valued self-energy operator. These are the two objects "free point mass" and "simple harmonic oscillator", regarding the cases we have considered so far. The complex-valued part of the self-energy operator is then used to describe the influence of the environment—the phenomenologically introduced friction in the above examples—that comes along with a loss of energy. An even more rigorous position would be the definition of the "free point mass" as the only interaction-free object of classical particle physics characterized by a vanishing Σ according to (2.245). All nonzero self-energy operators are then considered as lossless (the external force of the simple harmonic oscillator) or lossy (the friction) impacts on this idealized object from its environment. The usage of real-valued self-energy operators to characterize idealized objects exhibits already an analogy to the Hermitian operators of Quantum Mechanics, according to my mind.

2.5.3 *Kramers-Kronig Relation*

The Fourier transform (2.220) of the Green's function of the damped harmonic oscillator is within the focus of the following considerations. The situation is moreover restricted to a periodic external excitation, and that the oscillator is already in a steady state. This latter situation is obtained by shifting the lower integration boundary in Eq. (2.16) to $t = -\infty$, as already discussed in Sect. 2.2.2. And, finally, $m = 1$ is again chosen for simplicity. Since the Green's function depends only on the temporal difference $t - t'$ we have

$$x(t) = \int_{-\infty}^{t^+} G(t - t') \cdot \rho(t')\, dt' , \tag{2.248}$$

or, if introducing the new variable $\tau = t - t'$,

$$x(t) = \int_{0}^{\infty} G(\tau) \cdot \rho(t - \tau)\, d\tau . \tag{2.249}$$

We can use (2.233) as the relevant Green's function, for example, if the underdamped situation is considered. We know furthermore that both the expressions (2.249) and (2.16) are in agreement with Causality. Applying the convolution theorem to (2.249) provides

$$x(\bar{\omega}) = G(\bar{\omega}) \cdot \rho(\bar{\omega}) , \tag{2.250}$$

where

$$G(\bar{\omega}) = \int_{-\infty}^{\infty} G(\tau) \cdot e^{-i\bar{\omega}\tau}\, d\tau . \tag{2.251}$$

Because of

$$\rho(\bar{\omega}) = \int_{-\infty}^{\infty} \rho(t) \cdot e^{-i\bar{\omega}t}\, dt \tag{2.252}$$

and since we assume a periodic source with the external excitation frequency $\tilde{\omega}$ given by

$$\rho(t) = C \cdot e^{\pm i\tilde{\omega}t} \tag{2.253}$$

it follows that

$$\rho(\bar{\omega}) = 2\pi C \cdot \delta(\bar{\omega} \mp \tilde{\omega}) . \tag{2.254}$$

The damping term of the complex-valued amplitude of $x(t)$ and of the Fourier transform of the Green's function differ in sign if the lower sign in expression (2.253) is used. But it is identical for the upper sign in (2.253). This can be seen from Eqs. (2.104)/(2.105) and (2.109) in Sect. 2.2.2. We may therefore expect that the Kramers-Kronig relations (2.119) and (2.120) for the in general complex-valued amplitude can be translated into corresponding relations for the Fourier transform of the Green's function. Equations (2.220) and (2.251) are therefore in the center of our interest in what follows.

According to (2.224) the poles of the Fourier transform of the Green's function are located in the upper half of the complex $\bar{\omega}$-plane. In the lower complex $\bar{\omega}$-plane (2.251) reads

$$G(\bar{\omega}) \;=\; \int_{-\infty}^{\infty} G(\tau) \cdot e^{-i\bar{\omega}_r \tau \,-\, \bar{\omega}_i \tau}\, d\tau \;, \tag{2.255}$$

where we have $\bar{\omega} \;=\; \bar{\omega}_r - i\bar{\omega}_i$ and $\bar{\omega}_i \;\geq\; 0$. But this is a holomorphic function in the lower complex $\bar{\omega}$-plane since it is finite everywhere (also if $\bar{\omega} \;=\; 0$) and tends quickly to zero at the lower semi-circle as long as $\tau \;\geq\; 0$. This latter condition is justified by the Causality of $G(\tau)$ reflected in the Heaviside function $H(\tau)$. From Cauchy's integral formula it then follows that the integral in (2.255)—if closed at the lower semi-circle—becomes zero,

$$\oint_{\Gamma} G(\bar{\omega})\, d\bar{\omega} \;=\; 0 \;. \tag{2.256}$$

Now, instead of (2.256) let us consider the integral

$$\oint_{\Gamma'} \frac{G(\bar{\omega})}{\bar{\omega} - \bar{\omega}_0}\, d\bar{\omega} \tag{2.257}$$

with a single pole $\bar{\omega}_0$ located at the positive real axis, and with the closed integration path Γ' shown in Fig. 2.6. Since the pole $\bar{\omega}_0$ is outside this integration path (2.257) must also become zero. From Cauchy's integral formula it now follows that

$$\mathrm{pv} \int_{-\infty}^{\infty} \frac{G(\bar{\omega})}{\bar{\omega} - \bar{\omega}_0}\, d\bar{\omega} \;=\; -\,i\,\pi\, G(\bar{\omega}_0) \;. \tag{2.258}$$

The part of the integral that runs in mathematical positive sense along the semi-circle with radius $r \;=\; a$ around the pole $\bar{\omega}_0$ just provides $+i\pi \cdot \delta_c(\bar{\omega} - \bar{\omega}_0)$. The integral along the lower semi-circle at infinity in the lower plane, on the other hand, provides zero. The principal value integral along the real axis is defined according to

$$\mathrm{pv} \int_{-\infty}^{\infty} \frac{G(\bar{\omega})}{\bar{\omega} - \bar{\omega}_0}\, d\bar{\omega} \;:=\; lim_{a \to 0} \left[\int_{-\infty}^{\bar{\omega}-a} \frac{G(\bar{\omega})}{\bar{\omega} - \bar{\omega}_0}\, d\bar{\omega} \;+\; \int_{\bar{\omega}+a}^{\infty} \frac{G(\bar{\omega})}{\bar{\omega} - \bar{\omega}_0}\, d\bar{\omega} \right] . \tag{2.259}$$

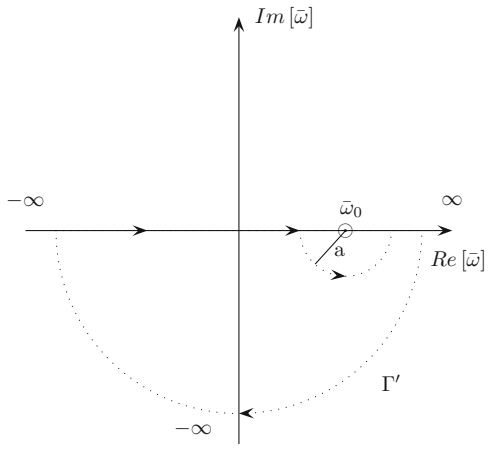

Fig. 2.6 Path of integration in the lower complex $\bar{\omega}$-plane related to the Kramers-Kronig relation

Splitting of the Fourier transform $G(\bar{\omega})$ into its real and imaginary part $G'(\bar{\omega}) + iG''(\bar{\omega})$ provides the Kramers-Kronig relations

$$G^{'}(\bar{\omega}_0) \;=\; -\frac{1}{\pi}\cdot \mathrm{pv}\int_{-\infty}^{\infty} \frac{G^{''}(\bar{\omega})}{\bar{\omega}\;-\;\bar{\omega}_0}\, d\bar{\omega} \tag{2.260}$$

$$G^{''}(\bar{\omega}_0) \;=\; \frac{1}{\pi}\cdot \mathrm{pv}\int_{-\infty}^{\infty} \frac{G^{'}(\bar{\omega})}{\bar{\omega}\;-\;\bar{\omega}_0}\, d\bar{\omega}\;. \tag{2.261}$$

These relations can further be modified and be expressed in terms of integrals over positive frequencies $\bar{\omega}$ alone. This is possible since

$$G^{*}(\bar{\omega}) \;=\; G(-\bar{\omega}) \tag{2.262}$$

holds. This follows from (2.251) and the fact that $G(\tau)$ is a pure real quantity. Regarding the real and imaginary part of $G(\bar{\omega})$ it follows from (2.262) that we have

$$G^{'}(\bar{\omega}) = G^{'}(-\bar{\omega}) \tag{2.263}$$

$$G^{''}(\bar{\omega}) = -\,G^{''}(-\bar{\omega})\;. \tag{2.264}$$

Splitting (2.220) into its real and imaginary part according to

$$G(\bar{\omega}) \;=\; G^{'}(\bar{\omega}) \;+\; i\,G^{''}(\bar{\omega})\;, \tag{2.265}$$

where

$$G'(\bar{\omega}) = \frac{(\omega^2 - \bar{\omega}^2)}{(\omega^2 - \bar{\omega}^2)^2 + 4\gamma^2\bar{\omega}^2} \tag{2.266}$$

$$G''(\bar{\omega}) = \frac{-2\gamma\bar{\omega}}{(\omega^2 - \bar{\omega}^2)^2 + 4\gamma^2\bar{\omega}^2} \tag{2.267}$$

is a direct way to justify relations (2.263) and (2.264) for the Green's function of our interest. Then, if multiplying the integrands in (2.260) and (2.261) by

$$1 = \frac{\bar{\omega} + \bar{\omega}_0}{\bar{\omega} + \bar{\omega}_0} \tag{2.268}$$

and if taking (2.263) and (2.264) into account we get finally the Kramers-Kronig relations

$$G'(\bar{\omega}_0) = -\frac{2}{\pi} \cdot \mathrm{pv} \int_0^\infty \frac{\bar{\omega} \cdot G''(\bar{\omega})}{\bar{\omega}^2 - \bar{\omega}_0^2}\, d\bar{\omega} \tag{2.269}$$

$$G''(\bar{\omega}_0) = \frac{2\bar{\omega}_0}{\pi} \cdot \mathrm{pv} \int_0^\infty \frac{G'(\bar{\omega})}{\bar{\omega}^2 - \bar{\omega}_0^2}\, d\bar{\omega}\,. \tag{2.270}$$

It should be noted that they differ from relations (2.119) and (2.120) in sign. This can be explained by the location of the poles of the complex amplitude of $x(t)$ in Sect. 2.2.2 in the lower complex plane. Thus we have to close the integration path at infinity in the upper complex plane. The pole $\bar{\omega}_0$ in (2.257) would thus be circled in mathematical negative sense. This would change the sign on the right-hand side of (2.258). It should be stated moreover that there is no damping in the time domain if the imaginary part of the Fourier transform of the Green's function is represented by Dirac's delta function, as already observed in Sect. 2.2.2. (Nussenzveig 1972) is highly recommended for further reading about Kramers-Kronig and other dispersion relations.

Let us summarize the results of this section:

- Causality is an essential precondition to derive the Kramers-Kronig relations for the Fourier transform of the Green's function.
- Due to Causality and in the presence of a periodic external excitation the Kramers-Kronig relations of the Green's function may be directly transferred to the complex-valued amplitude of $x(t)$.
- All the poles of the considered Fourier transform must be located either in the lower or in the upper complex plane. The Fourier transform must be a holomorphic function and must tend quickly to zero at infinity in the respective other half-plane.

- If the imaginary part of the Fourier transform of the Green's function is represented by Dirac's delta function no damping in the time domain can be observed. The imaginary part will take the form of a Lorentzian profile if there is a damping.

2.6 Temporal Boundary Value Problem of the Harmonic Oscillator

Initial condition problems of point masses have been exclusively considered so far. These initial conditions (initial position and initial momentum)—according to our understanding formulated in the Prologue—are provided by corresponding sources. The object itself was characterized by its Green's function $G(t, t')$. Its state, produced by a given source, was considered to be the result of relation (2.16). In other words and in accordance with the discussion at the end of Sect. 2.5.2: Our object of desire—so far—was the free point mass characterized by its Green's function G_0 according to (2.122). This point mass was subjected to different external influences (to an external force and/or to a phenomenologically introduced friction). In this section we will turn toward a different class of problems—so-called boundary value problems. For this purpose we consider once again the behaviour of the harmonic oscillator but in the presence of additional temporal conditions.

The following considerations are first aimed at a demonstration that an infinitely-countable number of simple harmonic oscillators—all subject to the same temporal boundary conditions—may be summarized into one superior object (let us call it a "super oscillator") with an infinitely-countable number of inner states (or degrees) of freedom. These inner states provide a complete physical characterization of this super oscillator. This will lead us already in this classical situation to an understanding of the abstract category **object** that is closely related to what is known from Quantum Mechanics. We faced a similar equivalence between a classical and a quantum mechanical point of view already at the end of Sect. 2.5.2 in conjunction with the self-energy operator. Second but not less important, the representation of the Green's function by a series expansion in terms of the eigenfunctions and with singularities at the eigenfrequencies usually employed in this situation will be critically scrutinized. The "source picture" of the Fourier series will be discussed as an alternative presentation. This will allow us to better express the point of view that a certain state of an object may be considered as the source for the state of another object from the same object class, as already mentioned in the Prologue.

Let us at first keep our attention focused on initial value problems, and let us consider the equation of motion (2.20) of the simple harmonic oscillator but now supplemented by the additional temporal conditions

$$x(t = 0) \; = \; x(t = t_1) \; = \; 0 \quad ; \; t_1 > 0 \; . \tag{2.271}$$

There exist an infinitely-countable number of oscillators with eigenfrequencies ω_n given by

$$\omega_n \;=\; \frac{n\,\pi}{t_1} \quad ;\; n = 1, 2, \cdots , \tag{2.272}$$

all of them subject to these additional conditions. The corresponding equation of motion that is in agreement with (2.271) reads therefore

$$\frac{d^2 x_n(t)}{dt^2} \;+\; \omega_n^2 \cdot x_n(t) \;=\; \frac{1}{m} \cdot \rho_n(t) \; . \tag{2.273}$$

Using (2.16), the Green's function

$$G_n(t, t') \;=\; \frac{\sin \omega_n (t - t')}{m \cdot \omega_n} \cdot H(t - t') \tag{2.274}$$

of the corresponding simple harmonic oscillator, and if assuming the source

$$\rho_n(t) \;=\; m \cdot v_n \cdot \delta(t) \tag{2.275}$$

with initial momentum $m\, v_n$ we obtain

$$x_n(t) \;=\; \frac{v_n}{\omega_n} \cdot \varphi_n(t) \; , \tag{2.276}$$

where

$$\varphi_n(t) \;=\; \sin \omega_n \, t \; . \tag{2.277}$$

All the solutions (2.276)—time harmonic oscillations with amplitudes $x_n \;=\; v_n/\omega_n$—obey the required temporal conditions. The functions $\varphi_n(t)\,;\; n = 1, 2, \cdots$ represent moreover an orthogonal basis in the temporal region $t \in [0, t_1]$. These are the eigensolutions of the homogeneous Eq. (2.273). ω_n^2 are the corresponding eigenvalues. Every function $x(t)$ subject to the temporal boundary conditions may therefore be expanded into the Fourier series

$$x(t) \;=\; \sum_{n=1}^{\infty} x_n \cdot \varphi_n(t) \tag{2.278}$$

in $t \in [0, t_1]$ with expansion coefficients x_n given by

$$x_n \;=\; \frac{v_n}{\omega_n} \; . \tag{2.279}$$

A specific expansion may therefore considered to be the result of the superposition of an in general infinitely-countable number of solutions of single oscillators, all excited at $t = 0$ with appropriate initial momenta.

$$x(t) \;=\; \sum_{n=1}^{\infty} \int_0^{t^+} G_n(t,t') \cdot \rho_n(t')\, dt' \tag{2.280}$$

with $G_n(t,t')$ according to (2.274) and $\rho_n(t')$ according to (2.275) represents therefore the Fourier series (2.278) as a result of an initial value problem related to the equation of motion (2.20) subject to the additional conditions (2.271). Now, let us see how this problem is usually solved in the literature by use of Green's functions (see Duffy (2001), for example).

Starting point is the equation of motion

$$\frac{\partial^2 G(t,t')}{\partial t^2} \;+\; \omega^2 \cdot G(t,t') \;=\; \frac{1}{m} \cdot \delta(t-t') \tag{2.281}$$

with not yet specified ω, and the additional temporal conditions

$$G(t=0,t') \;=\; G(t=t_1,t') \;=\; 0\,. \tag{2.282}$$

Representing the Green's function in $t \in [0,t_1]$ by the series expansion

$$G(t,t') \;=\; \sum_{n=1}^{\infty} G_n(t') \cdot \varphi_n(t) \tag{2.283}$$

in terms of the eigensolutions (2.277) will satisfy these conditions. The so far unknown expansion coefficients $G_n(t')$ are obtained from Eq. (2.281), and if using the corresponding Fourier series expansion

$$\delta(t-t') \;=\; \sum_{n=1}^{\infty} D_n(t') \cdot \varphi_n(t)\,, \tag{2.284}$$

of Dirac's delta function with expansion coefficients $D_n(t')$ given by

$$D_n(t') \;=\; \int_0^{t_1} \delta(t-t') \cdot \varphi_n(t)\, dt \;=\; \varphi_n(t')\,. \tag{2.285}$$

This representation of Dirac's delta function is also known as the "completeness relation". Inserting this representation in Eq. (2.281), we obtain for the expansion coefficients in (2.283)

$$G_n(t') \;=\; \frac{1}{m} \cdot \frac{\varphi_n(t')}{\omega^2 - \omega_n^2}\,. \tag{2.286}$$

The Green's function is therefore given by the bilinear expansion

$$G(t,t') \;=\; \frac{1}{m}\cdot\sum_{n=1}^{\infty}\frac{\varphi_n(t)\cdot\varphi_n(t')}{\omega^2-\omega_n^2} \;=\; \frac{1}{m}\cdot\sum_{n=1}^{\infty}G_n(\omega_n)\cdot\varphi_n(t)\cdot\varphi_n(t')\;. \tag{2.287}$$

Beside its poles at the eigenfrequencies (mathematically called its "point spectrum") this Green's function exhibits another interesting feature which makes it essentially differ from the Green's function (2.274) of the initial value problem. Equation (2.287) is now a symmetric function with respect to the time variables t and t'. It is therefore not in agreement with Causality, as required for the initial value problem. However, if we are interested in establishing a causal relation between a certain state $\rho(t)$ of an assumed source and the resulting state $x(t)$ of the considered object, and if all these states are time-periodic states restricted to the region $t\in[0,t_1]$, the Causality requirement applied to the initial value problems is not really necessary. Let us rather take up the position that the expansion coefficients of the state of the considered object—if expanded into a Fourier series in terms of the eigenfunctions (2.277)—are determined by an assumed source that is also expressed in terms of an appropriate Fourier series within $[0,t_1]$. This is exactly what I will call the "source picture" of the Fourier series. Applying Green's theorem (2.22) in region $[0,t_1]$ to the equation of motion, and if taking the temporal boundary conditions as well as the symmetry of (2.287) into account, it is straightforward to show that

$$x(t) \;=\; \frac{1}{m}\cdot\sum_{n=1}^{\infty}G_n(\omega_n)\cdot\int_0^{t_1}\varphi_n(t')\cdot\rho(t')\,dt'\cdot\varphi_n(t) \tag{2.288}$$

holds. This relation replaces (2.16). But, as already discussed in Sect. 2.1.2, there exists another possibility to directly derive (2.288) by introducing the inverse of the Green's function $G^{-1}(t,t')$ according to

$$G^{-1}(t,\bar{t})\odot G(\bar{t},t') \;=\; \frac{1}{m}\cdot\delta(t-t')\;. \tag{2.289}$$

Note that we have again to integrate from 0 to t_1 with respect to all time variables which appear twice! Comparison with (2.281) provides

$$G^{-1}(t,t') \;=\; \left[\frac{\partial^2}{\partial t^2}\;+\;\omega^2\right]\delta(t-t')\;. \tag{2.290}$$

This inverse of the Green's function is also symmetric with respect to t and t'. The equation of motion

$$\frac{d^2x(t)}{dt^2}\;+\;\omega^2\cdot x(t) \;=\; \frac{1}{m}\cdot\rho(t) \tag{2.291}$$

can be rewritten into

$$G^{-1}(t,\bar{t}) \odot x(\bar{t}) \;=\; \frac{1}{m} \cdot \rho(t) \;. \tag{2.292}$$

After multiplication of this equation with $G(\tilde{t},t)$, and if taking (2.287) as well as (2.289) into account we end up with (2.288).

Expression (2.288) is well-known from the literature (see Duffy (2001), for example). It is usually supplemented with the remark that, due to the resulting singularity, it cannot be used for any periodic source that provides an external excitation at the eigenfrequencies. This is justified by the observation that this situation runs into the resonance catastrophe, as already considered in Sect. 2.1.5. But, regarding this catastrophe we have seen that it is linear in time. That is, the amplitude becomes infinite only if t tends to ∞. One may therefore ask if (2.288) can be applied if this periodic source is acting only a finite time? Moreover, applying the source (2.275) in (2.288) provides the boring solution $x(t) = 0$ instead of (2.278) derived before. On the other hand, using the source

$$\rho(t) \;=\; m \cdot v_n \cdot \left(1 - \frac{\omega^2}{\omega_n^2}\right) \frac{d\delta(t)}{dt} \,, \tag{2.293}$$

in (2.288) provides exactly solution (2.278). This raises the question about the meaning of relation (2.288). The following considerations should be considered as an attempt to give an answer and to provide a first justification of the "source picture" of the Fourier series from a physical point of view.

The integral term on the right-hand side of Eq. (2.288) provides exactly the expansion coefficients ρ_n of a source function $\rho(t)$ if expanded in $[0,t_1]$ in terms of the orthogonal eigenfunctions $\varphi_n(t)$. Let us assume for a moment that $\omega \neq \omega_n$ holds. The series expansion

$$\rho(t) \;=\; \sum_{n=1}^{\infty} \rho_n \cdot \varphi_n(t) \tag{2.294}$$

of this source is then converted by Eq. (2.288) into the series expansion

$$x(t) \;=\; \sum_{n=1}^{\infty} x_n \cdot \varphi_n(t) \;, \tag{2.295}$$

of the sought solution in $[0,t_1]$ and with expansion coefficients x_n given by

$$x_n \;=\; \frac{1}{m} \cdot \frac{\rho_n}{\omega^2 - \omega_n^2} \;. \tag{2.296}$$

From a physical point of view we can therefore consider expression (2.288) as the representation of a causal relation between the state $\rho(t)$ of a given source and the state $x(t)$ of an object (the initially mentioned super oscillator) that is characterized by an infinitely-countable number of inner degrees of freedom subject to the additionally required temporal boundary conditions (2.271). But what happens if $\omega = \omega_n$ holds? Then we have again a singularity problem. But this problem can be avoided if every source is considered as an impressed source, and if it is chosen such that it produces every observable state of the super oscillator. Thus we may replace the pivotal relation (2.288) simply by

$$x(t) \;=\; \int_0^{t_1} \delta(t-t') \cdot \rho(t')\, dt' \;, \tag{2.297}$$

where the bilinear expansion

$$\delta(t-t') \;=\; \sum_{n=1}^{\infty} \varphi_n(t) \cdot \varphi_n(t') \tag{2.298}$$

is used for Dirac's delta function once the eigenfunctions $\varphi_n(t)$ are known. In that case, the source

$$\rho(t) \;=\; \sum_{n=1}^{\infty} \frac{v_n}{\omega_n} \cdot \varphi_n(t) \tag{2.299}$$

would be equivalent to the source (2.275) of the initial value problem since it produces the same state. In the case considered here this is only something like a tautological source since it results in an identical expansion of the state $x(t)$. In other words: In this situation (2.297)/(2.298) represents nothing but a mapping of a state $x(t)$ onto itself since we cannot distinguish between the acting source and the resulting state. Newton's cradle may be used to demonstrate this situation. In the steady state we cannot say which one of the outer balls is representing the considered object and the source. However, to demonstrate that the importance of (2.297)/(2.298) can go beyond such a simple tautological cause and event relation let us go back to the definition of Dirac's delta function by its sifting property

$$f(t) \;:=\; \int_0^{t_1} f(t') \cdot \delta(t'-t)\, dt' \;. \tag{2.300}$$

That is $\delta(t'-t)$ is acting as a sieve, selecting from all possible values of the function $f(t')$ its value at the point $t' = t$. On the other hand, if expanding a given function $f(t)$ into a Fourier series in terms of the orthonormal eigenfunctions $\varphi_n(t)$ we have

$$f(t) \;=\; \int_0^{t_1} \sum_{n=1}^{\infty} \varphi_n(t) \cdot \varphi_n(t') \cdot f(t')\, dt' \;. \tag{2.301}$$

A comparison of both expressions (2.300) and (2.301) provides the bilinear expansion (2.298) of Diracs delta function. However, the situation is different when it is only known that the function $f(t)$ is a result of the acting source

$$\rho(t) \;=\; \sum_{m=1}^{M} \rho_m \cdot \chi_m(t) \;. \tag{2.302}$$

Let us further assume that the expansion functions $\chi_m(t)$ may form another orthogonal basis in the temporal region $[0, t_1]$, and, moreover, that there are reasons (specific interactions which may result in specific boundary conditions, for example) to represent $f(t)$ by a Fourier series in terms of the eigenfunctions $\varphi_n(t)$. Well, I know that it is hard to imagine in case of the temporal boundary value problem considered here. But in some cases this is indeed possible, as we will see in Chap. 5. Then, from (2.297)/(2.298) we get

$$f(t) \;=\; \sum_{n,m} T_{nm} \cdot \rho_m \cdot \varphi_n(t) \;=\; \sum_{n} f_n \cdot \varphi_n(t) \;, \tag{2.303}$$

where the elements T_{nm} are given by

$$T_{nm} \;=\; \int_0^{t_1} \varphi_n(t) \cdot \chi_m(t)\, dt \;. \tag{2.304}$$

These are the elements of the so-called "T-matrix" $\mathbf{T}$ (the "transition matrix") we will encounter frequently in this book. Now it is more than a simple tautological mapping of the source onto the state.

To summarize: The bilinear expansion (2.298) (the completeness relation) of Dirac's delta function is a representation of all inner degrees of freedom of the object "simple harmonic super oscillator". This representation results from the eigenvalue problem

$$\hat{\mathbf{L}}\, \varphi_n(t) \;-\; \lambda_n \cdot \varphi_n(t) \;=\; 0 \tag{2.305}$$

related to the operator

$$\hat{\mathbf{L}} \;=\; \frac{d^2}{dt^2} \;. \tag{2.306}$$

In analogy to Quantum Mechanics we can therefore make the following statement: All possible/observable states of the object "simple harmonic super oscillator" are described by the Hermitian operator (2.306) in a space defined by $t \in [0, t_1]$ and the additional temporal boundary conditions at its boundaries. The eigenvalues and eigenfunctions in the considered situation are given by

$$\lambda_n \;=\; -\omega_n^2 \tag{2.307}$$

and

$$\varphi_n(t) \;=\; \sin\left(\omega_n\, t\right) \,. \tag{2.308}$$

Which states are excited with a certain amplitude in a certain experiment depends on the source, that is used in (2.297). The source itself is also described by a certain number of oscillator states. This is the justification for an understanding of (2.297) and (2.298) as a source picture of the Fourier series that establishes a causal relation between the given state of a source and the resulting state of the considered object. This point of view looks quite formal for the temporal boundary value problem of the simple harmonic oscillator. The equivalent initial value problem discussed at the beginning of this section appears more obvious. However, it was discussed already at this point to get a first impression of how to introduce a typical quantum mechanical point of view into classical physics. Let us conclude this section with a quick look at the damped harmonic oscillator.

Regarding the damped harmonic oscillator we have to take the complex-valued Fourier transform (2.247) of the self-energy operator additionally into account. This results in two effects—the lowering of the frequency and the damping of the state—as already discussed. Both effects can be observed in a real experiment. From (2.280), Green's function (2.99), and if applying the source (2.275) we get the series expansion

$$x(t) \;=\; e^{\,-\gamma\cdot t}\cdot\sum_{n=1}^{\infty}\frac{v_n}{\tilde{\omega}_n}\cdot\varphi_n(\tilde{\omega}_n,t) \,. \tag{2.309}$$

φ_n is again given by (2.277) but with ω_n replaced by $\tilde{\omega}_n$ according to

$$\tilde{\omega}_n^2 \;=\; \omega_n^2 \,-\, \gamma^2 \,. \tag{2.310}$$

This series expansion differs from (2.278) in the additional damping term that is independent of the eigenfrequency, and in the lower eigenfrequencies $\tilde{\omega}_n$. Please, note that $\tilde{\omega}_n$ was explicitly written as an argument of the eigenfunctions to indicate this latter difference. If the mass and the spring constants of the damped oscillators are those of the simple harmonic oscillators, then, instead of (2.271), each of the damped oscillators obeys the modified temporal boundary conditions

$$x(t=0) \;=\; x(t=t_1') \;=\; 0 \,, \tag{2.311}$$

where $t_1' > t_1$, and

$$t_1' \;=\; t_1\cdot\left(1 \,-\, \frac{\gamma^2\, t_1^2}{\pi^2}\right)^{-1/2} \,. \tag{2.312}$$

This enlargement of the period can be measured. But we have also the possibility to insist on the boundary conditions (2.271). Then, if the mass of the undamped system is used again, we have to replace the spring constants

$$k_n = m \cdot \left(\frac{n\pi}{t_1}\right)^2 \tag{2.313}$$

of the undamped system by

$$k'_n = m \cdot \left[\left(\frac{n\pi}{t_1}\right)^2 + \gamma^2\right] = k_n + m \cdot \gamma^2 \,. \tag{2.314}$$

The corresponding series (2.309) represents therefore a different object. That is, it is now impossible to maintain the position that the object (the simple harmonic super oscillator) remains the same but now exposed to the influence of its environment (the friction in our case), and that this influence may be studied by measuring the lowering of the eigenfrequencies and the damping of the amplitudes. And, in contrast to (2.287), it is also impossible to find a bilinear expansion of the Green's function with expansion coefficients $G_n(\omega_n)$ independent of t and t'. This is a consequence of the additional term

$$2\,\gamma \cdot \frac{\partial G(t,t')}{\partial t} \tag{2.315}$$

in the corresponding equation for the Green's function of the damped harmonic oscillator.

2.7 Two Simple Interaction Processes and Huygens' Principle

Two simple interaction mechanisms are within the focus of this section. It will be a first demonstration of how to incorporate these mechanisms into the Green's function formalism. In addition, it will be shown that these interactions may be replaced by equivalent but induced sources, according to our more general understanding of Huygens' principle mentioned in the Prologue. That they are local with respect to space and time is a characteristic property of the considered interactions. This will allow us to take up a typical position known from scattering theory. That is, information about the interaction may be obtained by comparing the "free states" of the considered object before and after the interaction.

2.7.1 Interaction with a Wall

First, let us consider the following very simple one-dimensional experimental situation: A point mass with mass m rests upon a horizontal plane. A primary source—an initial momentum according to (2.80)—is acting at time $t = t'$ on this point mass. As a result it starts moving forceless—let us say along the x-axis—with constant velocity v_1. There will be an interaction of the moving point mass with a wall at time $t = t_w > t'$. The wall is mounted perpendicularly to the x-axis. After this interaction, i.e., for times $t > t_w$, the point mass moves again forceless along the x-axis. The forceless motion with the constant velocity v_1 represents the "free state" of the point mass before the interaction. It can be compared with the primary incident acoustic or electromagnetic plane wave that is scattered on an obstacle. In scattering theory, this incident plane wave is usually assumed to be the given solution of the homogeneous wave equation, as we will see in Chap. 4. Regarding the forceless motion of the point mass we face the same situation. This state of motion is usually assumed to represent the solution of the homogeneous equation of motion $m \cdot \ddot{x} = 0$. However, a consistent Green's function approach requires necessarily a generating source for the plane wave as well as for the forceless motion. If not, there would be no plane wave or the point mass would freeze in place. Now, let us see how we can formulate this simple experiment by use of Green's functions. We decompose the Green's function $G(t, t')$ into the two parts

$$G(t, t') \;=\; G_0(t, t') \;+\; G_W(t, t_w) \cdot H(t - t_w) \;. \tag{2.316}$$

$G_0(t, t')$ is identical with (2.122), and, therefore, a solution of the inhomogeneous equation (2.131) before the interaction with the wall takes place. The interaction part $G_W(t, t_w)$, on the other hand, is assumed to be a solution of the homogeneous equation

$$\frac{\partial^2 G_W(t, t_w)}{\partial t^2} \;=\; 0 \;. \tag{2.317}$$

The Green's function after the interaction is thus the superposition of G_0 and G_W. Regarding the interaction part, we choose the general solution of the homogeneous equation

$$\frac{d^2 f(t)}{dt^2} \;=\; 0 \tag{2.318}$$

as an *ansatz*, i.e., we have

$$G_W(t, t_w) \;=\; A \;+\; B \cdot t \tag{2.319}$$

with so far unknown coefficients A and B. These coefficients are calculated from the two conditions

$$G(t_w - \epsilon, t') \;=\; G(t_w + \epsilon, t') \quad ;\; \epsilon \to 0 \tag{2.320}$$

and

$$c_p \cdot \left[\frac{\partial G(t,t')}{\partial t}\right]_{t=t_w-\epsilon} = \left[\frac{\partial G(t,t')}{\partial t}\right]_{t=t_w+\epsilon} \quad ;\; -1 \le c_p \le 1 \tag{2.321}$$

we impose additionally on the Green's function $G(t, t')$. These two conditions are representing the interaction of the point mass with the wall. Condition (2.320) indicates that there is no abrupt change in the position of the point mass. Parameter $c_p = -1$ in condition (2.321) characterizes an ideal elastic collision, whereas $-1 < c_p \le 0$ is characteristic for an inelastic collision. If $c_p = 1$ there will be no interaction—the point mass simply moves uniformly with its initial velocity v_1. And, finally, $0 < c_p < 1$ represents an interaction that results in a weakening of the initial momentum of the point mass but without a change in direction of its motion. Applying these condition we thus have

$$B \;=\; \frac{(c_p - 1)}{m} \tag{2.322}$$

$$A \;=\; -\frac{(c_p - 1)}{m} \cdot t_w \tag{2.323}$$

for the coefficients and

$$G_W(t, t_w) \;=\; \frac{(c_p - 1)}{m} \cdot (t \;-\; t_w) \tag{2.324}$$

for the interaction part of the Green's function. Inserting this expression into (2.316) provides finally for the total Green's function

$$G(t,t') \;=\; \frac{(t \;-\; t')}{m} \cdot H(t - t') \;+\; \frac{(c_p - 1)}{m} \cdot (t \;-\; t_w) \cdot H(t - t_w)\;. \tag{2.325}$$

By use of representation (2.16) it allows us to calculate the state $x(t)$ of the point mass at any time before or after the interaction. But we have to take into account that there is a restriction regarding the primary source. This source can only act up to the interaction time. The interaction part G_W of the Green's function could otherwise no longer considered to be a solution of the homogeneous equation. But this was a precondition in the above treatment. Now, let us consider two simple examples.

The impressed source (2.80) may act at time $t' = 0$ on a point mass that is at rest in $x = 0$. Its state of motion is then given by

$$x(t) \;=\; \int_0^{t^+} \frac{(t-t')}{m} \cdot \rho(t')\, dt' \;=\; v_1 \cdot t \tag{2.326}$$

for any observation time $t' < t < t_w$. If $t > t_w$ holds for the observation time, with Green's function (2.324) and if $c_p = -1$ is assumed (i.e., an interaction with an ideal elastic wall), we get on the other hand

$$x(t) \;=\; \int_0^{t^+} \frac{(t-t')}{m} \cdot \rho(t')\, dt' \;-\; 2 \cdot \int_0^{t^+} \frac{(t-t_w)}{m} \cdot \rho(t')\, dt' \;=\; v_1 \cdot (2\,t_w - t)\;. \tag{2.327}$$

Next, let us choose

$$\rho(t') \;=\; m \cdot a \cdot H(t_w - t') \tag{2.328}$$

as the primary impressed source that starts acting on the point mass at $t' = 0$ with a constant acceleration "a". If observation times $t < t_w$ are considered, we thus get

$$x(t) \;=\; \int_0^{t^+} \frac{(t-t')}{m} \cdot \rho(t')\, dt' \;=\; \frac{a}{2} \cdot t^2 \tag{2.329}$$

as the resulting state of motion. But for any observation times after the interaction with an ideal elastic wall

$$x(t) \;=\; \int_0^{t_w} \frac{(t-t')}{m} \cdot \rho(t')\, dt' \;-\; 2 \cdot \int_0^{t_w} \frac{(t-t_w)}{m} \cdot \rho(t')\, dt' \;=\; \frac{3a}{2}\,(t_w)^2 \;-\; a \cdot t_w \cdot t \tag{2.330}$$

is the corresponding state of motion. However, if the constant source (2.328) is acting on the point mass beyond t_w, for any observation time $t > t_w$ we have to use relation (2.16) with a source according to (2.81) but with initial momentum and initial position calculated from (2.329).

The question of energy conservation and its dependence on the parameter c_p can also be answered in a straightforward way. We have only to compare the kinetic energy before and after the interaction. If applied to the Green's function condition

$$\left[\frac{\partial G_0(t,t')}{\partial t}\right]^2 \;-\; \left[\frac{\partial G(t,t')}{\partial t}\right]^2 \;=\; 0 \tag{2.331}$$

must hold, with G_0 and G given by (2.122) and (2.325). As a result and in accordance with our experimental experience

$$c_p \;=\; \pm 1 \tag{2.332}$$

are the two cases (i.e., no interaction and the interaction with an ideal elastic wall) where we have energy conservation. Thus we may state that an energy-conserving interaction of a point mass with an ideal elastic wall is characterized by the two conditions (2.320) and (2.321) with the parameter $c_p = -1$.

This simple experiment allows us moreover to demonstrate the more general understanding of Huygens' principle discussed in the Prologue. According to this understanding we may replace the above considered interaction for any observation time $t > t_w$ by a corresponding induced source. That is, we can apply relation (2.16) with the Green's function $G(t, t')$ according to (2.122) and the—now induced!—source

$$\rho(t') \;=\; -m\, v_1 \cdot \delta(t' - t_w) \;+\; m\, v_1\, t_w \cdot \frac{d\delta(t' - t_w)}{dt'} \tag{2.333}$$

as the primary source, instead of the source (2.80). The second term on the right-hand side represents nothing but the initial position $x(t = t_w)$ at which the interaction with the wall takes place.

The interaction of the simple harmonic oscillator with a wall can be solved in exactly the same way as described above. But, now, G_0 according to (2.50) must be used in (2.316). The interaction part of the Green's function can again be calculated from the general solution (2.7) of the homogeneous equation of motion (2.5) and from the two conditions (2.320) and (2.321). Juggling with the addition theorems of the sine and cosine functions results finally in

$$\begin{aligned} G(t, t') \;&=\; \frac{1}{m\,\omega} \cdot \sin\omega(t - t') \cdot H(t - t') \\ &+ \frac{1}{m\,\omega} \cdot (c_p - 1) \cdot \cos\omega(t_w - t') \cdot \sin\omega(t - t_w) \cdot H(t - t_w)\;. \end{aligned} \tag{2.334}$$

$c_p = 1$ provides again the Green's function of the simple harmonic oscillator. That is, this represents the case of no interaction. From expression (2.334) we see moreover that switching on the interaction with the wall at a time t_w when the oscillator is in a turning point (this happens if $\cos\omega(t_w - t') = 0$!) has no impact on the state of motion. And, finally,

$$\left[\left(\frac{\partial G_0(t, t')}{\partial t}\right)^2 - \left(\frac{\partial G(t, t')}{\partial t}\right)^2\right] + \omega^2 \cdot \left(G_0^2(t, t') - G^2(t, t')\right) \;=\; 0 \tag{2.335}$$

is now the corresponding condition for energy conservation.

Exercise: Verify that (2.335) holds for the two parameters given by (2.332).

2.7.2 *Temporary Friction*

The second example is concerned with the following situation: The initial step is identical with the foregoing example. That is, a point mass of mass m rests on a horizontal plane at $x = 0$. The primary source (2.80) is again acting at time $t = t'$ on this point mass. As a result it starts moving with constant velocity v_1 along the x-axis as before. But, now, let us assume the existence of a temporary friction between $t = t_1^w$ and $t = t_2^w$. For times $t > t_2^w$ the point mass continues moving frictionless. The Green's function of the whole process is decomposed according to

$$G(t,t') \;=\; G_0(t,t') \;+\; G_W^{(R)}(t,t_1^w)\cdot H(t-t_1^w)\cdot H(t_2^w-t) \;+\; G_W(t,t_2^w)\cdot H(t-t_2^w)\;. \tag{2.336}$$

$G_0(t,t')$ therein represents again the part before the interaction (the friction). It is identical with (2.122). The interaction part $G_W^{(R)}(t,t_1^w)$ is constructed from the general solution of the homogeneous equation of motion

$$\frac{\partial^2 G_W^{(R)}(t,t_1^w)}{\partial t^2} \;+\; 2\,\gamma\cdot\frac{\partial G_W^{(R)}(t,t_1^w)}{\partial t} \;=\; 0 \tag{2.337}$$

in the presence of friction. This general solution reads

$$G_W^{(R)}(t,t_1^w) \;=\; A \;+\; B\cdot e^{-2\gamma t}\;. \tag{2.338}$$

The unknown coefficients A and B are determined by use of the additional conditions (2.320) and (2.321). Due to the smoothness requirement with respect to the momentum at $t = t_1^w$ these conditions must be applied with $c_p = 1$. A straightforward calculation provides

$$G_W^{(R)}(t,t_1^w) \;=\; G_0(t_1^w,t) \;+\; G_0^{(R)}(t,t_1^w)\;. \tag{2.339}$$

$G_0(t_1^w,t)$ and $G_0^{(R)}(t,t_1^w)$ are given by (2.122) and (2.127). We have to repeat this procedure at $t = t_2^w$ to cover the transition to the final frictionless motion. The general solution (2.319) of the homogeneous equation (2.317) is used as an *ansatz* for the part G_W of the Green's function in (2.336). The unknown coefficients are again calculated from the additional conditions (2.320) and (2.321) with $c_p = 1$. This gives

$$G_W(t,t_2^w) \;=\; G_0(t_1^w,t) \;+\; G_0^{(R)}(t_2^w,t_1^w) \;+\; e^{-2\gamma(t_2^w-t_1^w)}\cdot G_0(t,t_2^w)\;. \tag{2.340}$$

All parts of (2.336) are thus determined. Energy conservation (2.331) holds only if $\gamma = 0$ or if $t_1^w = t_2^w$, as one may expect. The above described procedure allows us

to couple several successive interaction processes. But let us now turn toward some more sophisticated interaction processes.

2.8 Particle Scattering on a Rigid Sphere and Kepler Problem

This section is concerned with the well-known scattering of a point mass on a rigid sphere but considered again through the glasses of a Green's function. It turns out that this Green's function is nothing but a slight modification of the Green's function of the simple harmonic oscillator. It is demonstrated moreover that the same Green's function in conjunction with an appropriate source can be used to solve the well-known Kepler problem.

2.8.1 Transformation of the Equation of Motion into Polar Coordinates

Starting from the conservation of the angular momentum polar coordinates are more appropriate for our purposes. That's because the plane of motion of both interaction processes is located perpendicularly to the angular momentum and thus restricted to a simpler 2-dim. situation. The relations between the unit vectors in Cartesian- and polar coordinates are summarized in Table 2.1. The same relations hold for the components of a given vector in one of these coordinate systems. But regarding the problems of our interest, in polar coordinates we face the additional difficulty of getting nonlinear equations of motion. This results from the fact that the unit vectors in polar coordinates are no longer constant with respect to time. Velocity and acceleration in polar coordinates are given by

$$\vec{v} = v_r \cdot \hat{r} + v_\phi \cdot \hat{\phi} = \dot{r} \cdot \hat{r} + r\dot{\phi} \cdot \hat{\phi} \tag{2.341}$$

and

$$\vec{a} = a_r \cdot \hat{r} + a_\phi \cdot \hat{\phi} = \left(\ddot{r} - r\dot{\phi}^2\right) \cdot \hat{r} + \left(r\ddot{\phi} + 2\dot{r}\dot{\phi}\right) \cdot \hat{\phi} \,. \tag{2.342}$$

Table 2.1 Relations between the unit vectors in Cartesian- and polar coordinates

	$\hat{x}$	$\hat{y}$
$\hat{r}$	$\cos\phi$	$\sin\phi$
$\hat{\phi}$	$-\sin\phi$	$\cos\phi$

The two equations of motion

$$\frac{d^2x(t)}{dt^2} = \frac{\rho_x(t)}{m} \tag{2.343}$$

$$\frac{d^2y(t)}{dt^2} = \frac{\rho_y(t)}{m} \tag{2.344}$$

in the x-y-plane of a Cartesian coordinate system are therefore transformed into the two equations

$$\ddot{r} - r\dot{\phi}^2 = \rho_r(t) \tag{2.345}$$

$$r\ddot{\phi} + 2\dot{r}\dot{\phi} = \frac{1}{r} \cdot \frac{d}{dt}\left(r^2\dot{\phi}\right) = \rho_\phi(t) \tag{2.346}$$

in polar coordinates, where

$$\rho_r(t) = \cos\phi \cdot \frac{\rho_x(t)}{m} + \sin\phi \cdot \frac{\rho_y(t)}{m} \tag{2.347}$$

$$\rho_\phi(t) = -\sin\phi \cdot \frac{\rho_x(t)}{m} + \cos\phi \cdot \frac{\rho_y(t)}{m} \,. \tag{2.348}$$

These are two coupled and nonlinear differential equations. It is therefore more convenient—and this is the usual way described in textbooks—to consider the inverse of the radius $u(\phi) = 1/r(\phi)$ as the state function , and the angle ϕ as the independent variable. It is moreover required that the source term $\rho_\phi(t)$ in equation (2.346) is identical zero. This corresponds to the initially assumed conservation of the angular momentum

$$|L| = m\,r^2\,\dot{\phi} = m \cdot h = const. \,. \tag{2.349}$$

A nonzero $\rho_\phi(t)$, on the other hand, would destroy the invariance of the Lagrangian with respect to rotation in space. Combining Eqs. (2.349) and (2.345) provides

$$\ddot{r} - \frac{h^2}{r^3} = \rho_r(t) \,. \tag{2.350}$$

Applying the chain rule

$$\dot{r} = \frac{dr(\phi)}{d\phi} \cdot \dot{\phi} \tag{2.351}$$

and taking once again $\dot{\phi}$ from Eq. (2.349) allows us to reformulate the two Eqs. (2.345) and (2.345) into

$$\dot{r} = \frac{h}{r^2} \cdot \frac{dr(\phi)}{d\phi} \tag{2.352}$$

$$\ddot{r} = \frac{h^2}{r^4} \cdot \frac{d^2 r(\phi)}{d\phi^2} - \frac{2\,h^2}{r^5} \cdot \left[\frac{dr(\phi)}{d\phi}\right]^2 . \tag{2.353}$$

Now, using $u(\phi) = 1/r(\phi)$ and the corresponding derivatives

$$\frac{dr(\phi)}{d\phi} = -\frac{1}{u^2} \cdot \frac{du(\phi)}{d\phi} \tag{2.354}$$

$$\frac{d^2 r(\phi)}{d\phi^2} = -\frac{1}{u^2} \cdot \frac{d^2 u(\phi)}{d\phi^2} + \frac{2}{u^3} \cdot \left[\frac{du(\phi)}{d\phi}\right]^2 , \tag{2.355}$$

Eq. (2.350) can finally be converted into

$$\frac{d^2 u(\phi)}{d\phi^2} + u(\phi) = -\frac{1}{u^2\,h^2} \cdot \rho_r(t) = \rho_u(\phi) . \tag{2.356}$$

In addition, from (2.352), (2.354), and (2.349) we get the relations

$$v_\phi = h \cdot u(\phi) \tag{2.357}$$

$$v_r = -h \cdot \frac{du(\phi)}{d\phi} . \tag{2.358}$$

for the components of the velocity in polar coordinates given by (2.341).

Equation (2.356) is still a nonlinear equation as one can see from the right-hand side. Let us therefore discuss some special sources which result in an elimination of this nonlinearity.

2.8.2 *Sources of the Scattering Problems*

The forceless, uniform motion of a point mass in distance b parallel to the x-axis of a Cartesian coordinate system is our first example (see Fig. 2.7). This state of motion represents the asymptotic free state before the interaction with the rigid sphere, according to our understanding of the considered scattering problem. We will therefore shift the corresponding primary impressed source with respect to time

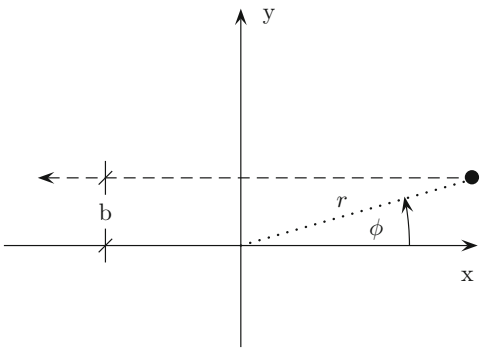

Fig. 2.7 Forceless motion of a point mass in distance b parallel to the x-axis if considered in polar coordinates

and position to infinity. That is, we use

$$\rho_x(t') = -m\, v_x \cdot \delta(t' + t'_\infty)\ ; \quad v_x > 0 \tag{2.359}$$

$$\rho_y(t') = 0 \tag{2.360}$$

as the primary impressed source in the Cartesian coordinate system (see also Sect. 2.1.5). This corresponds to an initial momentum $\vec{p} = -m \cdot v_x$ applied at time $t' = -t'_\infty = -\infty$ to the point mass that is at rest in $x = \infty$. By use of (2.360) and $x = \infty$ as the initial position $\phi' = 0$ holds for the initial angle in polar coordinates. ρ_ϕ in (2.348) thus becomes zero, i.e., the source (2.360) is in agreement with the required conservation of the angular momentum. Distance b denotes the so-called impact parameter. It can be related to the conservation of angular momentum. Taking (2.349), the initial momentum, and the conservation of the angular momentum into account provides the relations

$$h = b \cdot v_x \tag{2.361}$$

$$\dot{\phi} = u^2 \cdot h = const.\ . \tag{2.362}$$

Next we use the following relation that holds for Dirac's delta function:

$$\delta[\phi'(t')] = \frac{1}{\left[\frac{d\phi'(t')}{dt'}\right]_{t'=-t'_\infty}} \cdot \delta(t' + t'_\infty)\ . \tag{2.363}$$

The denominator is identical with (2.362). Equation (2.359) may therefore be replaced by

$$\rho_x(t') = -m\, v_x\, h\, u^2 \cdot \delta(\phi')\ . \tag{2.364}$$

Inserting this expression into (2.347) gives

$$\rho_r(t') \;=\; -\,v_x\,h\,u^2\cdot\delta(\phi')\;. \tag{2.365}$$

From (2.356) and (2.361) we thus get finally

$$\rho_u(\phi') \;=\; \frac{1}{b}\cdot\delta(\phi')\;. \tag{2.366}$$

This makes us very happy since the nonlinear term $1/u^2$ in (2.356) disappeared, and, due to a nonzero impact parameter b, the initial source is already endowed with an angular momentum. The source $\rho_u(\phi')$ which is equivalent to (2.366) but acting on the point mass that is initially at rest in a finite position x in distance b to the x-axis (this corresponds to the initial polar coordinates $\phi' = \phi_0$ and $r' = r_0$) is given without any comments. It reads

$$\rho_u(\phi') \;=\; \frac{\cos\phi_0}{b}\cdot\delta(\phi'-\phi_0) \;+\; \frac{\sin\phi_0}{b}\cdot\frac{d\delta(\phi'-\phi_0)}{d\phi'}\;. \tag{2.367}$$

We will see shortly that both initial sources result indeed in the same state of motion $u(\phi)$.

The Kepler problem and the corresponding asymptotic free states require the consideration of the forceless, uniform motion of a point mass as presented in Fig. 2.8. This straight line differs from the line shown in Fig. 2.7 in the angle ψ it forms with the x-axis. The corresponding primary source with an initial momentum—if again shifted to infinity—is then given by

$$\rho_u(\phi') \;=\; \frac{1}{b}\cdot\delta(\phi'-\psi)\;. \tag{2.368}$$

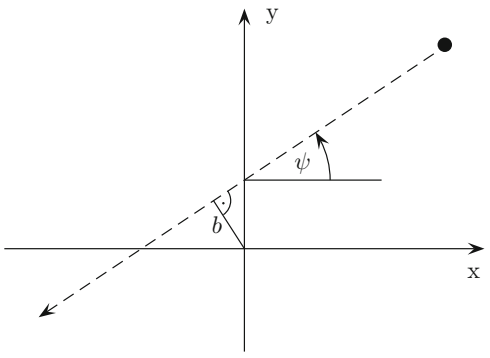

Fig. 2.8 Forceless motion of a point mass that must be considered to solve the Kepler problem

The relation (2.361) between h and the impact parameter b must accordingly be replaced by

$$h \;=\; b \cdot v_{r_\infty} \;=\; b \cdot v_x \cdot \cos\psi \tag{2.369}$$

that holds for large distances of the point mass from the scattering center. That is, $v_{r_\infty} = v_x \cdot \cos\psi$ expresses the radial projection of the velocity v_x in (2.361).

Another source results from the Newtonian potential. It results directly in a radially symmetric force that is proportional to $1/r^2$, and, thus, already proportional to u^2. $\rho_u(\phi')$ reads therefore

$$\rho_u(\phi') \;=\; \frac{K}{h^2}\,, \tag{2.370}$$

where

$$K \;=\; \gamma \cdot M\,. \tag{2.371}$$

M and γ therein denote the mass of the Sun (the central mass) and the gravitational constant. This source also avoids the nonlinear term in (2.356). Now we are prepared to solve the two scattering problems.

2.8.3 *Solving the Scattering Problems*

The equation of the Green's function related to (2.356) is given by

$$\frac{d^2G(\phi,\phi')}{d\phi^2} \;+\; G(\phi,\phi') \;=\; \delta(\phi-\phi')\,. \tag{2.372}$$

This equation is obviously identical with (2.21) of the simple harmonic oscillator if $m = k = 1$ is used, and if t, t' are replaced by ϕ, ϕ'. The solution of this latter equation is already known. It is given by (2.50). The corresponding solution of (2.372) reads therefore

$$G(\phi,\phi') \;=\; \sin(\phi-\phi') \cdot H(\phi-\phi')\,. \tag{2.373}$$

But we have to find out the conditions which will allow us to use relation

$$u(\phi) \;=\; \int_0^{\phi^+} G(\phi,\phi') \cdot \rho_u(\phi')\, d\phi' \tag{2.374}$$

together with Greens function (2.373) and the sources $\rho_u(\phi')$ considered above to calculate the state $u(\phi)$. To this end, let us go back to the situations depicted in

Figs. 2.7 and 2.8. Regarding Fig. 2.7 we get

$$u(\phi) \;=\; \frac{1}{r(\phi)} \;=\; \frac{\sin\phi}{b}\;, \tag{2.375}$$

and from Fig. 2.8 we get correspondingly

$$u(\phi) \;=\; \frac{1}{r(\phi)} \;=\; \frac{\sin(\phi-\psi)}{b}\;. \tag{2.376}$$

To find out whether the state $u(\phi)$ represents a uniform motion or an acceleration requires the knowledge of the temporal behaviour of the angle ϕ. Because of

$$x(t)\cdot\sin\phi(t) \;=\; b\cdot\cos\phi(t) \tag{2.377}$$

this is given by

$$\phi(t) \;=\; \operatorname{arccot}\left[\frac{x(t)}{b}\right] \tag{2.378}$$

for the motion of Fig. 2.7, for example. But independent of this aspect we have the following two characteristic features of these two motions in polar coordinates, and with ϕ as the independent variable:

- The independent variable ϕ is strictly monotonic increasing. Therefore, as already known from the relation between time and Causality, $\phi \geq \phi'$ holds with ϕ' and r' being the initial angle and radius related to the primary source. On the other hand, the point mass rests in a certain point of space if $\phi \leq \phi'$.
- If $\phi = 0$ and $\phi = \pi$, or if $\phi = \psi$ and $\phi = \pi + \psi$ (according to the motions depicted in Figs. 2.7 and 2.8) we have $u(\phi) = 0$. That is, in these asymptotic free cases before and after the interaction $r(\phi)$ becomes infinitely large. And, because of relation (2.357), the corresponding angular component of the velocity becomes zero but not its radial component.

Therefore and in agreement with the requirement for the Green's function of the harmonic oscillator with respect to time the smoothness condition

$$\lim_{\epsilon\to 0} G(\phi'+\epsilon,\phi') \;=\; 0 \tag{2.379}$$

with respect to ϕ is also required for the Green's function of (2.372). Due to the above mentioned features, and by use of Green's theorem (2.22) and the Reciprocity condition (2.23) (with t replaced by ϕ in these last two relations!) we are indeed able to derive the integral relation (2.374) with the Green's function (2.373). The derivation follows the same way described already for the simple harmonic oscillator. One may get a first confirmation of the correctness of this relation if the known solution (2.375) may be derived from the sources (2.366) and (2.367). That

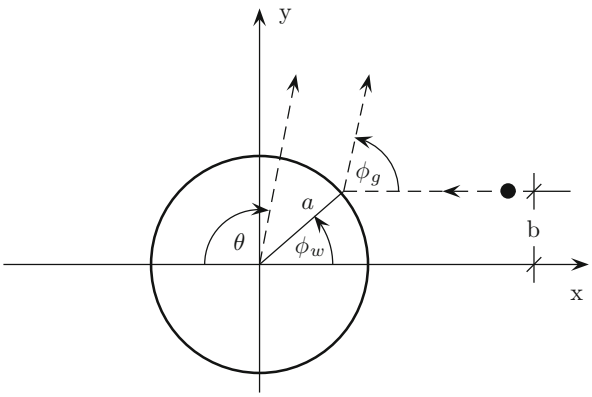

Fig. 2.9 Geometry of particle scattering on a rigid sphere

this really happens if (2.366) is used together with (2.373) in (2.374) is easy to see. On the other hand, using (2.367) results at first in

$$u(\phi) \;=\; \frac{1}{b}\cdot[\cos\phi_0\cdot\sin(\phi-\phi_0) \;+\; \sin\phi_0\cdot\cos(\phi-\phi_0)] \;. \tag{2.380}$$

Applying the addition theorems of $\sin(\phi - \phi_0)$ and $\cos(\phi - \phi_0)$ provides again (2.375). It is exactly the second term of (2.367) with its first derivative of Dirac's delta function that makes sure that despite of condition (2.379) $u(\phi') > 0$ for every finite initial angle ϕ' !

Exercise: Show that the solution (2.376) follows also from (2.373), (2.374), and the source (2.368).

Let us now turn toward the solution of the scattering problems of our actual interest. The geometry of the scattering problem of a point mass on a rigid sphere with radius $r = a$ is depicted in Fig. 2.9. The point mass hits the surface of the sphere at an angle of ϕ_w. Regarding the assumption of a rigid sphere we require the smoothness of the tangential component of the velocity in this surface point. Due to the spherical geometry the tangential vector agrees with the unit vector $\hat{\phi}$ in polar coordinates. Because of (2.357) and in analogy to (2.320) we thus have the additional condition

$$G(\phi_w-\epsilon,\phi') \;=\; G(\phi_w+\epsilon,\phi') \quad ;\, \epsilon\to 0\;. \tag{2.381}$$

The normal component of the velocity agrees with the radial unit vector $\hat{r}$ in case of a spherical scatterer. Due to the jump of this component it follows from (2.358) and in analogy to (2.321)

$$c_p\cdot\left[\frac{\partial G(\phi,\phi')}{\partial\phi}\right]_{\phi=\phi_w-\epsilon} = \left[\frac{\partial G(\phi,\phi')}{\partial\phi}\right]_{\phi=\phi_w+\epsilon} \quad ;\, -1\le c_p\le 1\;. \tag{2.382}$$

$c_p = -1$ must be used for the rigid sphere, and $c_p = 1$ corresponds to "no sphere" (i.e., to "no scattering"). The two features with respect to the angles we mentioned above in conjunction with the motions represented in Figs. 2.7 and 2.8 are still valid for the scattering problems at hand. Regarding the scattering problem on a rigid sphere, and in dependence on the impact parameter b, angle ϕ can take only values between 0 and π. A limiting angle of $\phi_g = \pi$ belongs to the asymptotic free state after the scattering process and is the result of an impact parameter $b \geq a$ (i.e., there is in fact no scattering). However, if $b < a$ we have $\phi_g < \pi$. This limiting angle is asymptotically achieved if r tends to infinity after the scattering. It can therefore be calculated from

$$u(\phi) \; = \; 0 \; . \tag{2.383}$$

The Green's function of this scattering process follows directly from (2.334) but with all time variables replaced by corresponding angles. This provides

$$G(\phi, \phi') \; = \; G_0(\phi, \phi') \; + \; G_W(\phi, \phi') \cdot H(\phi - \phi_w) \; , \tag{2.384}$$

where

$$G_W(\phi, \phi') \; = \; (c_p - 1) \cdot \cos(\phi_w - \phi') \cdot \sin(\phi - \phi_w) \; , \tag{2.385}$$

and with $G_0(\phi, \phi')$ according to (2.373). If $\phi > \phi_w$ holds, i.e., after the interaction with the sphere, we thus get from (2.374), by use of the source (2.366), and from (2.384)

$$u(\phi) \; = \; \frac{1}{b} \cdot \left[c_p \cdot \cos\phi_w \cdot \sin(\phi - \phi_w) \; + \; \sin\phi_w \cdot \cos(\phi - \phi_w) \right] \; . \tag{2.386}$$

In case of a rigid sphere with $c_p = -1$, $u(\phi) = 0$ if $\phi = 2\phi_w$. The limiting angle is accordingly given by

$$\phi_g \; = \; 2 \cdot \phi_w \; . \tag{2.387}$$

This corresponds with our experimental experience. The scattering angle θ can be introduced via the relation

$$\theta \; := \; \pi \; - \; \phi_g \; . \tag{2.388}$$

In case of the rigid sphere we thus get

$$\theta \; = \; \pi \; - \; 2 \cdot \phi_w \tag{2.389}$$

(see Fig. 2.9). At the interaction point on the surface of the sphere we have on the other hand

$$\sin\phi_w = \frac{b}{a} . \tag{2.390}$$

Then, from (2.389) and (2.390) we get the relation

$$b(\theta) = a \cdot \sin\left[\frac{(\pi - \theta)}{2}\right] = a \cdot \cos\frac{\theta}{2} \tag{2.391}$$

between the impact parameter b and the scattering angle θ. If the scattering angle is measured in a certain scattering experiment with a rigid sphere and a known impact parameter we are then able to deduce the radius of the sphere. Especially this last situation reflects the importance of scattering experiments—to gain information about the interaction process by looking at the asymptotic free state after the interaction. However, such an scattering experiment with only one point mass and one given impact parameter is not very effective. It is much more convenient to send a large number of point masses with different impact parameters toward the rigid sphere. Without going into details (we are mainly interested in describing well-known processes in terms of Green's functions) it should be mentioned that the so-called "differential scattering cross-section" is then an appropriate quantity to characterize such a statistical scattering experiment. It is defined according to

$$\frac{d\sigma}{d\Omega} := \frac{b(\theta)}{\sin\theta} \cdot \left|\frac{db(\theta)}{d\theta}\right| , \tag{2.392}$$

where $d\Omega = \sin\theta d\theta d\phi$ denotes the differential solid angle in spherical coordinates. The angle $\phi \in [0, 2\pi]$ therein represents the azimuthal angle in spherical coordinates and should not be confused with the angle ϕ of the considered polar coordinate system. Angle $\theta \in [0, \pi]$ in $d\Omega$ can on the other hand be identified with the scattering angle introduced before. From (2.391) it follows

$$\frac{d\sigma}{d\Omega} = \frac{a^2}{4} . \tag{2.393}$$

The integral

$$\sigma = \int \left(\frac{d\sigma}{d\Omega}\right) d\Omega \tag{2.394}$$

denotes the "total scattering cross-section". This quantity is also of some importance in scattering experiments. Scattering of point masses on a rigid sphere of radius $r = a$ thus provides

$$\sigma = \pi \cdot a^2 . \tag{2.395}$$

That is, the total scattering cross-section is independent of θ and identical with the corresponding circular cross-section. We will come back to these quantities at the end of Chap. 4. To conclude and before we will center our attention on the Kepler problem it may be useful to mention some situations which go beyond scattering on a rigid sphere.

The approach described above can be applied without major changes to the scattering problem of a point mass on an inelastic sphere. This scattering process is characterized by a coefficient $c_p > -1$. The limiting angle ϕ_g can be determined numerically from Eq. (2.386) and condition $u(\phi) = 0$. But we will not end up with relation (2.387). This may be considered as a hint that scattering on an inelastic sphere comes along with a deformation of the spherical boundary around the impact point. $b(\theta)$ and its dependence on the coefficient c_p can also be determined in the same way. This would allow us to deduce the coefficient c_p from a corresponding scattering experiment if the radius of the sphere is given. A major effort is required if particle scattering on a rigid but non-spherical object is considered. This applies to the spheroidal object presented in Fig. 2.10, for example. The characteristic behaviour of an monotoneously increasing angle ϕ for the ongoing motion of the point mass is still valid. This allows us to use (2.373) as the unperturbed Green's function even in this case. But the interaction part of the Green's function cannot be taken from (2.385). This part must be calculated again by use of the method described in Sect. 2.7. This becomes necessary since the conditions (2.381) and (2.382) are no longer valid. This is due to the fact that the unit vectors $\hat{r}$ and $\hat{\phi}$ in polar coordinates are no longer identical with the tangential and normal vector at a certain surface point of the nonspherical object. The tangential plane and the normal vector at a certain surface point are now the result of a combination of these unit vectors. Only afterwards the smoothness condition of the tangential component and the jump condition of the normal component can be applied . This can be done only numerically in most of the cases.

Exercise: Development of a numerical algorithm to study particle scattering on a rigid spheroidal body—wouldn't it be a nice project in numerical physics?

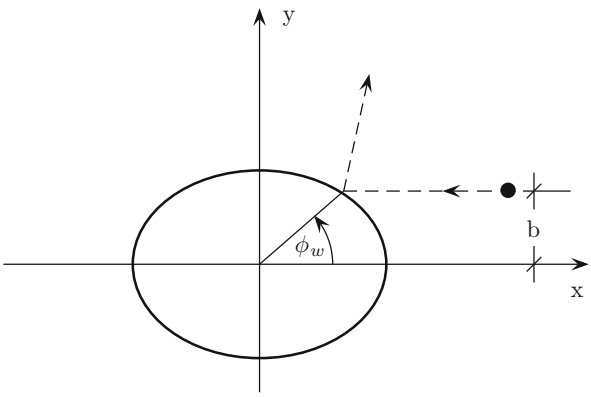

Fig. 2.10 Geometry of particle scattering on a spheroidal object located with its major axis on the x-axis

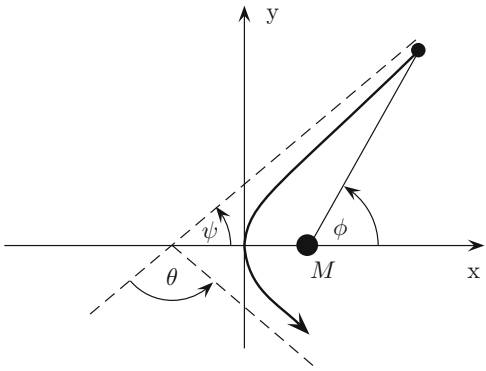

Fig. 2.11 Geometry of the motion of a point mass on a Kepler hyperbola in the gravitational field of a central mass M fixed at the focal point on the x-axis

Hint: The boundary surface of a spheroidal body is given by

$$r(\theta) \;=\; a \cdot \left[\cos^2\theta \;+\; \left(\frac{a}{b}\right)^2 \cdot \sin^2\theta \right]^{-1/2} \tag{2.396}$$

in spherical coordinates (see Chap. 4), where "a" denotes the semi-axis along the z-axis, and "b" denotes the semi-axis along the x-axis. The aspect ratio is given by

$$av \;=\; \frac{a}{b}\,. \tag{2.397}$$

$av \;<\; 1$ **and** $av \;>\; 1$ **are the aspect ratios of oblate and prolate spheroids, respectively.** $av \;=\; 1$ **provides the spherical body with radius** $r \;=\; a$**. Note that, in contrast to the spherical body the tangential plane at each surface point becomes a combination of the unit vectors** $\hat{\mathbf{r}}$ **and** $\hat{\boldsymbol{\theta}}$**. Calculate the tangential planes first and apply the law of reflection afterwards if the rigid spheroidal body is considered.**

The motion of a point mass on a Kepler hyperbola in the gravitational field of a mass M fixed at a focal point is depicted in Fig. 2.11. The primary source that causes the initial motion of the point mass at infinity may be given by the initial momentum (2.368), according to the situation depicted in Fig. 2.8. This source is required since the gravitational force alone is unable to induce a motion of a point mass that is initially located at an infinite distance from the central mass M. Without (2.368) the point mass would simply rest at infinity. The sum of both sources (2.368) and (2.370) are therefore needed to describe the motion of the point mass in the gravitational field. The state of motion $u(\phi)$ is then obtained from

$$u(\phi) \;=\; \int_{\psi}^{\phi} \sin(\phi \;-\; \phi') \cdot \left[\frac{\delta(\phi' - \psi)}{b} \;+\; \frac{K}{h^2} \right] d\phi'\,. \tag{2.398}$$

This gives

$$u(\phi) = \frac{K}{h^2} \cdot \left[1 + \frac{h^2}{K\,b} \cdot \sin(\phi - \psi) - \cos(\phi - \psi) \right] . \tag{2.399}$$

Now, let us transform this last expression into

$$u(\phi) = \frac{K}{h^2} \cdot [\,1 + \epsilon \cdot \cos(\phi - \Phi_0)] \ , \tag{2.400}$$

or rather

$$r(\phi) = \frac{h^2/K}{1 + \epsilon \cdot \cos(\phi - \Phi_0)} \ , \tag{2.401}$$

since these expressions are more appropriate to discuss the Kepler motion. Applying the addition theorems to (2.399) and (2.400) results in the following to equations to determine ϵ and Φ_0:

$$\epsilon \cdot \cos \Phi_0 = - \left(\cos \psi + \frac{h^2}{K\,b} \cdot \sin \psi \right) \tag{2.402}$$

$$\epsilon \cdot \sin \Phi_0 = \sin \psi - \frac{h^2}{K\,b} \cdot \cos \psi \ . \tag{2.403}$$

From Fig. 2.11 we can see moreover that the smallest distance between the moving point mass and the fixed mass M is achieved if $\phi = \pi$. Since the smallest value of $r(\phi)$ results on the other hand from (2.401) and $\phi = \Phi_0$ we choose $\Phi_0 = \pi$. Inserting this value into (2.402) and (2.403) gives

$$\epsilon = \cos \psi + \frac{h^2}{K\,b} \cdot \sin \psi \tag{2.404}$$

$$0 = \sin \psi - \frac{h^2}{K\,b} \cdot \cos \psi \ , \tag{2.405}$$

to determine ϵ. To this end we have to take the square of both equations and have to add the results subsequently. Then

$$\epsilon^2 = 1 + \left(\frac{h^2}{K\,b} \right)^2 \ , \tag{2.406}$$

or

$$\epsilon = \pm \left[1 + \left(\frac{h^2}{K\,b} \right)^2 \right]^{1/2} \ . \tag{2.407}$$

Instead of (2.401) we may therefore write

$$r(\phi) \;=\; \frac{h^2/K}{1 \,-\, \epsilon \cdot \cos\phi} \;, \tag{2.408}$$

with ϵ given by (2.407) but with the positive sign according to Fig. 2.11. This is the well-known expression in polar coordinates that is used in many textbooks to discuss the Kepler motion. The different cases—motion on a hyperbola, on a parabola, and the elliptical orbit around M—are then the result of $\epsilon > 1$, $\epsilon = 1$, and $\epsilon < 1$, or of the related energies $E > 0$, $E = 0$, and $E < 0$, respectively. In what follows we will therefore derive the relation between ϵ and the energy as well as the dependence of the impact parameter on the scattering angle θ for the motion on a hyperbola.

The initial momentum acting on the point mass with mass m that rests in an infinite distance from mass M transfers the initial energy

$$E_i \;=\; \frac{m}{2} \cdot v_{r_\infty}^2 \tag{2.409}$$

to this point mass. Or, if taking (2.369) into account, we may also write

$$E_i \;=\; \frac{m\,h^2}{2\,b^2} \;. \tag{2.410}$$

The gravitational potential of Mass M does not contribute to this energy at the beginning, due to the infinite distance. But in the further course of motion and as a consequence of (2.341) and the energy conservation we get

$$\frac{m}{2} \cdot v_{r_\infty}^2 \;=\; \frac{m}{2} \cdot \left(\dot{r}^2 \,+\, r^2\,\dot{\phi}^2\right) \,-\, \frac{m\,K}{r} \;. \tag{2.411}$$

Inserting (2.410) into (2.406) results in

$$\epsilon^2 \;=\; 1 \,+\, \frac{2\,h^2}{m\,K^2} \cdot E_i \;. \tag{2.412}$$

This combines the parameter ϵ with the initial energy. Thus it becomes clear that such an initial momentum and in the absence of any loss in the further course of motion (by friction or by active deceleration, for example) an elliptical orbit of the point mass around M is impossible. The point mass escapes asymptotically to infinity, as shown in Fig. 2.11. The final asymptotic motion is again characterized by $u(\phi) = 0$ or $r(\phi) = \infty$. From (2.408) we thus get the following relation between the two angles $\pm\psi$ the initial and final asymptote form with the x-axis, and for the parameter ϵ:

$$\cos(\pm\psi) \;=\; \frac{1}{\epsilon} \;. \tag{2.413}$$

The scattering angle θ reads on the other hand

$$\theta \;=\; \pi \;-\; 2\,\psi \;. \tag{2.414}$$

Equation (2.413) can therefore be rewritten into

$$\sin\frac{\theta}{2} \;=\; \frac{1}{\epsilon}\;. \tag{2.415}$$

Using relations

$$\tan\alpha \;=\; \frac{\sin\alpha}{(1-\sin^2\alpha)^{1/2}}\;, \tag{2.416}$$

(2.369), and (2.412) allows us again to relate the scattering angle to the impact parameter b, as already done in conjunction with particle scattering on a rigid sphere. We obtain

$$b(\theta) \;=\; \frac{K\,m}{2\,E_i}\cdot\frac{1}{\tan\frac{\theta}{2}}\;. \tag{2.417}$$

And, finally, the differential scattering cross-section (2.392) for the gravitational potential (as well as for the Coulomb-potential if K is taken adequately) gives

$$\frac{d\sigma}{d\Omega} \;=\; \left(\frac{K\,m}{4\,E_i\,\sin^2\frac{\theta}{2}}\right)^2\;. \tag{2.418}$$

This is the well-known Rutherford scattering cross-section. But due to the θ-dependent denominator in (2.418) the corresponding total cross-section (2.394) is now becoming divergent if θ tends to zero. This raises the question about the experimental importance of the total cross-section for such potentials with an infinite range. The scattering of a point mass into the forward direction $\theta = 0$ would require an infinitely large initial energy or an impact parameter b that is infinitely far away from the central mass M.

The above described treatment of the Kepler problem by use of a Green's function allows me to be more specific about an aspect discussed in the Prologue from a more general point of view. It is concerned with the importance of the source/cause within the idea of Green's functions and the resulting possibility to relate different levels of our experimental or theoretical experience. Within the framework of Classical Mechanics only states of motions are considered the sources/causes of which are not explained by the theory itself. These impressed sources/causes are only justified by our experimental experience. This experience can be gathered, for example, by testing the correctness of relation (2.418) and the used model for the gravitational potential as the impressed source. We have

to think about this source seriously if a discrepancy between the observations and the model is detected. It is exactly the situation that comes across with Mercury's precession that cannot be described by Newtonian's gravitational potential alone. A more precise description is provided within the framework of General Relativity. Using the Schwarzschild metric, for example, it can be shown that we get a much better quantitative agreement with the observations if the term

$$V(r) = \frac{K\,|L|^2}{r^3} \tag{2.419}$$

is added to Newtonian's gravitational potential (for details see Carroll (2003), for example). That is, the Schwarzschild metric can be considered as a theory of the source of Mercury's motion. However, in General Relativity the mass M of the central body, or more general, the stress-energy tensor is now considered as an impressed source that is justified only by our experience. It cannot be derived by the theory itself. By the way, regarding the scattering of a point mass on a rigid sphere we face a similar situation. The interaction with the surface of the sphere—expressed in terms of the special boundary conditions (2.381) and (2.382)—are also justified by our experimental experience only.

Regarding Newtonian's physics there is another aspect frequently discussed in the literature. It is concerned with the point of view that it implies instantaneous action at a distance. That is, according to this point of view a planet would respond without delay to an abrupt displacement of the sun. But I am sceptic about this interpretation of Newtonian's mechanics. I am rather convinced that we should not make such a statement within this theory since it is concerned with the nature of the source (2.370) (the sun in our example), and, therefore, outside this theory. According to my understanding Newtonian's mechanics tacitly assumes the existence of this source (this is what we called an impressed source in the Prologue), justified by the experience, that this source together with the underlying equation of motions can be brought within a certain accuracy into correspondence with our observations. It is not quite clear to me how to solve the above mentioned problem of an abrupt displacement of the sun and the resulting effect on a planet within Newtonian mechanics. To my mind only General Relativity provides an approach to this problem. The situation seems to me comparable to what is known from steady state theories of classical fields, like plane wave scattering, for example. The question of how to accomplish such a steady state situation cannot be answered within a steady state theory itself. It is used only as an appropriate *ansatz* to separate the time dependence. Its success is again justified only by the agreement with corresponding experiments.

Chapter 3
Green's Functions of Classical Fields

Metaphysics is the desperate attempt of the physicist to escape Faraday's cage of rationality

Solving boundary value problems of electromagnetic fields was the historical starting point for the development of the Green's function formalism. The person after whom these functions were named—George Green—published an essay in 1828 in which he introduced special functions to solve certain boundary value problems of the Poisson equation (Green 1850, 1852, and 1854). Unfortunately, this essay sank into oblivion shortly after its publication until it was rediscovered in 1846 by the later Lord Kelvin. In a paper, published in 1993, F. Dyson considered the invention of these functions as a methodical revolution in physics which was as important as the invention of computers in our days (Dyson 1993).

Today there exist a vast amount of literature concerned with classical fields and the corresponding mathematical tools and solution methods. I want to mention only the two volumes "Methods of Theoretical Physics" by P.M. Morse and H. Feshbach (Morse and Feshbach 1953) and the book "Partial Differential Equations in Physics" by A. Sommerfeld (Sommerfeld 1949) since these books were constant companions during my scientific activities. Because of the wealth of material the considerations in the following two chapters are restricted to a selected number of field equations and the corresponding Green's functions. However, the discussed solution methods are quite general and applicable also to other problems. Regarding the scattering problems considered in the next chapter we place a particular focus on the S- and T-matrix as the decisive elements of the corresponding Green's functions. But let us start this chapter with a few comments on the field concept in physics which are related to the points of view formulated in the Prologue.

3.1 Comments on the Field Concept

It is not even a simple task to find a satisfactory definition of the term **field** in physics. Looking back on my time at the university, the fields of physical interest have been essentially defined as a **characteristic state of space or part of the space that will affect a physical object in this space** (apply a force to it, etc.). Other

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definitions coincide more or less with this definition. A quite instructive historical overview of the field concept in physics can be found in (McMullin 2002), for example. Accepting this definition as a first guess, and from the discussion of the categories **object** and **state** in the Prologue we are thus running into the strange situation that not the **field** but the **space** represents the corresponding object with the **field** being its **state**—as well as we have considered the state of motion $x(t)$ as the characteristic state of the object **point mass** in the foregoing chapter. That in General Relativity the **space** itself has become the object of investigation is an argument in favour of this point of view. And also the notation **Green's function of the free space** (this is the Green's function of the equation under consideration but with no additional boundary conditions involved) we will frequently encounter in this chapter seems to support this idea at least linguistically. On the other hand, our entire sensory perception, and, therefore, our entire physical experience is related to space and time. That is, space and time establish the framework of our physical experience, as expressed by the term **laboratory system** and the related measure and boundary conditions. Such a laboratory system can often be represented by a three-dimensional Cartesian coordinate system and a clock and must not be confused with the space of the General Relativity that results from a given stress-energy tensor. Throughout this book, **space** will therefore be understood as an appropriate laboratory system that fits the problem we intend to solve. By the way, also Quantum Mechanics is such a "laboratory system-related" theory.

Starting from a given laboratory system the field can be considered as a nonlocal object within this laboratory system that is characterized by a state that depends on position and time, in general. Especially since the work of Faraday, Maxwell, and Einstein the **field** has become a substantial part of our physical reality and is considered as an object of its own. Since that time field theories form an essential part of modern physics. And also our everyday life is infused with fields—especially with electromagnetic fields. But despite their ubiquity it is quite difficult to get a clear idea of electromagnetic fields. In the second volume of the "Feynman Lectures on Physics" Feynman wrote: *I see some kind of vague shadowy, wiggling lines—here and there is an "E" and "B" written on them somehow, and perhaps some of the lines have arrows on them—an arrow here or there which disappears when I look to closely at it* (Feynman et al. 1989). However, it is in fact not the electromagnetic field we perceive with our senses or measure with our instruments but their effect, even if the underlying theory is a theory of the fields. A consequence of this is the necessity to link the field to the quantities we really measure in an experiment. Regarding the scattering problems considered in the next chapter the differential or total scattering cross-sections are such observable quantities, for example. They are related to the square of the state of the field in the far field. The same holds for the probabilities in Quantum Mechanics calculated from the square of the probability state vector. That this concept is also applicable to specific probability experiments with classical objects is demonstrated in the Chap. 5. In contrast to this, the state of motion $x(t)$ of a point mass in the foregoing chapter was a directly observable quantity.

However, it is our main goal also in this chapter to relate the state $\psi(\mathbf{x}, t)$ of a certain field at position $\mathbf{x}$ and time t of a laboratory system to its generating source $\rho(\mathbf{x}', t')$ via the integral expression

$$\psi(\mathbf{x}, t) = \int_0^{t^+} \int_{\Gamma'} G(\mathbf{x}, t; \mathbf{x}', t') \cdot \rho(\mathbf{x}', t') \, d\Gamma' \, dt' \, . \tag{3.1}$$

Γ' represents the volume within volume Γ of the laboratory system that is occupied by the source. With this relation we take up again the position that without any source there will be no state of a field. Since the considered laboratory system is also defined by its enclosing boundaries special conditions on these boundaries must be taken into account to end up with (3.1). It is important to note that these conditions are justified only by our experimental experience. They are not a priori given. Moreover and as already done in the foregoing chapter, the a priori existence of any initial state $\psi(\mathbf{x}, 0)$ and/or initial "velocity" $[\partial \psi(\mathbf{x}, t)/\partial t]_{t=0}$ of the state is excluded from the very beginning. These initial conditions will again be related to corresponding sources. But it will be demonstrated by several examples that inhomogeneous boundary conditions can also be related to corresponding sources. And, finally, beside the principle of contiguous action we have to take again Causality and Reciprocity as basic principles of our physical experience appropriately into account.

3.2 The Elastic String

Although the elastic string represents a quite simple physical object it allows us in a straightforward way to discuss and demonstrate some of the methodical and conceptual aspects regarding Green's functions of classical fields. It is moreover an example of a state—the displacement from its rest position—that can directly be observed, i.e., that avoids transferring this state into an observable quantity by an additional procedure. It is moreover demonstrated in this section that for the 1-dim. situation the "classical method" of deriving the Green's function, as it was described in Sect. 2.5.1 of the foregoing chapter, can also be applied with benefit to the Poisson equation, the wave equation, the Klein-Gordon equation, the equation of telegraphy, and, as a limiting case of the latter, the diffusion equation. For problems which do not depend on time (static problems or steady state problems with a separable time dependence) we choose an *ansatz* that is in correspondence with the principle of Reciprocity, i.e., with the experience that one can interchange source- and observation points without changing the final observation. A similar approach was used in the foregoing chapter, where the principle of Causality was taken into account by the Heaviside function $H(t - t')$ in *ansatz* (2.166). The principle of contiguous action is considered by an appropriate *ansatz* for all the time-dependent problems. It guarantees that only the physically meaningful time-like solutions are

taken into account. For the reader who may be interested in more complex problems of strings and membranes I want to call the attention to the book "Wave Motion in Elastic Solids" by K.F. Graff (1991). But let us now start with the problem of an ideal elastic string under the influence of a static force (the problem of the clothes line).

3.2.1 One-Dimensional Poisson Equation

We are interested in the solution of the equation

$$\frac{d^2\psi(x)}{dx^2} = \rho(x) \tag{3.2}$$

with $\rho(x)$ representing again the source function which is now a function of position. The corresponding equation of the Green's function reads

$$\frac{d^2G(x,x')}{dx^2} = \delta(x-x') \; . \tag{3.3}$$

It is an essential experience that it has no effect on our final observation if the source- and observation points are interchanged. That is, the observation (the measurable quantity) depends only on the spatial distance between source- and observation point. This symmetry is again called Reciprocity, but now with respect to position (and not with respect to time, as considered in the foregoing chapter). Applying this experience to the Green's function we require the fulfillment of the Reciprocity condition

$$G(x,x') = G(x',x) \; . \tag{3.4}$$

This condition is obviously fulfilled if

$$G(x,x') = F(|x-x'|) = F(u) \tag{3.5}$$

is used as an *ansatz* with the so far unknown function F. At this point I want to add the following remark: The fact that the considered field equation and the related boundary conditions allow the mathematical proof of relation (3.4) is in the physical literature often discussed as the proof of Reciprocity. But this will put the cart before the horse, according to my understanding formulated in the Prologue. This is because such a symmetry is primarily owed to our experimental experience within a certain object space. Expressing this experience by an appropriate mathematical condition is "only" a subsequent step. A different experience would us possibly lead to a different equation and different boundary conditions which do not result in (3.4). Or, in other words, an experience can never be proven. We can only accept it. I will come back to this aspect in the chapter when discussing the Unitarity of the S-matrix of scattering processes and its relation to energy conservation.

But, now, let us ask for the function F of the Poisson equation. To this end we insert *ansatz* (3.5) into Eq. (3.3), where we have to take the derivative (2.54) of the absolute value u into account. We thus get

$$\frac{dF(u)}{dx} \;=\; F_x \;=\; F_u \cdot u_x \;=\; F_u \cdot \big[H(x-x') \;-\; H(x'-x)\big] \tag{3.6}$$

and

$$\begin{aligned} F_{xx} \;&=\; F_{uu} \cdot u_x^2 \;+\; 2 \cdot F_u \cdot \delta(x-x') \;= \\ &F_{uu} \;+\; 2 \cdot F_u \cdot \delta(x-x') \;=\; \delta(x-x') \;. \end{aligned} \tag{3.7}$$

Please, note the abbreviation used for the derivatives. This will save some paperwork and will be applied frequently in what follows! Next, we require that the function F must be a solution of the homogeneous equation

$$F_{uu} \;=\; 0 \;. \tag{3.8}$$

This gives the general solution

$$F(u) \;=\; C_1 \cdot u \;+\; C_2 \;. \tag{3.9}$$

From the integration of the remaining part of (3.7) with respect to x from $-\infty$ to ∞ we obtain the additional condition

$$[F_u]_{u=0} \;=\; \frac{1}{2} \;. \tag{3.10}$$

We thus get the Green's function

$$G(x,x') \;=\; F(u) \;=\; \frac{1}{2} \cdot u \;+\; C_2 \;=\; \frac{1}{2} \cdot |x-x'| \;+\; C_2 \;. \tag{3.11}$$

Regarding the discontinuity of its first derivative at the source point x' we have again

$$\left[\frac{dG(x,x')}{dx}\right]_{x=x'-\epsilon}^{x=x'+\epsilon} \;=\; 1 \tag{3.12}$$

(see also (2.52) if $m \;=\; 1$!). As known from potential theory, potentials are determined except for an arbitrary constant. Let us therefore choose $C_2 \;=\; 0$ and consider

$$G(x,x') \;=\; F(u) \;=\; \frac{1}{2} \cdot u \;=\; \frac{1}{2} \cdot |x-x'| \tag{3.13}$$

as the free-space Green's function of the 1-dim. Poisson equation.

To solve the problem of the ideal elastic string fixed at two points (let us say at $x = 0$ and $x = L$) we have to take the homogeneous Dirichlet conditions

$$\psi(x = 0) \;=\; \psi(x = L) \;=\; 0 \tag{3.14}$$

additionally into account. $0 \leq x \leq L$ is therefore the spatial region of our interest. $\rho(x)$ represents the force applied to this string. For the corresponding Green's function we require also the fulfillment of these two boundary conditions,

$$G(x = 0, x') \;=\; G(x = L, x') \;=\; 0\,. \tag{3.15}$$

We add the general solution of the homogeneous equation to (3.13), as already done in Sect. 2.7 of the last chapter,

$$G(x, x') \;=\; \frac{1}{2} \cdot |x - x'| \;+\; \tilde{C}_1 \cdot x \;+\; \tilde{C}_2\,. \tag{3.16}$$

This is nothing but an application of the well-known fact that the general solution of the inhomogeneous equation can be represented by the sum of the general solution of the homogeneous equation and a special solution of the inhomogeneous equation. Constants $\tilde{C}_1$ and $\tilde{C}_2$ are determined afterwards by application of conditions (3.15). Thus we get finally

$$G(x, x') \;=\; \frac{1}{2} \cdot |x - x'| \;-\; \frac{1}{2} \cdot (x + x') \;+\; \frac{x \cdot x'}{L}\,. \tag{3.17}$$

It is obvious that conditions (3.4) and (3.12) are fulfilled. Moreover and in accordance with our experience, it can be seen that the string has its strongest displacement in x' (see Fig. 3.1). Thus we have found the Green's function that represents the object "ideal elastic string fixed at the two points $x = 0$ and $x = L$". It is yet to be determined how we can find the solution of Eq. (3.2) by use of (3.17) and for a given source $\rho(x)$. But to demonstrate that the Reciprocity relation (3.4) follows from the homogeneous Dirichlet problem of the Poisson equation is also

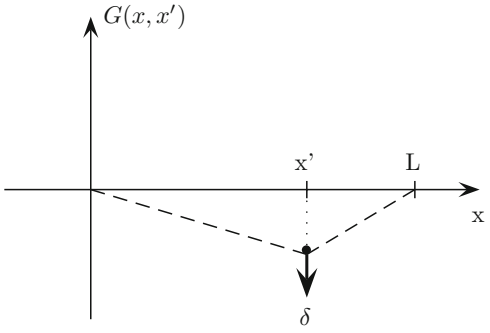

Fig. 3.1 Green's function of an ideal elastic string that is fixed at the two points $x = 0$ and $x = L$. An elementary force is applied in x' (the problem of an elementary sock on the clothes line)

of our interest. As the attentive reader may possibly be surmise—these questions are answered by use of Green's theorem in close analogy to the way described in Sect. 2.1.2.

$\Psi(x)$ and $\Phi(x)$ are any two functions defined in the spatial region of our interest. Green's theorem is then given by

$$\int_0^L \left[\Psi(x) \cdot \frac{d^2\Phi(x)}{dx^2} - \Phi(x) \cdot \frac{d^2\Psi(x)}{dx^2} \right] dx = \int_0^L \frac{d}{dx} \left[\Psi(x) \cdot \frac{d\Phi(x)}{dx} - \Phi(x) \cdot \frac{d\Psi(x)}{dx} \right] dx = \left[\Psi(x) \cdot \frac{d\Phi(x)}{dx} - \Phi(x) \cdot \frac{d\Psi(x)}{dx} \right]_0^L . \tag{3.18}$$

In contrast to (2.22) the integration must now be performed over the entire spatial region $x \in [0, L]$. Replacing $\Phi(x)$ by the Green's function $G(x, x')$ and $\Psi(x)$ by $\psi(x)$, applying the homogeneous Dirichlet conditions (3.14) and (3.15), and if taking Reciprocity relation (3.4) into account results in the integral relation

$$\psi(x) = \int_0^L G(x, x') \cdot \rho(x')\, dx' \tag{3.19}$$

we are looking for.

Exercise: Show that the Reciprocity relation (3.4) can be derived in exactly the same way by replacing $\boldsymbol{\Psi}(\mathbf{x})$ by $\mathbf{G}(\mathbf{x}, \mathbf{x}')$ and $\boldsymbol{\Phi}(\mathbf{x})$ by $\mathbf{G}(\mathbf{x}, \mathbf{x}'')$, and if take again the homogeneous Dirichlet conditions for both these Green's functions into account.

Let us now consider the simple example of a constant force acting at a certain point x_q. This source is given by

$$\rho(x) = C \cdot \delta(x - x_q) . \tag{3.20}$$

From (3.19) we thus get with (3.17)

$$\psi(x) = \frac{C}{2} \cdot |x - x_q| - \frac{C}{2} \cdot (x + x_q) + C \cdot \frac{x \cdot x_q}{L} \tag{3.21}$$

for the displacement of the string under the influence of (3.20). It agrees with the situation represented in Fig. 3.1. This is a nice example to demonstrate the experience of Reciprocity. For this purpose we want to answer the following question: The dashed line in Fig. 3.2 represents the solution (3.21), i.e., the solution, if the force is acting in x_q. Can we use this knowledge to construct the solution if the same force is acting in the observation point x_M? Based on the experience of Reciprocity the answer is a clear "yes"'! First, we have to measure the displacement a in x_M if the force is acting in x_q. Reciprocity expresses our experimental experience

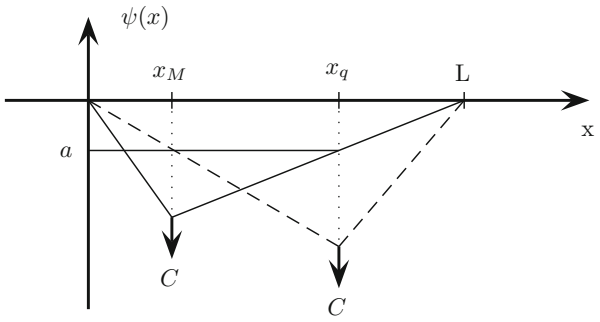

Fig. 3.2 Demonstration of Reciprocity for the clothes line problem under the influence of force (3.20). The *dashed and full line* represent the displacement if this source is acting in x_q and x_M, respectively

that the same displacement is observed in x_q if the same source is acting in x_M. This will allow us to construct the full line of Fig. 3.2. The experience of Reciprocity—beside those simple applications—can be applied with benefit to estimate the accuracy of numerical solutions of certain boundary value problems. This has been demonstrated in (Rother and Kahnert 2013), for example, where it was applied to plane wave scattering on nonspherical objects. We will come back to this special aspect at the end of Chap. 4.

The next example is concerned with the clothes line problem under the influence of a constant gravitational force given by

$$\rho(x) \;=\; \frac{\rho_c}{T} \cdot g \;=\; C_g \;. \tag{3.22}$$

ρ_c is a material parameter that represents the mass of the string per unit of length, T is the tension of the string under the influence of an external force, and g is the gravity acceleration. Using again (3.19) and (3.17) results in

$$\psi(x) \;=\; \frac{C_g}{2} \cdot x \cdot (x \,-\, L) \;. \tag{3.23}$$

We have now a parabolic displacement which is deepest at $x \;=\; L/2$. As these examples show, Green's functions can also be applied with benefit to run the household.

Only homogeneous Dirichlet conditions have been considered so far. But what happens with homogeneous von Neumann conditions, i.e., if the first derivative of the displacement $\psi(x)$ at $x \;=\; 0$ and $x \;=\; L$ is required to become zero? One may expect that solving this problem should be also possible since the last term of (3.18) becomes identical zero. Thus we would again end up with relation (3.19). However, it can be seen from *ansatz* (3.16) that it does not work! This is because constant $\tilde{C}_2$ will always vanish for the first derivative. Thus we have only constant $\tilde{C}_1$ that can be matched to one condition at a certain point. Regarding the Poisson equation von Neumann conditions are therefore not of our interest. But it is of our interest to see what is going on if we have to consider an inhomogeneous Dirichlet condition for

the displacement, i.e., if

$$\begin{aligned} \psi(x=0) &= 0 \\ \psi(x=L) &= C_L \;=\; konst. \end{aligned} \tag{3.24}$$

must hold while the homogeneous Dirichlet conditions (3.15) still apply to the Green's function. From Green's theorem (3.18) it follows that the solution of (3.2) is given by

$$\psi(x) \;=\; \psi_1(x) \;+\; \psi_2(x) \;=\; \int_0^L G(x,x')\cdot\rho(x')\,dx' \;+ \\ C_L\cdot\left[\frac{\partial G(x,x')}{\partial x'}\right]_{x'=L}. \tag{3.25}$$

The second term on the right-hand side contains the derivative of the Green's function (3.17) with respect to the source point and provides the additional contribution

$$\psi_2(x) \;=\; \frac{C_L}{L}\cdot x\,. \tag{3.26}$$

But the second term on the right-hand side of expression (3.25) can be replaced by relation (3.19) if introducing the source

$$\rho_L(x') \;=\; -\,C_L\cdot\frac{d\delta(x'-L)}{dx'} \tag{3.27}$$

acting in $x'=L$, and if replacing $\psi(x=L)=C_L$ by $\psi(x=L)=0$. This gives

$$\psi_2(x) \;=\; \int_0^L G(x,x')\cdot\rho_L(x')\,dx'\,. \tag{3.28}$$

Here we have a further example of how to replace an inhomogeneous condition by an appropriate source, as already discussed in the context of an initial position and initial momentum of the simple harmonic oscillator. Let us now turn our attention to time dependent problems of other 1-dim. equations which can be used to describe wave phenomena of the taut elastic string.

3.2.2 *One-Dimensional Wave-, Klein-Gordon-, Telegraphy-, and Diffusion Equation*

We start with the 1-dim. wave equation

$$\frac{1}{c^2}\cdot G_{tt}(x,t;x',t') \;-\; G_{xx}(x,t;x',t') \;=\; \delta(x-x')\cdot\delta(t-t') \tag{3.29}$$

for the Green's function. This equation is invariant under Lorentz transformation. c denotes the velocity of a constant wave front (phase velocity). Regarding the taut elastic string it is given by (see Graff (1991), for example)

$$c = \sqrt{\frac{T}{\rho_c}} . \tag{3.30}$$

Next, we have to find an appropriate *ansatz* that will allow us again to apply our "classical method" to derive the Green's function. To this end we have to think about the propagation of an effect caused by a source that is switched on in x' at time t'. Since we are generally interested in causal cause and effect relations we restrict our considerations to the time-like region of the x-ct-plane represented in Fig. 3.3. In this region we have

$$x' - c\tau \leq x \leq x' + c\tau , \tag{3.31}$$

where $\tau = (t - t') \geq 0$. This can be rewritten into

$$\tau \geq \frac{1}{c} \cdot |x - x'| . \tag{3.32}$$

In view of $ds^2 = c^2 \cdot dt^2 - dx^2 \geq 0$, that holds in the time-like region, we introduce the variable

$$v = \left[(t - t')^2 - \frac{1}{c^2} \cdot (x - x')^2 \right]^{1/2} \geq 0 . \tag{3.33}$$

A second variable u is introduced by

$$u = (t - t') - \frac{1}{c} \cdot |x - x'| . \tag{3.34}$$

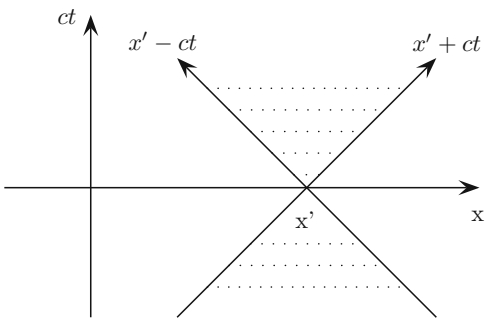

Fig. 3.3 Time-like region (*dotted area*) in the x-ct-plane with $ds^2 = c^2 \cdot dt^2 - dx^2 \geq 0$. This region allows causal relations

Choosing

$$G(x,t;x',t') \;=\; F(v)\cdot H(u) \tag{3.35}$$

as an appropriate *ansatz* for the Green's function of the 1-dim. wave equation, where $H(u)$ is again the Heaviside function, is then justified by the fact that it ensures the restriction of the solution to the time-like region from the very beginning. *A confession is appropriate at this point: I did not came to this ansatz in the way described above. I was first simply looking at the known solution for the Green's function of the 1-dim. wave equation. Only afterwards I was seeking for a justification from a more general point of view. But I was ultimately convinced from the usefulness of this ansatz when I discovered that it can successfully be applied to derive also the Green's functions of the other 1-dim. equations, as we will see shortly.*

Starting from *ansatz* (3.35) the first and second derivative of the Green's function with respect to position and time are given by

$$G_x \;=\; F_v\cdot v_x\cdot H \;+\; F\cdot H_u\cdot u_x \tag{3.36}$$

$$G_t \;=\; F_v\cdot v_t\cdot H \;+\; F\cdot H_u\cdot u_t \tag{3.37}$$

and

$$\begin{aligned} G_{xx} \;=\; & F_{vv}\cdot H\cdot v_x^2 \;+\; F_v\cdot v_{xx}\cdot H \;+\; H_{uu}\cdot F\cdot u_x^2 \;+ \\ & H_u\cdot u_{xx}\cdot F \;+ 2\cdot F_v\cdot H_u\cdot v_x\cdot u_x \end{aligned} \tag{3.38}$$

$$\begin{aligned} G_{tt} \;=\; & F_{vv}\cdot H\cdot v_t^2 \;+\; F_v\cdot v_{tt}\cdot H \;+\; H_{uu}\cdot F\cdot u_t^2 \;+ \\ & H_u\cdot u_{tt}\cdot F \;+ 2\cdot F_v\cdot H_u\cdot v_t\cdot u_t\;. \end{aligned} \tag{3.39}$$

Please, note that the arguments of the functions involved have been omitted for the sake of convenience. But the arguments are identical with the variables of the derivation (i.e., F is a function of v, H of u, u of x,t, and v in x,t). From (3.33) and (3.34) we have furthermore

$$v_t \;=\; \frac{(t-t')}{v} \tag{3.40}$$

$$v_x \;=\; -\frac{1}{c^2}\cdot\frac{(x-x')}{v} \tag{3.41}$$

$$v_{tt} \;=\; \frac{1}{v} \;-\; \frac{(t-t')^2}{v^3} \tag{3.42}$$

$$v_{xx} \;=\; -\frac{1}{c^2}\cdot\left[\frac{1}{v} \;+\; \frac{1}{c^2}\cdot\frac{(x-x')^2}{v^3}\right] \tag{3.43}$$

as well as

$$u_t = 1 \tag{3.44}$$

$$u_x = -\frac{1}{c} \cdot \left[H(x-x') - H(x'-x)\right] \tag{3.45}$$

$$u_{tt} = 0 \tag{3.46}$$

$$u_{xx} = -\frac{2}{c} \cdot \delta(x-x') \tag{3.47}$$

and

$$H_u = \delta(u) \tag{3.48}$$

$$u \cdot \delta(u) = 0\,. \tag{3.49}$$

From (3.29) it follows

$$\frac{1}{c^2} \cdot G_{tt} - G_{xx} = \frac{1}{c^2} \cdot \left[F_{vv} + \frac{F_v}{v}\right] \cdot H + \frac{2}{c} \cdot F \cdot \delta(u) \cdot \delta(x-x') = \frac{1}{c^2} \cdot \left[F_{vv} + \frac{F_v}{v}\right] \cdot H + \frac{2}{c} \cdot F \cdot \delta(t-t') \cdot \delta(x-x') = \delta(t-t') \cdot \delta(x-x')\,. \tag{3.50}$$

This equation can now be used to determine the unknown function $F(v)$.

$$F(v) = C_1 \cdot \ln(v) + C_2 \tag{3.51}$$

is the general solution of the homogeneous equation

$$F_{vv} + \frac{F_v}{v} = 0\,. \tag{3.52}$$

This equation is identical with the equation in the square brackets in (3.50). The constant C_1 is set to zero since we are interested in a solution that do not diverge if $v = 0$. From the remaining part of (3.50) we find

$$C_2 = \frac{c}{2}\,. \tag{3.53}$$

We thus get finally for the free-space Green's function of the 1-dim. wave equation

$$G(x,t;x',t') = \frac{c}{2} \cdot H(u)\,, \tag{3.54}$$

with u given by (3.34). The Reciprocity condition

$$G(x,t;x',t') \;=\; G(x',-t';x,-t)\;, \tag{3.55}$$

that holds obviously for this Green's function, is a combination of (2.23) and (3.4).

There is an interesting relation that can be derived from the Green's function (3.54). For this purpose we write (3.54) once again but by introducing the always positive spatial distance

$$x_d \;=\; |x-x'|\;. \tag{3.56}$$

Since (3.54) reads explicitly

$$G(x,t;x',t') \;=\; \frac{c}{2}\cdot H\left[(t-t') \;-\; \frac{1}{c}\cdot x_d\right] \tag{3.57}$$

it is straightforward to show that relation

$$\frac{1}{c}\frac{\partial G}{\partial t} \;+\; \frac{\partial G}{\partial x_d} \;=\; 0 \tag{3.58}$$

holds for the Green's function of the 1.-dim. wave equation. What makes this relation so interesting? To answer this question let us forget for a moment that we are dealing with the Green's function of the wave equation, and let us assume that we have a Green's function given by the general expression

$$G(x,t;x',t') \;=\; \frac{c}{2}\cdot e^{-i\omega(t-t')}\cdot \bar{G}(x_d)\;. \tag{3.59}$$

This is exactly the *ansatz* we will use later on in this chapter to discuss the Helmholtz equation. Then, if applying relation (3.58) to this Green's function, we get

$$\frac{\partial \bar{G}(x_d)}{\partial x_d} \;-\; \frac{i\omega}{c}\cdot \bar{G}(x_d) \;=\; 0\;. \tag{3.60}$$

But this can directly be compared to Sommerfeld's radiation condition

$$\lim_{|x|\to\infty}\left(\frac{\partial f}{\partial |x|} \;-\; i\,k\,f\right) \;=\; 0 \tag{3.61}$$

required for the scattering solution of the 1.-dim. Helmholtz equation in open spaces, as we will see later on. I found it of some interest that Sommerfeld's radiation condition can be considered as a consequence of the Green's function of the wave equation and its restriction to time-like regions. This condition is usually derived for scattering problems by energy considerations at infinity (see Sommerfeld (1949), Sect. 28 therein), i.e., that any sources within a finite spatial region can only act as sources and not as sinks of energy at infinity.

Beside its importance in Quantum Mechanics, in the theory of vibrating strings the Klein-Gordon equation

$$\frac{1}{c^2}\cdot\left[G_{tt}(x,t;x',t') + a^2\cdot G(x,t;x',t')\right] - G_{xx}(x,t;x',t') = \delta(x-x')\cdot\delta(t-t') \tag{3.62}$$

allows one to couple the elastic string to an elastic support. This support produces a restoring force that causes dispersion effects. It is now straightforward to derive the Green's function by use of the *ansatz* (3.35). From (3.36)–(3.49) it follows the equation

$$\frac{1}{c^2}\cdot\left[F_{vv} + \frac{F_v}{v} + a^2\cdot F\right]\cdot H + \frac{2}{c}\cdot F\cdot\delta(t-t')\cdot\delta(x-x') = \delta(t-t')\cdot\delta(x-x') \tag{3.63}$$

to determine the function $F(v)$. Next we are looking again for the general solution of the homogeneous equation

$$F_{vv}(v) + \frac{F_v(v)}{v} + a^2\cdot F(v) = 0\,. \tag{3.64}$$

within the square brackets of (3.63). Applying the substitution

$$z = a\cdot v \tag{3.65}$$

gives the ordinary differential equation

$$F_{zz}(z) + \frac{F_z(z)}{z} + F(z) = 0\,. \tag{3.66}$$

This is nothing but Bessel's differential equation of zeroth order. Since we are again interested in a solution that do not diverge if $z = 0$, and from the remaining part of (3.63) we find

$$F(z) = F(a\,v) = \frac{c}{2}\cdot J_0(a\,v) \tag{3.67}$$

($J_0(z)$ is Bessel's function of zeroth order for which we have $J_0(0) = 1$ whereas the other independent solution of (3.66) becomes divergent if $z = 0$). The free-space Green's function of the 1-dim. Klein-Gordon equation reads therefore

$$G(x,t;x',t') = \frac{c}{2}\cdot J_0(a\,v)\cdot H(u)\,. \tag{3.68}$$

Equation

$$\frac{1}{c^2}\cdot\left[G_{tt}(x,t;x',t') \;+\; 2\,\gamma\cdot G_t(x,t;x',t')\right] \;-\; G_{xx}(x,t;x',t') \;=\; \delta(x-x')\cdot\delta(t-t') \tag{3.69}$$

represents the 1-dim. equation of telegraphy that can be used to describe wave motions of an elastic string in the presence of a viscous damping. Using the decomposition

$$G(x,t;x',t') \;=\; e^{-\gamma\cdot(t-t')}\cdot\hat{G}(x,t;x',t') \tag{3.70}$$

(3.69) can be rewritten as follows:

$$\frac{1}{c^2}\cdot\left[\hat{G}_{tt}(x,t;x',t') \;-\; \gamma^2\cdot\hat{G}(x,t;x',t')\right] \;-\; \hat{G}_{xx}(x,t;x',t') \;=\; e^{\gamma\cdot(t-t')}\cdot\delta(x-x')\cdot\delta(t-t')\;. \tag{3.71}$$

This equation looks similar to the Klein-Gordon equation. With *ansatz* (3.35), now applied to $\hat{G}(x,t;x',t')$, we thus get the equation

$$\frac{1}{c^2}\cdot\left[F_{vv} \;+\; \frac{F_v}{v} \;-\; \gamma^2\cdot F\right]\cdot H \;+\; \frac{2}{c}\cdot F\cdot\delta(t-t')\cdot\delta(x-x') \;=\; e^{\gamma\cdot(t-t')}\cdot\delta(t-t')\cdot\delta(x-x') \tag{3.72}$$

to determine $F(v)$. Substitution

$$z \;=\; i\cdot\gamma\cdot v \tag{3.73}$$

gives again Bessel's differential equation of zeroth order,

$$F_{zz}(z) \;+\; \frac{F_z(z)}{z} \;+\; F(z) \;=\; 0\;, \tag{3.74}$$

but now for complex arguments. Looking for a solution that is regular in $z = 0$ we thus get

$$F(z) \;=\; \frac{c}{2}\cdot J_0(z) \tag{3.75}$$

Alternatively we have

$$F(v) \;=\; \frac{c}{2}\cdot I_0(\gamma\, v)\;, \tag{3.76}$$

where I_0 denotes the modified Bessel function of zeroth order. The free-space Green's function of the 1-dim. equation of telegraphy is therefore given by

$$G(x,t;x',t') \;=\; \frac{c}{2}\cdot e^{-\gamma\cdot(t-t')}\cdot I_0(\gamma\, v)\cdot H(u)\;. \tag{3.77}$$

The Green's function (3.54) of the 1-dim. wave equation follows from the limiting case $\gamma \to 0$ and the fact that $I_0(0) = 1$.

Starting from the Green's function (3.77) but with the substitution

$$\gamma \;=\; \frac{1}{2}\cdot c^2\cdot a^2\;, \tag{3.78}$$

and if we consider the limiting case $c \to \infty$ we can quickly derive the free-space Green's function of the 1-dim. diffusion equation

$$a^2\cdot G_t(x,t;x',t') \;-\; G_{xx}(x,t;x',t') \;=\; -\,\delta(x-x')\cdot\delta(t-t')\;. \tag{3.79}$$

In so doing, we have only to take the approximations

$$I_0(z) \;\approx\; \frac{e^z}{\sqrt{2\,\pi\, z}} \tag{3.80}$$

and

$$(1\;-\;x)^{1/2} \;\approx\; 1\;-\;\frac{x}{2}\quad ;\; x << 1 \tag{3.81}$$

into account. This provides

$$G(x,t;x',t') \;=\; F(x,t;x',t')\cdot H(t-t')\;, \tag{3.82}$$

where

$$F(x,t;x',t') \;=\; \frac{1}{\sqrt{4\,\pi\, a^2\,(t-t')}}\cdot e^{-\frac{a^2}{4}\cdot\frac{(x-x')^2}{(t-t')}} \tag{3.83}$$

is a solution of the homogeneous diffusion equation

$$a^2\cdot F_t(x,t;x',t') \;-\; F_{xx}(x,t;x',t') \;=\; 0\;. \tag{3.84}$$

Since $c \to \infty$ was assumed in the course of deriving this function the principle of contiguous action does not applies to the diffusion equation! An alternative derivation of the Green's function of the diffusion equation will be discussed in the final chapter of this book.

I hope that I could convince the reader by and by from the usefulness of the "classical method" to derive the Green's functions. We will come back to this method later on in this chapter in conjunction with the Poisson- and Helmholtz equations of higher dimensions. The method of the Fourier- or Laplace transform that is usually applied in the literature is much more laborious. But, now, let us see the Green's function of the 1-dim. wave equation in action by looking at a few wave phenomena of the elastic string.

3.2.3 *Reciprocity and General Solution of the One-Dimensional Wave Equation*

By application of Green's theorem for spatio-temporal problems and the requirement of homogeneous boundary conditions we first want to derive the Reciprocity condition (3.55). The same procedure is applied to express the solution of the inhomogeneous wave equation by the integral relation (3.1). To start with the first task we consider the two equations

$$\frac{1}{c^2} \cdot G_{tt}(x,t;x',t') \; - \; G_{xx}(x,t;x',t') \; = \; \delta(x-x') \cdot \delta(t-t') \tag{3.85}$$

and

$$\frac{1}{c^2} \cdot G_{tt}(x,-t;x'',-t'') \; - \; G_{xx}(x,-t;x'',-t'') \; = \; \delta(x-x'') \cdot \delta(t-t'') \; . \tag{3.86}$$

Regarding the integration with respect to time ($t = 0$ is again chosen as the initial time, and it is further assumed that $t'' \geq t'$ holds) we proceed in a way similar to what was done with expression (2.26). Regarding the integration with respect to x the time-like region $\Gamma_z = \Gamma'_z \cap \Gamma''_z$ that is common to both Green's functions (see Fig. 3.4) must be considered. This provides

$$\int_0^{t''+} dt \int_{\Gamma_z} dx \left[G(x,-t;x'',-t'') \cdot \frac{\partial^2 G(x,t;x',t')}{\partial x^2} - G(x,t;x',t') \cdot \frac{\partial^2 G(x,-t;x'',-t'')}{\partial x^2} + \frac{1}{c^2} \cdot G(x,t;x',t') \cdot \frac{\partial^2 G(x,-t;x'',-t'')}{\partial t^2} - \frac{1}{c^2} \cdot G(x,-t;x'',-t'') \cdot \frac{\partial^2 G(x,t;x',t')}{\partial t^2} \right] = G(x'',t'';x',t') \; - \; G(x',-t';x'',-t'') \; . \tag{3.87}$$

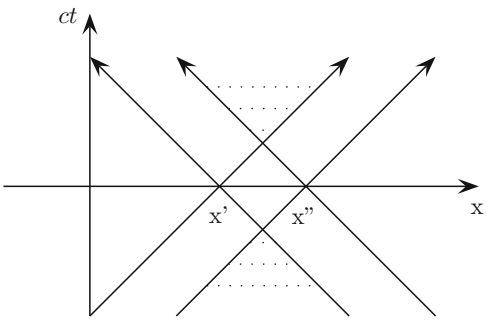

Fig. 3.4 Time-like region $\Gamma_z = \Gamma'_z \cap \Gamma''_z$ (*dotted area*) that is common to both Green's functions $G(x,t;x',t'=0)$ and $G(x,t;x'',t''=0)$

The integration with respect to x and t on the left-hand side can be partially accomplished and gives

$$\int_0^{t''+} dt \left[G(x,-t;x'',-t'') \cdot \frac{\partial G(x,t;x',t')}{\partial x} - G(x,t;x',t') \cdot \frac{\partial G(x,-t;x'',-t'')}{\partial x} \right]_{x \in \partial\Gamma_z} + \frac{1}{c^2} \cdot \int_{\Gamma_z} dx \left[G(x,t;x',t') \cdot \frac{\partial G(x,-t;x'',-t'')}{\partial t} - G(x,-t;x'',-t'') \cdot \frac{\partial G(x,t;x',t')}{\partial t} \right]_{t=0}^{t=t''+} . \tag{3.88}$$

As already discussed in Sect. 2.1.2, these two terms become identical zero due to the requirement of Causality with respect to the temporal boundaries of the time-like region and the assumed homogeneous boundary conditions with respect to its spatial boundaries. The Reciprocity relation

$$G(x'',t'';x',t') = G(x',-t';x'',-t'') \tag{3.89}$$

follows immediately. Restricting the derivation to homogeneous boundary conditions emphasizes once again the insistence on the point of view that every inhomogeneous boundary condition may be replaced by an appropriate source, as demonstrated in conjunction with the 1-dim. Poisson equation.

If using the two equations

$$\frac{1}{c^2} \cdot \psi_{t't'}(x',t') - \psi_{x'x'}(x',t') = \rho(x',t') \tag{3.90}$$

and

$$\frac{1}{c^2} \cdot G_{t't'}(x,t;x',t') - G_{x'x'}(x,t;x',t') = \delta(x-x') \cdot \delta(t-t') , \tag{3.91}$$

and if calculating once again the integral expression

$$\int_0^{t^+} dt' \int_{\Gamma_z'} dx' \left[G(x,t;x',t') \cdot \frac{\partial^2 \psi(x',t')}{\partial x'^2} - \psi(x',t') \cdot \frac{\partial^2 G(x,t;x',t')}{\partial x'^2} + \frac{1}{c^2} \cdot \psi(x',t') \frac{\partial^2 G(x,t;x',t')}{\partial t'^2} - \frac{1}{c^2} \cdot G(x,t;x',t') \cdot \frac{\partial^2 \psi(x',t')}{\partial t'^2} \right] =$$

$$\psi(x,t) - \int_0^{t^+} dt' \int_{\Gamma_z'} dx' \, G(x,t;x',t') \cdot \rho(x',t') \tag{3.92}$$

we get

$$\begin{aligned} \psi(x,t) \; = \; & \int_0^{t^+} dt' \int_{\Gamma_z'} dx' \, G(x,t;x',t') \cdot \rho(x',t') \; + \\ & \int_0^{t^+} dt' \left[G(x,t;x',t') \cdot \frac{\partial \psi(x',t')}{\partial x'} \right]_{x' \in \partial \Gamma_z'} - \\ & \int_0^{t^+} dt' \left[\psi(x',t') \cdot \frac{\partial G(x,t;x',t')}{\partial x'} \right]_{x' \in \partial \Gamma_z'} + \\ & \frac{1}{c^2} \cdot \int_{\Gamma_z'} dx' \, G(x,t;x',0) \cdot \left[\frac{\partial \psi(x',t')}{\partial t'} \right]_{t'=0} - \\ & \frac{1}{c^2} \cdot \int_{\Gamma_z'} dx' \, \psi(x',0) \cdot \left[\frac{\partial G(x,t;x',t')}{\partial t'} \right]_{t'=0} \end{aligned} \tag{3.93}$$

for the general solution of the inhomogeneous wave equation. The last two terms are the result of performing the integration with respect to time. $\psi(x',0)$ and $[\partial \psi(x',t')/\partial t']_{t'=0}$ represent the initial conditions of the field at $t = 0$. That is, these two expressions are the equivalent to the initial position and the initial velocity of the point mass. The corresponding two terms at the upper temporal boundary condition $t' = t^+$ are again zero because of the requirement of Causality. It should be noted that even the last term of (3.93) bears already a strong resemblance to the propagator concept in Quantum Mechanics. That is, a given field distribution $\psi(x',0)$ at the initial time $t' = 0$ causes a field distribution

$$\psi(x,t) \; = \; \int_{\Gamma_z'} P(x,t;x',t') \cdot \psi(x',0) \, dx' \tag{3.94}$$

at a later time $t > t'$, where

$$P(x,t;x',t') \; = \; \frac{1}{c^2} \cdot \left[\frac{\partial G(x,t;x',t')}{\partial t'} \right]_{t'=0} \tag{3.95}$$

represents the "propagator". Expression (3.94) makes also clear that the propagator cannot be represented by any conventional function. It is rather a distribution since $P(x,t;x',t')$ must become Dirac's delta function $\delta(x-x')$ if $t \to 0$. However and as already noted: Each of the last 4 terms of (3.93) may be replaced by corresponding sources. But before this will be demonstrated by three examples it should be also emphasized that the Klein-Gordon equation as well as the equation of telegraphy can be iteratively solved by use of the Lippmann-Schwinger equation if the parameters a and γ result only in small disturbations from the wave equation. Regarding the 1-dim. Klein-Gordon equation and if assuming in general homogeneous boundary conditions with respect to space and time the Lippmann-Schwinger equation reads

$$G^{(KG)}(x'',t'';x',t') \;=\; G_0(x'',t'';x',t') \;- \\ \frac{a^2}{c^2}\int_{t'}^{t''+} dt \int dx\; G_0(x,t;x',t')\cdot G^{(KG)}(x'',t'';x,t)\;. \tag{3.96}$$

For the equation of telegraphy we have on the other hand

$$G^{(TG)}(x'',t'';x',t') \;=\; G_0(x'',t'';x',t') \;+ \\ \frac{2\,\gamma}{c^2}\int_{t'}^{t''+} dt \int dx\; G_0(x,t;x',t')\cdot \frac{\partial G^{(TG)}(x'',t'';x,t)}{\partial t}\;. \tag{3.97}$$

$G_0(x'',t'';x',t')$ represents in both cases the Green's function of the 1-dim. wave equation. How we can take a spatial disturbance from a spherical scatterer geometry by use of a Lippmann-Schwinger equation into account is discussed in the next chapter.

3.2.4 *Examples of Simple Sources*

The first and most simple source is given by

$$\rho(x',t') \;=\; \frac{2}{c}\cdot\delta(t')\cdot\delta(x')\;. \tag{3.98}$$

From the first term on the right-hand side of (3.93),

$$\psi(x,t) \;=\; \int_0^{t+}\int_{-\infty}^{\infty} G(x,t;x',t')\cdot\rho(x',t')\,dx'\,dt'\;, \tag{3.99}$$

and by use of the Green's function (3.54) we get the solution

$$\psi(x,t) \;=\; H(t-|x|/c)\;. \tag{3.100}$$

Starting in $x = 0$, this is simply the step function $\psi(x,t) = 1$ that becomes broader in both the positive and negative x-direction for an increasing observation time t.

As a second example, let us consider the source

$$\rho(x',t') \;=\; \psi(a,t') \cdot \delta_{x'}(x'-a) \;-\; \psi(-a,t') \cdot \delta_{x'}(x'+a)\;. \tag{3.101}$$

The first derivative of the Green's function (3.54) with respect to x' provides

$$G_{x'}(x,t;x',t') \;=\; \frac{1}{2} \cdot \delta(t-t'-|x-x'|/c) \cdot \big[H(x-x') \;-\; H(x'-x)\big]\;. \tag{3.102}$$

From (3.99) and if taking the definition of the derivative of Dirac's delta function into account (see (2.44)!) we get therefore the final solution

$$\begin{aligned}\psi(x,t) \;=\; -\frac{1}{2} \cdot \psi(a,t'=t-|x-a|/c) \cdot [H(x-a) \;-\; H(a-x)] \;+\\ \frac{1}{2} \cdot \psi(-a,t'=t-|x+a|/c) \cdot [H(x+a) \;-\; H(-a-x)]\;.\end{aligned} \tag{3.103}$$

Let us now assume that $\psi(a,t-|x-a|/c) = \psi(-a,t-|x+a|/c) = 1$ holds at the spatial boundaries $x' = \pm a$, and at any time t' earlier than the observation time t. This provides the step function $\psi(x,0) = 1$ in the spatial region $x \in [-a,a]$ and at observation time $t = 0$, for example, as shown in the upper part of Fig. 3.5. Examples of boundary values along $x' = \pm a$ at three earlier times t' which

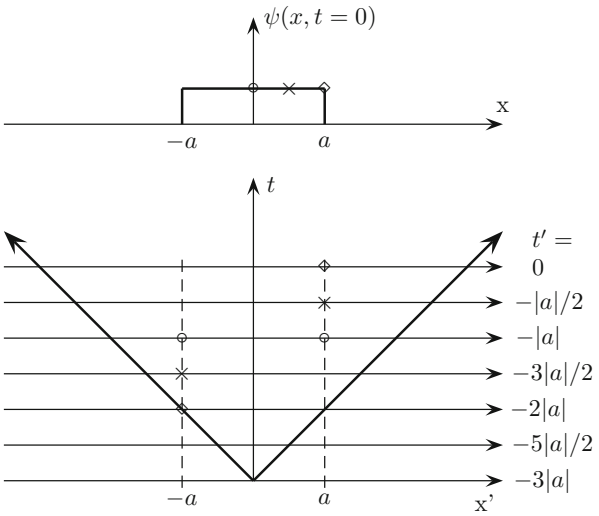

Fig. 3.5 Huygens' principle and the solution (3.103) of the 1-dim. wave equation. The marks along $x' = \pm a$ are the values of Eqs. (3.104)–(3.106) at some earlier times $t' < 0$ which contribute to the step function at observation time $t = 0$. All other values on the two boundaries $x' = \pm a$ and at times $t' < -2|a|$ (i.e., the values outside the time-like region) cancel each other

contribute to the step function at $t = 0$ are shown in the lower part. That is, we have

$$\psi(0,0) = \frac{1}{2} \cdot \left[\psi(a, t' = -|a|) + \psi(-a, t' = -|a|)\right] = 1 \quad (3.104)$$

$$\psi(a/2,0) = \frac{1}{2} \cdot \left[\psi(a, t' = -|a|/2) + \psi(-a, t' = -3|a|/2)\right] = 1 \quad (3.105)$$

$$\psi(a,0) = \frac{1}{2} \cdot \left[\psi(a, t' = 0) + \psi(-a, t' = -2|a|)\right] = 1\,. \quad (3.106)$$

Please, note that $c = 1$ was used for simplicity! All the constant values along $x' = \pm a$ but for times $t' < -2|a|$—these are points outside the time-like region!—cancel each other and do not contribute to the step function at $t = 0$. This example can be considered as an expression of Huygens' principle for the 1-dim. wave equation. But it reveals moreover that solution (3.103) produced by the source (3.101) can also be obtained from the third term on the right-hand side of (3.93) if the inhomogeneous Dirichlet conditions $\psi(a, t - |x - a|/c) = \psi(-a, t - |x + a|/c) = 1$ are required. On the other hand, the second term on the right-hand side will become zero for the homogeneous von Neumann conditions

$$\left[\psi_{x'}(x', t')\right]_{x'=\pm a} = 0\,. \quad (3.107)$$

The last example is concerned with the well-known d'Alembert solution of the elastic string. To this end, let us consider the source

$$\rho(x', t') = \frac{2}{c^2} \cdot \left\{\left[\psi_{t'}(x', t')\right]_{t'=0} \cdot \delta(t') + \psi_0(x') \cdot \delta_{t'}(t')\right\} \quad (3.108)$$

which is appropriate to replace the last two terms on the right-hand side of (3.93). $\psi_0(x')$ and $[\psi_{t'}(x', t')]_{t'=0}$ are the initial conditions. The source (3.108) can therefore be compared to the initial value problems considered in Sect. 2.1.5. Using the Green's function (3.54) and the source (3.108) in (3.99) provides

$$\psi(x,t) = \frac{1}{c} \cdot \int_{-\infty}^{\infty} \left\{\left[\psi_{t'}(x', t')\right]_{t'=0} \cdot H(t - 1/c \cdot |x - x'|) + \psi_0(x') \cdot \delta(t - 1/c \cdot |x - x'|)\right\} dx'\,. \quad (3.109)$$

Taking the properties

$$\delta(\alpha\, x) = \frac{\delta(x)}{|\alpha|} \quad (3.110)$$

$$\delta[f(x)] = \sum_n \frac{1}{|f_x(x_n)|} \cdot \delta(x - x_n) \quad (3.111)$$

of Dirac's delta function into account, where x_n represent the zeroes of the function $f(x)$ and f_x denotes the first derivative of this function with respect to x, gives the d'Alembert solution

$$\psi(x,t) \;=\; \frac{1}{c}\cdot\int_{x-ct}^{x+ct} \left[\psi_{t'}(x',t')\right]_{t'=0}\, dx' + \left[\psi_0(x+ct) \;+\; \psi_0(x-ct)\right] \;. \qquad (3.112)$$

We see that an initial displacement of $2\cdot\psi_0(x = x')$ at $t = 0$ results from the superposition of the two functions $\psi_0(x-ct)$ and $\psi_0(x+ct)$ which move in opposite directions along the elastic string for an increasing observation time $t > 0$ but without changing the form (i.e., without dispersion).

3.2.5 *Reflection of d'Alembert's Solution From a Fixed Boundary*

The reflection of an initial displacement from a fixed boundary is studied in what follows. By introducing a mirror source this example offers a further possibility to discuss the more general understanding of Huygens' principle formulated in the Prologue. The fixed boundary is assumed to be located in $x = 0$. It is characterized by the homogeneous Dirichlet condition

$$G(x = 0, t; x', t') \;=\; 0 \qquad (3.113)$$

that must additionally be fulfilled by the Green's function (3.54) of the 1-dim. wave equation. The initial displacement $\psi_0(x')$ is assumed to be restricted to a finite region on the positive x-axis. The positive x-axis is therefore the spatial region of our interest. Furthermore, $t' = 0$ is used as the initial time. The corresponding source is given by

$$\rho(x',t') \;=\; \frac{2}{c^2}\cdot\psi_0(x')\cdot\delta_{t'}(t') \;. \qquad (3.114)$$

The following *ansatz* is chosen for the Green's function of this problem:

$$G_+(x,t;x',t') \;=\; G_0(x,t;x',t') \;+\; G_r(x,t;x',t') \;, \qquad (3.115)$$

where G_0 represents the known free-space Green's function (3.54). G_r, on the other hand, represents the so far unknown reflected part. This part is once again assumed to represent an appropriate solution of the 1-dim. but homogeneous wave equation. The term $\psi_0(x + ct)$, that results from G_0 and the source (3.114), describes the part of the d'Alembert solution that moves away from x' but toward $x = 0$ for an increasing observation time t. This is the only term that can actually approach the fixed boundary at $x = 0$. Contrary, the term $\psi_0(x - ct)$ moves into the opposite

direction starting from $x = x'$. This term is therefore unable to approach the fixed boundary. The Green's function (3.54) can be split accordingly into two parts. The one part, $G_0^<(x,t;x',t')$, is given by

$$G_0^<(x,t;x',t') \;=\; \frac{c}{2}\cdot H\left[(t-t') \;-\; \frac{(x'-x)}{c}\right] , \tag{3.116}$$

or, because of the restriction to $t' = 0$,

$$G_0^<(x,t;x') \;=\; \frac{c}{2}\cdot H\left[t \;-\; \frac{(x'-x)}{c}\right] . \tag{3.117}$$

It is a solution of the homogeneous, 1-dim. wave equation, as the reader may verify by himself. Let us assume that the argument of the Heaviside function in Eq. (3.117) is given by the positive constant ϵ,

$$t \;-\; \frac{(x'-x)}{c} \;=\; \epsilon \; . \tag{3.118}$$

Then we have

$$x \;=\; c\cdot\epsilon \;+\; x' \;-\; ct \; , \tag{3.119}$$

and

$$x_2 \;<\; x_1 \quad \text{if} \quad t_2 \;>\; t_1 \tag{3.120}$$

holds. That is, it is the part of the Green's function that corresponds with $\psi_0(x+ct)$. Indeed, if using $G_0^<(x,t;x',t')$ and source (3.114) in the integral relation (3.99), and if taking the property (3.110) into account it is not difficult to see that we end up with $\psi(x,t) = \psi_0(x+ct)$. The other part is given by

$$G_0^>(x,t;x',t') \;=\; \frac{c}{2}\cdot H\left[(t-t') \;-\; \frac{(x-x')}{c}\right] . \tag{3.121}$$

Now, if the argument of the Heaviside function with $t' = 0$ is again replaced by ϵ,

$$t \;-\; \frac{(x-x')}{c} \;=\; \epsilon \; , \tag{3.122}$$

we have

$$x \;=\; -c\cdot\epsilon + x' \;+\; ct \tag{3.123}$$

so that

$$x_2 \;>\; x_1 \quad \text{if} \quad t_2 \;>\; t_1 \tag{3.124}$$

holds. This is the part that corresponds with $\psi_0(x - ct)$. That is, now we end up with $\psi(x,t) = \psi_0(x - ct)$ if using $G_0^>(x,t;x',t')$ and source (3.114) in the integral relation (3.99). This part is also a solution of the homogeneous, 1-dim. wave equation. Both these Green's functions are not appropriate to represent the reflected part G_r since $G_0^<$ expresses the unperturbed problem of the initial source that moves in the opposite direction of the reflected part caused by the fixed boundary, and since $G_0^>$ will never come in touch with this boundary. However, if replacing the initial position x' of an elementary displacement on the positive x-axis by $-x'$ on the negative x-axis we have the two other solution

$$\widehat{G}_0^<(x,t;x',t') = \frac{c}{2} \cdot H\left[(t-t') + \frac{(x'+x)}{c}\right] \tag{3.125}$$

and

$$\widehat{G}_0^>(x,t;x',t') = \frac{c}{2} \cdot H\left[(t-t') - \frac{(x+x')}{c}\right] \tag{3.126}$$

of the homogeneous, 1-dim. wave equation. And it is only $\widehat{G}_0^>(x,t;x',t')$ that is appropriate to represent the reflected part. This is due to the fact that it provides a solution that travels away from the fixed boundary along the positive x-axis.

$$G_r(x,t;x',t') = C_r \cdot \widehat{G}_0^>(x,t;x',t') \tag{3.127}$$

with the so far unknown constant C_r is therefore the expression used for the reflected part in *ansatz* (3.115). This constant is determined by application of condition (3.113). Since only $G_0^<$ is the relevant part of G_0 at the boundary in $x = 0$, and since

$$G_0^<(x=0,t;x',t') = \widehat{G}_0^>(x=0,t;x',t') \tag{3.128}$$

holds we have

$$C_r = -1\,. \tag{3.129}$$

$$G_+(x,t;x',t') = G_0(x,t;x',t') - \frac{c}{2} \cdot H\left[t - t' - \frac{(x+x')}{c}\right] \tag{3.130}$$

is therefore the Green's function of the problem under consideration.

Figure 3.6 shows the situation of a rectangular pulse as the initial displacement on the positive x-axis. The corresponding source is given by (3.114) with

$$\psi_0(x') = H(x'-a) \cdot H(b-x') \tag{3.131}$$

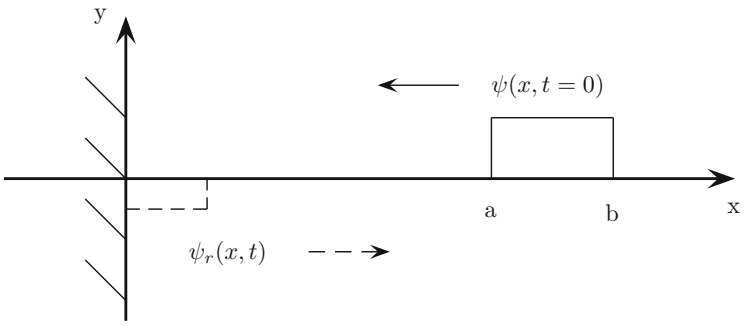

Fig. 3.6 Reflection of a rectangular pulse on a fixed boundary at $x = 0$

Half of the initial rectangular pulse $\psi(x, t = 0) = 2\,\psi_0(x')$ generated by this source moves toward the fixed boundary according to

$$\psi(x,t) \;=\; H(x + ct - a) \cdot H(b - x - ct) \tag{3.132}$$

for an increasing observation time t, as already discussed. The reflected part results from the integral relation

$$\psi_r(x,t) \;=\; \int_0^{t^+} \int_{-\infty}^{\infty} G_r(x,t;x',t') \cdot \rho(x',t')\, dx'\, dt' \tag{3.133}$$

with G_r given by (3.127)/(3.129). Thus we get from (3.114) and (3.131)

$$\psi_r(x,t) \;=\; -\,\psi_0(ct - x) \;=\; -H(ct - x - a) \cdot H(b + x - ct)\;. \tag{3.134}$$

Starting from $t = a/c$ in $x = 0$ this reflected solution moves along the positive x-axis but with the reversed sign of the initial rectangular pulse, as shown in Fig. 3.7. The complete solution is obtained from the superposition of this reflected part with the initial solution (3.132) produced by $G_0^<$. This superposition reads

$$\psi_+(x,t) \;=\; \psi(x,t) \;+\; \psi_r(x,t) \;=$$
$$H(x + ct - a) \cdot H(b - x - ct) \;-\; H(ct - x - a) \cdot H(b + x - ct) \tag{3.135}$$

and guarantees the fulfillment of the fixed boundary condition in $x = 0$.

Exercise: Development of a computer program to demonstrate the temporal behaviour of a rectangular pulse and its reflection from a fixed boundary according to Eq. (3.135). Generalize the above equations and the computer program to the situation of a second but fixed boundary so that the initial pulse generated in between these two boundaries at initial time t = 0 will be reflected back and forth. Note, that both the initial solutions $\psi_0(x - ct)$ and $\psi_0(x + ct)$

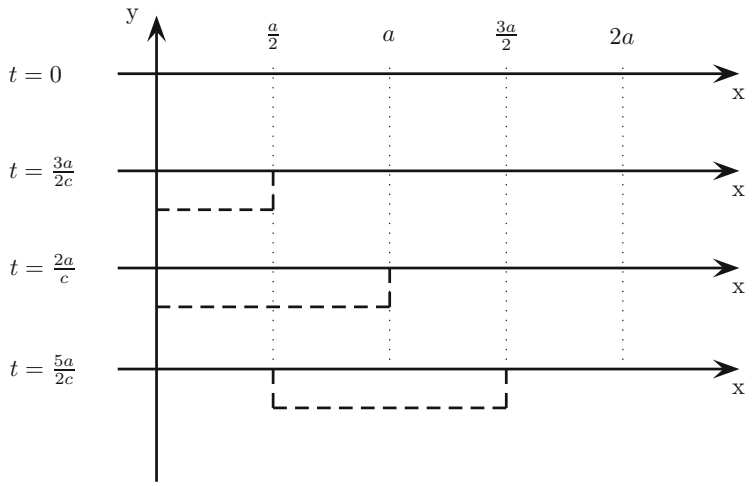

Fig. 3.7 Sequence of the reflected part (3.134) on the positive x-axis (if $b = 2a$ is used) for 4 different observation times

have to be considered in this case (see also Sect. 3.4.4)! Choose the temporal resolution appropriately to generate a movie of this motion.

In the method described above the Green's function was splitted into the two parts G_0 and G_r according to *ansatz* (3.115). After determination of its reflected part the single source (3.114) was applied in our pivotal integral relation. But the same solution on the positive x-axis can alternatively be obtained with only the free-space Green's function G_0 of the 1-dim. wave equation by introducing a second source—a so-called "mirror source"—beside the original source (3.114). This mirror source, if applied to G_0, generates the correct reflected part of the solution if it is given by

$$\rho_m(x', t') = \frac{2}{c^2} \cdot \phi_0(x') \cdot \delta_{t'}(t') \,, \tag{3.136}$$

where

$$\phi_0(x') = -\psi_0(-x') \tag{3.137}$$

(see Fig. 3.8 for the rectangular pulse). Now, the fixed boundary condition does not applies to the Green's function G_0 but to the superposition of the solutions generated by each of these two sources. This is a further example of the fact that an interaction—the interaction with a fixed boundary in our case—can be replaced by a corresponding source according to the more general understanding of Huygens' principle discussed in the Prologue.

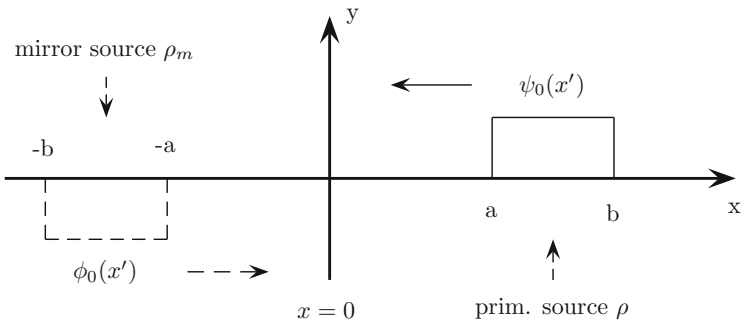

Fig. 3.8 Position of the mirror source related to the problem of the reflection of a rectangular pulse on a fixed boundary at $x = 0$

Another aspect of interest is the rate of transfer of energy across a certain observation point x. This rate is given by

$$P(x,t) := -T \cdot \frac{\partial \psi_+}{\partial x} \cdot \frac{\partial \psi_+}{\partial t} \tag{3.138}$$

(see Graff (1991), Chap. 1 or Morse and Feshbach (1953), Vol 1, Sect. 2.1, for example). Applied to the solution (3.135) the resulting expression for the initial part $\psi(x,t) = \psi_0(ct + x)$ gives

$$P(x,t) = -c\,T \cdot \left[\frac{\partial \psi_0}{\partial u}\right]^2 \tag{3.139}$$

while the corresponding expression for the reflected part $\psi_r(x,t) = -\psi_0(ct - x)$ gives

$$P_r(x,t) = c\,T \cdot \left[\frac{\partial \psi_0}{\partial u}\right]^2 . \tag{3.140}$$

Please, note that u represents the respective argument of ψ_0 in these two expressions! Thus we have finally

$$P_+(x,t) = P(x,t) + P_r(x,t) = 0 \tag{3.141}$$

as an expression of energy conservation.

3.2.6 *Reflection and Transmission of d'Alembert's Solution at a Discontinuity*

The last example is concerned with the behaviour of d'Alembert's solution in the presence of a discontinuity. For this purpose, let us consider two strings with different material parameters linked together at $x = 0$. On the negative x-axis we have the string with the characteristic phase velocity c_-. The other string with the characteristic phase velocity c_+ agrees with the positive x-axis. The source (3.114) of an initial displacement in x' on the positive x-axis at $t' = 0$ is moreover used. Thus we have to replace c by c_+ in (3.114) as well as in the corresponding solution $\psi_+(x,t)$ on the positive x-axis that is given by (3.135). Beside the reflected part we may now expect the existence of an additional transmitted part $\psi_t(x,t)$ that moves along the negative x-axis starting from $x = 0$ at time $t = x'/c_+$. I hope that the reader will not become confused with the subindex "t" that is used to denote the transmitted part of the solution as well as the time derivative. The meaning should become clear from the context. *Ansatz* (3.115) with G_0 and G_r according to (3.54) and (3.127) (with c again replaced by c_+) can still be used for the Green's function on the positive x-axis. On the other hand,

$$G_-(x,t;x',t') \;=\; C_t \cdot \frac{c_-}{2} \cdot H\left[t - t' \;-\; \frac{x'}{c_+} \;+\; \frac{x}{c_-}\right] \tag{3.142}$$

is used as an appropriate *ansatz* for the Green's function on the negative x-axis that can be related to the transmitted solution. This Green's function is now a solution of the homogeneous wave equation

$$\frac{1}{c_-^2} \cdot [G_-]_{tt}(x,t;x',t') \;-\; [G_-]_{xx}(x,t;x',t') \;=\; 0\,. \tag{3.143}$$

The term x'/c_+ in (3.142) considers the fact that the transmitted part cannot be observed before $t = x'/c_+$. This is the time the initial displacement in x' at time $t' = 0$ needs to move to $x = 0$. To determine the constants C_r and C_t of the reflected and transmitted part we require the fulfillment of the two additional conditions

$$G_+(x = 0,t;x',t') \;=\; G_-(x = 0,t;x',t') \tag{3.144}$$

and

$$\left[\frac{\partial G_+(x,t;x',t')}{\partial x}\right]_{x=0} = \left[\frac{\partial G_-(x,t;x',t')}{\partial x}\right]_{x=0} \tag{3.145}$$

at $x = 0$. From these conditions we obtain

$$1 \;-\; C_r = C_t \tag{3.146}$$

$$1 \;+\; C_r = \kappa \cdot C_t\,, \tag{3.147}$$

where

$$\kappa \;=\; \frac{c_-}{c_+} \tag{3.148}$$

denotes the ratio of the phase velocities. This gives

$$C_r = \frac{\kappa - 1}{\kappa + 1} \tag{3.149}$$

$$C_t = \frac{2}{\kappa + 1}\,. \tag{3.150}$$

The reflected part of the solution on the positive x-axis reads

$$\psi_r(x,t) \;=\; C_r \cdot \psi_0(c_+ \cdot t - x)\,. \tag{3.151}$$

The transmitted part can be calculated from

$$\psi_t(x,t) \;=\; \int_0^{t^+} \int_{-\infty}^{\infty} G_-(x,t;x',t') \cdot \rho(x',t')\,dx'\,dt'\,. \tag{3.152}$$

This gives

$$\psi_t(x,t) \;=\; \tilde{C}_t \cdot \psi_0\left(c_+ \cdot t + \frac{x}{\kappa}\right)\,, \tag{3.153}$$

where

$$\tilde{C}_t \;=\; \frac{2\,\kappa}{\kappa + 1}\,. \tag{3.154}$$

Applied to the rectangular pulse given in (3.131) this reads

$$\psi_t(x,t) \;=\; \tilde{C}_t \cdot H\left(c_+ \cdot t + \frac{x}{\kappa} - a\right) \cdot H\left(2a - c_+ \cdot t - \frac{x}{\kappa}\right)\,. \tag{3.155}$$

C_r and $\tilde{C}_t$ are the reflection and transmission coefficients of the solutions. The following relation holds for these coefficients:

$$1 \;=\; C_r^2 \;+\; \frac{1}{\kappa} \cdot \tilde{C}_t^{\,2}\,. \tag{3.156}$$

With the definition

$$S \;:=\; S_r + i\,S_i \;=\; C_r \;+\; i\,\sqrt{\kappa} \cdot C_t \tag{3.157}$$

this can be rewritten into

$$S^* \cdot S \;=\; 1\;, \tag{3.158}$$

It is again an expression of energy conservation. Alternatively, by taking relation (3.156) into account it is straightforward to show that instead of (3.141)

$$P_+(x,t) \;=\; P_t(x,t) \tag{3.159}$$

holds for the energy flow defined in (3.138). However, these relations do not hold if the strings are embedded in a viscous environment. This would require the usage of the Green's function (3.77) in the above considered derivations. But the boundary conditions (3.113) and (3.144)/(3.145) are still be applicable. From (3.153) we see moreover that, in dependence on κ the transmitted solution ψ_t is stretched or compressed compared to the primary solution ψ_0. The former holds for $\kappa > 1$ while the latter applies to $\kappa < 1$. This can nicely be seen from (3.155). And also the two limiting cases of only a reflection if $c_- = 0$, and of no interaction at all if $c_- = c_+$ are also correctly covered by the coefficients C_r and $\tilde{C}_t$.

3.3 Poisson Equations of Higher Dimensions

The objective of this section is to derive the free-space Green's functions of the Poisson equation

$$\nabla^2 G(\mathbf{r},\mathbf{r}') \;=\; \delta(\mathbf{r}-\mathbf{r}') \tag{3.160}$$

in two and three dimensions. The inhomogeneity on the right-hand side is in Cartesian coordinates correspondingly given by

$$\delta(\mathbf{r}-\mathbf{r}') \;=\; \delta(x-x')\cdot\delta(y-y') \tag{3.161}$$

and

$$\delta(\mathbf{r}-\mathbf{r}') \;=\; \delta(x-x')\cdot\delta(y-y')\cdot\delta(z-z')\;. \tag{3.162}$$

It is of special interest to find out if our "classical method" can successfully be applied also in the cases of polar and spherical coordinates. We will discover moreover an interesting relation between the Green's functions of the Poisson equation in one- and three dimensions. But, first, let us consider Dirac's delta function and the **unit source** in polar- and spherical coordinates.

3.3.1 Dirac's Delta Function and Unit Sources in Polar- and Spherical Coordinates

The integral

$$\int_{\Gamma} f(\mathbf{r}) \cdot \delta(\mathbf{r} - \mathbf{r}')\, d\Gamma \; := f(\mathbf{r}') \tag{3.163}$$

is the generalization of the definition of the 1-dim. Dirac's delta function to higher dimensions. $\mathbf{r}'$ and $\mathbf{r}$ are the corresponding vectors to two points inside the higher-dimensional space Γ. This integral should provide 1 if $f(\mathbf{r}) = 1$. Regarding polar coordinates, we have

$$\begin{aligned} x &= R \cdot \cos\phi \\ y &= R \cdot \sin\phi \;, \end{aligned} \tag{3.164}$$

where $R \in [0, \infty[$, and $\phi \in [0, 2\pi]$. For spherical coordinates we have on the other hand

$$\begin{aligned} x &= R \cdot \sin\theta \cdot \cos\phi \\ y &= R \cdot \sin\theta \cdot \sin\phi \\ z &= R \cdot \cos\theta \;, \end{aligned} \tag{3.165}$$

where $R \in [0, \infty[$, $\phi \in [0, 2\pi]$, and $\theta \in [0, \pi]$. Suppose that the origin of the coordinate system is identical with the source point. Then, Dirac's delta functions as well as the free-space Green's functions are only functions of the radius R and independent of the angular coordinates. This simplifies the calculation of the Green's function, as we will see shortly. The origin of the coordinate system can be shifted afterwards to an arbitrary position. To calculate the integral (3.163) with $f(\mathbf{r}) = 1$ in this special situation we have to take the integral

$$\int_0^{2\pi} R\, d\phi \;=\; 2\,\pi\, R \tag{3.166}$$

in the case of polar coordinates, and the integral Integral

$$\int_0^{2\pi} \int_0^{\pi} R^2 \cdot \sin\theta\, d\theta\, d\phi \;=\; 4\,\pi\, R^2 \tag{3.167}$$

in the case of spherical coordinates into account. The corresponding Dirac's delta functions read therefore (see Duffy (2001), Sect. 1.2 therein, for example)

$$\delta_p(R) = \frac{1}{2\,\pi\,R} \cdot \delta(R) \tag{3.168}$$

$$\delta_s(R) = \frac{1}{4\,\pi\,R^2} \cdot \delta(R)\ . \tag{3.169}$$

If the radially dependent delta function $\delta(R)$ is normalized to unity according to

$$\int_0^\infty \delta(R)\,dR\ =\ 1\ , \tag{3.170}$$

we thus have

$$\int_0^\infty \int_0^{2\pi} R \cdot \delta_p(R)\,dR\,d\phi\ =\ 1 \tag{3.171}$$

$$\int_0^\infty \int_0^{2\pi} \int_0^{\pi} R^2 \cdot \sin\theta \cdot \delta_s(R)\,dR\,d\phi\,d\theta\ =\ 1\ . \tag{3.172}$$

Next we want to clarify the understanding of a unit source located in the origin of the coordinate system. The yield of such a source is defined as the outward flow of the field $\psi(R)$ (the gradient $\partial\psi(R)/\partial R$) across a closed surface surrounding the source point. The field itself as well as the corresponding Green's function is characterized by a discontinuity (1-dim. case) or a singularity (higher dim. case) if the observation point approaches the source point. For our purpose we have to surround the source point by a circle of an arbitrarily small radius R_ϵ in case of polar coordinates or by the surface of a sphere of an arbitrarily small radius R_ϵ in case of spherical coordinates. Normalization of this flow to unity if integrated over the circle or the spherical surface provides the following conditions for the unit source (see Sommerfeld (1949), Chap. II, for example):

- 1-dim. case:

$$\left[\frac{dG(x,x')}{dx}\right]_{x=x'-\epsilon}^{x=x'+\epsilon} = 1 \tag{3.173}$$

- polar coordinates:

$$\left[R \cdot \frac{dG^{(2)}(R)}{dR}\right]_{R_\epsilon} = \frac{1}{2\,\pi} \tag{3.174}$$

- spherical coordinates:

$$\left[R^2 \cdot \frac{dG^{(3)}(R)}{dR}\right]_{R_\epsilon} = \frac{1}{4\,\pi}\ . \tag{3.175}$$

These three conditions can be considered to be the analog to condition (2.52). They will again be used in our "classical method" to determine the constants of the general solutions of the respective homogeneous equations, as we will see now.

3.3.2 Green's Function of the Two-Dimensional Poisson Equation

Assuming that the source point agrees with the origin of the polar coordinate system the Poisson equation for the Green's function $G^{(2)}(R)$ reads

$$G^{(2)}_{RR}(R) + \frac{1}{R} \cdot G^{(2)}_{R}(R) = 2\,\delta_p(R) = \frac{1}{\pi\,R} \cdot \delta(R)\,. \tag{3.176}$$

Please, note that we have used once again the symbolic notation for the first and second derivative with respect to R. From our experience of the second chapter it seems promising to use

$$G^{(2)}(R) = F(R) \cdot H(R) \tag{3.177}$$

as an appropriate *ansatz*. It seems as if the Heaviside function $H(R)$ can be omitted since $R \geq 0$. But according to our classical method we have to calculate the first and second derivative of the Green's function. In so doing $H(R)$ produces the required Dirac's delta function. However, $H(R)$ can be omitted in the final result, i.e., once we have determined $F(R)$. Using (3.177) in (3.176) we find

$$\left[F_{RR}(R) + \frac{F_R(R)}{R}\right] \cdot H(R) + 2 \cdot F_R(R) \cdot \delta(R) = \frac{1}{\pi\,R} \cdot \delta(R)\,. \tag{3.178}$$

The unknown function $F(R)$ can be determined by looking for the general solution of the homogeneous equation in the square brackets, i.e., of the ordinary differential equation

$$F_{RR}(R) + \frac{F_R(R)}{R} = 0\,. \tag{3.179}$$

$$F(R) = C_1 \cdot \ln(R) + C_2 \tag{3.180}$$

is its general solution. Constant C_1 can now be determined by applying condition (3.174). This gives

$$C_1 = \frac{1}{2\,\pi}\,. \tag{3.181}$$

If C_2 is again set to zero, as already done in the 1-dim. case in Sect. 3.2.1, the free-space Green's function of the 2-dim. Poisson equation is given by

$$G^{(2)}(R) \;=\; \frac{1}{2\,\pi}\cdot \ln(R)\cdot H(R)\;. \tag{3.182}$$

It is not difficult to show that this Green's function is indeed a solution of (3.176). But it becomes also clear that only the inhomogeneity $2\,\delta_p(R)$ produces a solution that is in correspondence with condition (3.174) of the unit source. On the other hand, using the inhomogeneity $\delta_p(R)$ would result in

$$G^{(2)}(R) \;=\; \frac{1}{4\,\pi}\cdot \ln(R)\cdot H(R) \tag{3.183}$$

which is not in correspondence with (3.174). We have to replace R by $|\mathbf{r}-\mathbf{r}'|$ in (3.182) if the source point does not agrees with the origin of the coordinate system. Since

$$|\mathbf{r}\,-\,\mathbf{r}'| \;=\; \left[(x-x')^2\,+\,(y-y')^2\right]^{1/2}\;, \tag{3.184}$$

and if using (3.164) we thus get

$$G^{(2)}(\mathbf{r},\mathbf{r}') \;=\; \frac{1}{2\,\pi}\cdot \ln\left\{\left[R^2\,+\,R'^2\,-\,2\,R\,R'\cdot\cos(\phi-\phi')\right]^{1/2}\right\} \tag{3.185}$$

for the free-space Green's function of the 2-dim. Poisson equation. It contains the solution (3.182) as a special case if $R' = 0$.

3.3.3 *Green's Function of the Three-Dimensional Poisson Equation*

$$G^{(3)}_{RR}(R)\,+\,\frac{2}{R}\cdot G^{(3)}_{R}(R) \;=\; \delta_s(R) \tag{3.186}$$

is the equation of the Green's function of the 3-dim. Poisson equation in spherical coordinates. The source point is again assumed to be located in the origin of the coordinate system. From *ansatz*

$$G^{(3)}(R) \;=\; F(R)\cdot H(R) \tag{3.187}$$

it follows the equation

$$\left[F_{RR}(R) + \frac{2}{R}\cdot F_R(R)\right]\cdot H(R) + \left[2\cdot F_R(R) + \frac{F(R)}{R}\right]\cdot \delta(R) = \frac{\delta(R)}{4\,\pi\,R^2} \tag{3.188}$$

to determine $F(R)$. The general solution of the corresponding homogeneous differential equation

$$F_{RR}(R) + \frac{2}{R}\cdot F_R(R) = 0\,, \tag{3.189}$$

that results from the expression in the square brackets of the first term on the left-hand side of (3.188), is given by

$$F(R) = \frac{C_1}{R} + C_2\,. \tag{3.190}$$

Constant C_1 can now be determined from condition (3.175). This gives

$$C_1 = -\frac{1}{4\,\pi}\,. \tag{3.191}$$

Constant C_2 is again set to zero. Thus we get for the free-space Green's function of the 3-dim. Poisson equation in spherical coordinates the expression

$$G^{(3)}(R) = -\frac{1}{4\,\pi\,R}\cdot H(R)\,. \tag{3.192}$$

It is indeed a solution of (3.186) as a straightforward calculation demonstrates. If the source point is located outside the origin of the coordinate system we have on the other hand

$$G^{(3)}(\mathbf{r},\mathbf{r}') = -\frac{1}{4\,\pi\,|\mathbf{r}-\mathbf{r}'|}\,, \tag{3.193}$$

where

$$|\mathbf{r}-\mathbf{r}'| = \left[(x-x')^2 + (y-y')^2 + (z-z')^2\right]^{1/2}\,. \tag{3.194}$$

Next, let us consider the modified 1-dim. Poisson equation

$$G_{RR}(R) = \delta(R) \tag{3.195}$$

that is the radially dependent analog to (3.3). Its solution is given by

$$G(R) = R\cdot H(R) \tag{3.196}$$

as the reader may verify by himself by insertion. It differs from (3.13) in the absence of the factor $1/2$ and is in accordance with the 1-dim. condition

$$\left[\frac{dG(R)}{dR}\right]_{R=0^+} = 1 \tag{3.197}$$

of a unit source. The Green's function (3.192) of the 3-dim. Poisson equation can be related to this 1-dim. Green's function by

$$G^{(3)}(R) = -\frac{1}{4\,\pi\,R}\cdot G_R(R)\ . \tag{3.198}$$

We will see later on in this chapter that this relation also applies to other equations. I want to point out also the typical logarithmic singularity in the 2-dim. case and the $1/R$ singularity in the 3-dim. case. For all the scalar fields considered in this book these singularities are uncritical and in accordance with the conditions of the unit source. The situation becomes much more complicate if vector fields be involved in the problems under consideration, as we have in electromagnetic wave scattering, for example. Then the singularities may become much stronger and require a special treatment with essential consequences also for the numerical procedures. But since vector fields are outside the interest of this book I just want to mention the two references Van Bladel (1991) and Fikioris (2004) which consider strong singularities of electromagnetic fields in detail. Especially the latter reference provides a very good introduction (according to my very personal mind) to this topic.

3.4 Wave Equations of Higher Dimensions

We are now interested in the derivation of the Green's functions of the 2-dim. wave equation

$$\frac{1}{c^2}G^{(2)}_{tt}(R;t,t') - G^{(2)}_{RR}(R;t,t') - \frac{1}{R}\cdot G^{(2)}_R(R) = \delta(R)\cdot\delta(t-t') \tag{3.199}$$

in polar coordinates, and the 3-dim. wave equation

$$\frac{1}{c^2}G^{(3)}_{tt}(R;t,t') - G^{(3)}_{RR}(R;t,t') - \frac{2}{R}\cdot G^{(3)}_R(R) = \delta(R)\cdot\delta(t-t') \tag{3.200}$$

in spherical coordinates with the source point assumed again to be located in the origin of the coordinate system. The solutions are well-known. Looking into the relevant literature tells us that these are given by

$$G^{(2)}(R;t,t') = \frac{H(u)}{2\pi\,v} \tag{3.201}$$

and

$$G^{(3)}(R;t,t') \;=\; \frac{\delta(u)}{4\pi R}\;, \tag{3.202}$$

where

$$u \;=\; (t-t') \;-\; \frac{R}{c}\cdot H(R) \tag{3.203}$$

and

$$v \;=\; \left[(t-t')^2 \;-\; \frac{R^2}{c^2}\right]^{1/2} \tag{3.204}$$

in analogy to (3.33) and (3.34) (see Morse and Feshbach (1953), Duffy (2001), for example). For the corresponding radially dependent, 1-dim. wave equation

$$\frac{1}{c^2}G_{tt}(R;t,t') \;-\; G_{RR}(R;t,t') \;=\; \delta(u)\cdot\delta(R) \;=\; \delta(t-t')\cdot\delta(R) \tag{3.205}$$

we have on the other hand

$$G(R;t,t') \;=\; c\cdot H(u) \tag{3.206}$$

which differs again from (3.54) by the absent factor of $1/2$. The Heaviside function $H(R)$ that appears in (3.203) can again be omitted in the final expression. But if we want to prove the correctness of solution (3.206) by insertion into (3.205), for example, we have to take it into account since it produces the required Dirac's delta functions in the corresponding derivatives u_R and u_{RR}, as already shown in Sect. 3.2.2 in connection with u_x and u_{xx}. However, when I tried to derive the above given Green's functions of the 2- and 3-dim. wave equation by the "classical method" I was unable to accomplish it, and I faced the following problem: In all the situations considered so far (including the 1-dim. wave equation) we succeeded in deriving the Green's functions by a shirtsleeves handling of the Heaviside- and Dirac's delta function—shirtsleeves at least from the point of view of a mathematician. On the other hand, this handling is well accepted among physicists. It was therefore my goal to insist in this method and to find out the point where it fails. Frankly speaking, I cannot offer a satisfactory answer to this problem. I consider my restricted in-depth knowledge of the mathematical background of the theory of distributions as the most likely cause of this invidious situation. However, reading the physical literature I have got the impression that I am not alone with this problem, and that it is often swept under the carpet or even ignored. That is, if we try to prove the correctness of (3.201) and (3.202) by insertion into (3.199) and (3.200), respectively, we fail to end up with the correct inhomogeneities. But these inhomogeneities are important to derive the

pivotal relation (1.1), as demonstrated already not only in the last but also in this chapter. And, regarding (3.201), this is not even a solution of the corresponding homogeneous equation. Before I will offer something like a **D**esperate **E**xplanation of **P**lausibility (DEP) to insist in the "classical method" by its combination with the Fourier transform method with respect to time, let us see how these Green's function are usually derived in the physical literature.

3.4.1 Three-Dimensional Wave Equation

In Morse and Feshbach (1953) Chap. 7.3 therein, for example, it is first required that the radially dependent part of the 3-dim. Green's function of the wave equation must behave like the Green's function of the 3-dim. Poisson equation if R tends to 0. That is, condition

$$lim_{R\to 0}\, G^{(3)}(R;t,t') \;=\; \frac{\delta(t-t')}{4\pi R} \tag{3.207}$$

must hold. This condition, the fact that

$$C_1 \cdot \frac{F_1[(t-t')-R/c]}{R} \;+\; C_2 \cdot \frac{F_[(t-t')+R/c]}{R} \tag{3.208}$$

represents the general solution of the 3-dim. but homogeneous wave equation for any two functions F_1 and F_2 (d'Alembert's solution is raising its head!), and the restriction to the time-like region (i.e., $C_2 = 0$) results finally in the solution (3.202). In Duffy (2001) this Green's function is obtained by applying the Laplace transform to the time dependence and the Fourier transform to the Cartesian coordinates.

However, the third and most simple way to determine (3.202) consists in the application of relation (3.198) to the 1-dim. Green's function (3.206), as already mentioned in the foregoing section. The same holds for the 3-dim. Klein-Gordon equation if using the radially dependent, 1-dim. Green's function

$$G(R;t,t') \;=\; c\cdot J_0(a\,v)\cdot H(u) \tag{3.209}$$

instead of (3.68) in relation (3.198). The free-space Green's function of the 3-dim. Klein-Gordon equation is then given by

$$G^{(3)}(R;t,t') \;=\; \frac{\delta(u)}{4\pi R} \;-\; \frac{aJ_1(a\,v)}{4\pi c v}\cdot H(u)\;. \tag{3.210}$$

Exercise: Apply the same procedure to determine the Green's function of the 3-dim. equation of telegraphy.

3.4.2 Two-Dimensional Wave Equation

At first glance it seems possible to apply the procedure of Morse and Feshbach (1953) also to the 2-dim. situation. But looking at the different singularities of the Green's functions (3.182) and (3.201) of the 2-dim. Poisson- and wave equations if R tends to zero reveals that this is not feasible. Interestingly, when we try to apply the "classical method" to the 2-dim. wave equation by choosing *ansatz* (3.35) but with u and v given by (3.203) and (3.204) we end up with the general solution $C \cdot H(u)/v$ of the corresponding homogeneous differential equation. This agrees already with the general structure of (3.201). But the determination of the constant C by integration of the remaining expression and the inhomogeneity on the right-hand side fails.

One method in the literature to determine this Green's function is called the "Hadamard method of descent" (see Morse and Feshbach (1953), for example). In so doing, we have to integrate the Green's function (3.202) of the 3-dim. wave equation with respect to one coordinate—let us say the z-coordinate—according to

$$G^{(2)}(\hat{R}; t, t') \;=\; \int_{-\infty}^{\infty} G^{(3)}(R; t, t')\, dz\,, \tag{3.211}$$

where $\hat{R} = \sqrt{x^2 + y^2}$ and $R = \sqrt{\hat{R}^2 + z^2}$. Expressed in Cartesian coordinates, we have to calculate the integral

$$G^{(2)}(\hat{R}; t, t') \;=\; \frac{1}{4\pi} \cdot \int_{-\infty}^{\infty} \frac{\delta[(t - t') - 1/c \cdot \sqrt{\hat{R}^2 + z^2}]}{\sqrt{\hat{R}^2 + z^2}}\, dz\,. \tag{3.212}$$

Integration can be performed by employing relation (3.111), where the zeroes $z_{1,2}$ are given by

$$z_{1,2} \;=\; \pm\sqrt{c^2\,(t - t')^2 - \hat{R}^2}\,, \tag{3.213}$$

and with the restriction

$$\hat{R} \;<\; c \cdot (t - t') \tag{3.214}$$

that must hold for the time-like region. This gives the Green's function (3.201). An alternative method is discussed in Duffy (2001). This method applies the Laplace transform to the time variable and the Fourier transform to the x-coordinate only. The y-coordinate remains unchanged. The inversion is accomplished by the not even simple Cagniard-de Hoop technique.

These are some of the methods one can find in the literature to calculate the free-space Green's functions of the 2- and 3-dim. wave equation. But, according to my mind, the initially mentioned problem with reproducing the correct inhomogeneities on the right-hand side of these equations remains still open.

3.4.3 *Fourier Transform Method in Infinite Regions*

One possibility to act as if everything is okay with the inhomogeneities of the solutions (3.201) and (3.202) without going into the details of the theory of distributions consists in the application of the Fourier transform method to the time variable only. In so doing, we have to discover the frequency dependent Green's functions of the resulting Helmholtz equations. This can again be accomplished by our "classical method". Integration over these frequency dependent Green's functions results finally in the Green's functions of the wave equations. This final step is the reason for calling it also the "superposition method". This method is described in Morse and Feshbach (1953) and applied to the transient motion of a circular membrane and to the derivation of (3.202). That it can be applied with benefit also to other equations is demonstrated in what follows and also in the last chapter of this book when dealing with the 1-dim. diffusion- and Schrodinger equation. In Wladimirow (1972) (unfortunately only in German) one can find a mathematical justification of this method by operating with the direct product of distributions. However, the Fourier transform method is applied in this book to the space dependent part.

We start with the integral representations (the inverse of the Fourier transformations)

$$\delta(t-t') \;=\; \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega(t-t')}\,d\omega \tag{3.215}$$

of the time dependent Dirac's delta function and

$$G(\mathbf{r},t;\mathbf{r}',t') \;=\; \frac{1}{2\pi}\int_{-\infty}^{\infty} G(\mathbf{r},\mathbf{r}';\omega)\cdot e^{-i\omega(t-t')}\,d\omega \tag{3.216}$$

of the time dependent part of the Green's function. In case of the 1-, 2-, and 3-dim. wave equation the following space dependent Dirac's delta functions are used:

$$\delta(\mathbf{r}-\mathbf{r}') \;=\; \delta(x-x')\;, \tag{3.217}$$

$$\delta(\mathbf{r}-\mathbf{r}') \;=\; 2\cdot\delta_p(R)\;, \tag{3.218}$$

and

$$\delta(\mathbf{r}-\mathbf{r}') \;=\; \delta_s(R)\;, \tag{3.219}$$

where $\delta_p(R)$ and $\delta_s(R)$ are given by (3.168) and (3.169). That the unit source is located in the origin of the polar and spherical coordinate system is assumed in the last two expressions. Applied to the wave equation

$$\frac{1}{c^2}\cdot G_{tt}(\mathbf{r},t;\mathbf{r}',t') \;-\; \nabla^2 G(\mathbf{r},t;\mathbf{r}',t') \;=\; \delta(t-t')\cdot\delta(\mathbf{r}-\mathbf{r}') \tag{3.220}$$

provides the following Helmholtz equations:

- 1-dim. case:

$$G_{xx}(x,x';\omega) \; + \; k^2\, G(x,x';\omega) \; = \; -\,\delta(x-x')\,, \tag{3.221}$$

- 2-dim. case (polar coordinates):

$$\nabla_p^2 G^{(2)}(R;\omega) \; + \; k^2\, G^{(2)}(R;\omega) \; = \; -\,2\cdot\delta_p(R) \tag{3.222}$$

- 3-dim. case (spherical coordinates):

$$\nabla_s^2 G^{(3)}(R;\omega) \; + \; k^2\, G^{(3)}(R;\omega) \; = \; -\,\delta_s(R)\;. \tag{3.223}$$

The wave number k therein is given by

$$k \; = \; \frac{\omega}{c}\;, \tag{3.224}$$

and the radially dependent parts ∇_p^2 and ∇_s^2 of the Laplace operator in polar- and spherical coordinates agree with the left-hand sides of the 2- and 3-dim. Poisson equations (3.176) and (3.186). Next we have to find the solutions of these equations. As already mentioned, and as will be demonstrated in detail in the next section, this can again be accomplished by our "classical method". In this section we will consider these Green's functions to be given. That these functions are in fact the correct solutions can be proven by insertion into the respective Helmholtz equation. The Green's functions read

$$G(x,x';\omega) \; = \; \frac{i}{2k}\cdot e^{\,ik|x-x'|}\;, \tag{3.225}$$

$$G^{(2)}(R;\omega) \; = \; \frac{i}{4}\cdot H_0^{(1)}(kR)\cdot H(R)\;, \tag{3.226}$$

and

$$G^{(3)}(R;\omega) \; = \; \frac{1}{4\pi R}\cdot e^{\,ikR}\cdot H(R)\;. \tag{3.227}$$

$H_0^{(1)}(kR)$ in (3.226) denotes the Hankel function of first kind and zeroth order. The Heaviside functions in (3.226) and (3.227) can again be omitted if used in (3.216). But they have to be taken into account for the proof of correctness. And, as it happened for the Poisson- and wave equation, relation (3.198) holds also for the 3-dim. Green's function of the Helmholtz equation if the solution

$$G(R;\omega) \; = \; \frac{i}{k}\cdot e^{\,ikR\,H(R)} \tag{3.228}$$

of the radially dependent, 1-dim. Helmholtz equation

$$G_{RR}(R;\omega) \; + \; k^2\, G(R;\omega) \; = \; -\,\delta(R) \tag{3.229}$$

is used instead of (3.225).

It is now straightforward to derive the Green's function of the 3-dim. wave equation by substituting (3.227) into (3.216). That is, we have to calculate

$$G^{(3)}(R;t,t') \; = \; \frac{1}{8\pi^2 R} \int_{-\infty}^{\infty} e^{\,ikR} \cdot e^{\,-i\omega(t-t')}\, d\omega \;, \tag{3.230}$$

or, if using (3.224),

$$G^{(3)}(R;t,t') \; = \; \frac{1}{8\pi^2 R} \int_{-\infty}^{\infty} e^{\,-i\omega[(t-t')-R/c]}\, d\omega \;. \tag{3.231}$$

Application of (3.215) results finally in (3.202).

Regarding the 2-dim. situation in polar coordinates we have to solve

$$G^{(2)}(R;t,t') \; = \; \frac{i}{8\pi} \int_{-\infty}^{\infty} H_0^{(1)}(kR) \cdot e^{\,-i\omega(t-t')}\, d\omega \;. \tag{3.232}$$

The following integral representation is known for the Hankel function of first kind and zeroth order (see Abramowitz and Stegun (1984), for example):

$$\begin{aligned} H_0^{(1)}(z) \; &= \; -\,\frac{2\,i}{\pi} \int_1^{\infty} \frac{e^{\,iz\alpha}}{\sqrt{\alpha^2-1}}\, d\alpha \; = \\ &-\,\frac{2\,i}{\pi} \int_{-\infty}^{\infty} \frac{e^{\,iz\alpha}}{\sqrt{\alpha^2-1}} \cdot H(\alpha-1)\, d\alpha \quad ; \; z>0 \end{aligned} \tag{3.233}$$

Substituting this expression into (3.232) and taking (3.215) into account provides

$$G^{(2)}(R;t,t') \; = \; \frac{c}{2\pi R} \int_{-\infty}^{\infty} \frac{\delta(\frac{c(t-t')}{R}-\alpha)}{\sqrt{\alpha^2-1}} \cdot H(\alpha-1)\, d\alpha \;. \tag{3.234}$$

Since $H\{c/R[(t-t')-R/c]\} = H[(t-t')-R/c]$ (3.201) follows immediately.

To derive the Green's function of the 1-dim. wave equation we have to calculate

$$G(x,t;x',t') \; = \; \frac{i}{4\pi} \int_{-\infty}^{\infty} \frac{e^{\,ik|x-x'|} \cdot e^{\,-i\omega(t-t')}}{k}\, d\omega \tag{3.235}$$

or

$$G(x,t;x',t') \; = \; \frac{i\,c}{4\pi} \int_{-\infty}^{\infty} \frac{e^{\,-i\omega[(t-t')-\frac{|x-x'|}{c}]}}{\omega}\, d\omega \tag{3.236}$$

if applying (3.224). Substitution of ω by

$$\omega = -\bar{\omega} - i\epsilon \quad ; \quad \epsilon > 0 \tag{3.237}$$

results in

$$G(x,t;x',t') = \frac{c}{4\pi i} e^{-\epsilon\,[(t-t') - \frac{|x-x'|}{c}]} \int_{-\infty}^{\infty} \frac{e^{i\bar{\omega}[(t-t') - \frac{|x-x'|}{c}]}}{\bar{\omega} + i\epsilon} d\bar{\omega} \,. \tag{3.238}$$

On the other hand, integral representation

$$H(x) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{i\bar{\omega}x}}{\bar{\omega} + i\epsilon} d\bar{\omega} \tag{3.239}$$

is known for the Heaviside function. Then (3.54) follows from (3.238) and from $\epsilon \to 0$.

It seems that this method works quite well. But the following aspect should not be swept under the carpet: In contrast to the inverse (2.56) of the Fourier transform defined with $exp[+\,i\omega(t-t')]$ in Sect. 2.1.4, in representation (3.216) $e^{-i\omega(t-t')}$ was used instead. The fact that we have to look for solutions in the time-like region is the reason for this difference. This becomes impossible if $exp[+\,i\omega(t-t')]$ would have been used. This can be seen from the derivation of the 1-dim. wave equation considered above. Instead of (3.235) we would then get

$$G(x,t;x',t') = \frac{i}{4\pi} \int_{-\infty}^{\infty} \frac{e^{ik|x-x'|} \cdot e^{i\omega(t-t')}}{k} d\omega \,, \tag{3.240}$$

and, therefore, $(t-t') + \frac{|x-x'|}{c}$ as the argument of the Heaviside function. It seems as if the requirement of Causality fixes the sign in the exponent of the Fourier transform if applied to problems in time and space!

Next we want to clarify if this method can also be applied to problems in finite regions. For this purpose, let us consider the example of a finite elastic string with fixed ends. The Green's function of the Helmholtz equation, or, better, its approximation by a bilinear expansion in terms of the corresponding eigensolutions, possesses poles at the eigenfrequencies. This was already demonstrated in Sect. 2.6.

3.4.4 *Fourier Transform Method in Finite Regions*

The eigenvalue problem of Helmholtz' equation for the finite elastic string fixed at $x = 0$ and $x = L$ will be discussed in more detail in the next section. Here it will

again considered to be given. The corresponding bilinear expansion of the Green's function reads

$$G(x, x'; \omega) \;=\; c^2 \cdot \sum_{n=1}^{\infty} \frac{\varphi_n(x) \cdot \varphi_n(x')}{\omega^2 - \omega_n^2} \;, \tag{3.241}$$

where

$$\varphi_n(x) \;=\; \sqrt{\frac{2}{L}} \cdot \sin(k_n x) \tag{3.242}$$

and

$$k_n \;=\; \frac{\omega_n}{c} \;=\; \frac{n\pi}{L} \tag{3.243}$$

are the normalized eigenfunctions and eigenvalues. From (3.216) we thus get

$$G(x, t; x', t') \;=\; i\, c^2 \sum_{n=1}^{\infty} \varphi_n(x) \cdot \varphi_n(x') \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \cdot \frac{e^{-i\omega(t-t')}}{\omega^2 - \omega_n^2} \tag{3.244}$$

for the Green's function of the 1-dim. wave equation. A similar integral was already considered in Sect. 2.1.4 when deriving the Green's function of the simple harmonic oscillator by use of the Fourier transform method. Due to the negative sign of the exponent in (3.244) this method must be modified accordingly to meet the requirement of Causality. That is, now we have to close the path of integration in the lower complex ω-plane. Another possibility to solve this integral offers the complex-valued Dirac's delta function, as described in Sect. 2.5.2. Both these methods provide finally "$\sin[\omega_n(t - t')]/\omega_n$" that can be compared to (2.66). The Green's function reads therefore

$$G(x, t; x', t') \;=\; c^2 \sum_{n=1}^{\infty} \frac{\sin[\omega_n(t - t')]}{\omega_n} \cdot H(t - t') \cdot \varphi_n(x) \cdot \varphi_n(x') \;, \tag{3.245}$$

where we have multiplied the time dependent Heaviside function $H(t-t')$ to indicate that $t > t'$ must hold. By use of this Green's function we are now able to solve temporal problems for the finite elastic string fixed at $x = 0$ and $x = L$. As an example, let us again consider the d'Alembert problem of an initial displacement $\psi_0(x')$ at time $t' = 0$ given by the source (3.114). We thus get from (3.99)

$$\psi(x, t) \;=\; \sum_{n=1}^{\infty} \cos(\omega_n t) \cdot \varphi_n(x) \cdot \int_0^L 2 \cdot \psi_0(x') \cdot \varphi_n(x')\, dx' \;. \tag{3.246}$$

In doing so

$$\frac{\sin(\omega_n t)}{\omega_n} \cdot \delta(t) \;=\; 0 \tag{3.247}$$

was taken into account. The integral in (3.246) just provides the expansion coefficients A_n of the initial displacement $2 \cdot \psi_0(x')$ if expanded in terms of the eigensolutions $\varphi_n(x')$. These eigensolutions are even or odd functions with respect to $x' = L/2$ if n is odd or even. For the reason of simplicity let us further assume that $\psi_0(x')$ represents an even function with respect to $x' = L/2$. Only odd expansion coefficients will then become nonzero. We have therefore

$$2 \cdot \psi_0(x') \;=\; \sum_{n=1}^{\infty} A_{2n-1} \cdot \varphi_{2n-1}(x') \;, \tag{3.248}$$

and, finally,

$$\psi(x,t) \;=\; \sum_{n=1}^{\infty} \cos\left[\frac{(2n-1)\pi}{L} ct\right] \cdot A_{2n-1} \cdot \varphi_{2n-1}(x) \;. \tag{3.249}$$

This expression describes the temporal behaviour of the d'Alembert solution. To see if its behaviour is in correspondence with our experience let us consider the discrete observation times

$$t \;=\; \frac{mL}{c} \quad ; \quad m = 1, 2, \cdots \;. \tag{3.250}$$

Since

$$\cos\left[(2n-1)m\pi\right] \;=\; (-1)^m \tag{3.251}$$

we find

$$\psi(x, t = mL/c) \;=\; (-1)^m \cdot \sum_{n=1}^{\infty} A_{2n-1} \cdot \varphi_{2n-1}(x) \;, \; m = 1, 2, \cdots \;. \tag{3.252}$$

If m is an even number we can observe the initial displacement. On the other hand, if m is an odd number we can observe the initial displacement but mirrored around the x-axis. This agrees indeed with our observations and the result obtained in Sect. 3.2.5.

3.5 The Scalar Helmholtz Equation

The Helmholtz equation

$$\nabla^2 \psi(\mathbf{r}) \; + \; k^2 \, \psi(\mathbf{r}) \; = \; - \rho(\mathbf{r}) \tag{3.253}$$

results from the Fourier transformation of the wave equation with respect to time, as we have seen in the last section.

$$\nabla_{\mathbf{r}}^2 G(\mathbf{r}, \mathbf{r}') \; + \; k^2 \, G(\mathbf{r}, \mathbf{r}') \; = \; - \delta(\mathbf{r} - \mathbf{r}') \tag{3.254}$$

is the corresponding equation of its Green's function. This equation is of our special interest in this section as well as in the next chapter. It plays a major role in different fields of physics. Scattering of acoustic and electromagnetic waves, eigenvalue problems of strings as well as of waveguides in the microwave region and in integrated optics are only a few examples which are also of considerable practical importance. In this section we will essentially focus on the derivation of the Green's functions of the 1-, 2-, and 3-dim. Helmholtz equation by use of the "classical method" while the next chapter addresses the application to different scattering problems.

3.5.1 Green's Functions of the One-Dimensional Helmholtz Equation

Let us first derive the free-space Green's function of the 1-dim. Helmholtz equation

$$G_{xx}(x, x') \; + \; k^2 \, G(x, x') \; = \; - \delta(x - x') \tag{3.255}$$

in an infinite region. According to our classical method *ansatz* (3.5) is used to this end. This gives the equation

$$F_{uu} \; + \; k^2 \cdot F \; + \; 2 \cdot F_u \cdot \delta(x - x') \; = \; - \delta(x - x') \tag{3.256}$$

with $u \; = \; |x - x'|$. The unknown function $F(u)$ is then the general solution of the homogeneous, ordinary differential equation

$$F_{uu} \; + \; k^2 \cdot F \; = \; 0 \; . \tag{3.257}$$

Its solution reads

$$F(u) \; = \; C_1 \cdot e^{\, ik|x - x'|} \; + \; C_2 \cdot e^{\, -ik|x - x'|} \tag{3.258}$$

and meets already the requirement of Reciprocity. But we need a further condition to reject one of the two constants to make the solution unique. This condition is the so-called "Sommerfeld's radiation condition". It was already mentioned in connection with the d'Alembert solution in the presence of a fixed boundary. The radiation condition expresses our physical experience that any time harmonic source located within a finite distance from the origin of the coordinate system can only produce effects that move away from this source. There will be no effect that moves toward this source coming from infinity. In the 1-dim. case, and if the time dependence $exp(-i\omega t)$ is considered this condition reads

$$\lim_{|x|\to\infty} \left(\frac{\partial G(x,x')}{\partial |x|} - i\,k\,G(x,x') \right) = 0 \tag{3.259}$$

(see Sommerfeld (1949)). From (3.258) we have to choose the one solution that is in accordance with this condition. This is obviously

$$F(u) = C_1 \cdot e^{ik|x-x'|} \,. \tag{3.260}$$

Constant C_1 is then the result of the integration of the remaining part of equation (3.256) with respect to x. This gives

$$C_1 = \frac{i}{2k} \,. \tag{3.261}$$

This constant can alternatively be determined by application of condition (3.173) of the unit source in one dimension. But, please, note that we have to replace $+1$ on the right-hand side of (3.173) by -1, due to the negative sign on the right-hand side of (3.255). Thus we have the free-space Green's function

$$G(x,x') = \frac{i}{2k} \cdot e^{ik|x-x'|} \tag{3.262}$$

of the 1-dim. Helmholtz equation in an infinite region subject to the radiation condition (3.259). This agrees with (3.225).

A slight modification of this procedure can be applied to derive the Green's function of the 2-dim. Helmholtz equation subject to the periodicity condition

$$G(x=0,y;x',y') = G(x=L,y;x',y') \tag{3.263}$$

with respect to the x-coordinate. Regarding the y-coordinate we still consider the infinite region and the radiation condition. This Green's function is of importance for solving the problem of a perpendicularly incident plane wave scattered on a periodic grid, amongst others (see Rother and Kahnert (2013), Chap. 6 therein, for example). Since

$$\varphi_n(x) = \frac{1}{\sqrt{L}} \cdot e^{ik_{xn}\,x} \tag{3.264}$$

with

$$k_{xn} \;=\; \frac{2\pi n}{L} \tag{3.265}$$

are normalized eigenfunctions in the interval $x \in [0, L]$ we can expand Dirac's delta function as well as the Green's function according to

$$\delta(x - x') \;=\; \frac{1}{L} \sum_{n=-\infty}^{\infty} e^{\,ik_{xn}\,(x-x')} \tag{3.266}$$

and

$$G(x, y; x', y') \;=\; \frac{1}{L} \sum_{n=-\infty}^{\infty} e^{\,ik_{xn}\,(x-x')} \cdot G_n(y, y') \;. \tag{3.267}$$

$G_n(y, y')$ are so far unknown expansion coefficients. Substitution in the 2-dim. Helmholtz equation

$$G_{xx}(x, y; x', y') \;+\; G_{yy}(x, y; x', y') \;+\; k^2\, G(x, y; x', y') \;=\; -\,\delta(x - x') \cdot \delta(y - y') \tag{3.268}$$

provides the 1-dim. Helmholtz equation

$$\frac{d^2 G_n(y, y')}{dy^2} \;+\; k_{yn}^2\, G_n(y, y') \;=\; -\,\delta(y - y') \;, \tag{3.269}$$

where

$$k_{yn} \;=\; \begin{cases} \sqrt{k^2 - k_{xn}^2} \;; & \text{if } k^2 > k_{xn}^2 \\ i\sqrt{k_{xn}^2 - k^2} \;; & \text{if } k_{xn}^2 > k^2 \;. \end{cases} \tag{3.270}$$

Its solution is identical with (3.262) but with k and $|x-x'|$ replaced by k_{yn} and $|y-y'|$. The Green's function of the 2-dim. Helmholtz equation subject to the periodicity condition with respect to x and to the radiation condition with respect to y reads therefore

$$G(x, y; x', y') \;=\; \frac{i}{2L} \sum_{n=-\infty}^{\infty} \frac{1}{k_{yn}} \cdot e^{\,ik_{xn}\,(x-x')} \cdot e^{\,ik_{yn}\,|y-y'|} \;. \tag{3.271}$$

Moreover, the Reciprocity condition

$$G(x, y; x', y') \;=\; G(x', y'; x, y) \tag{3.272}$$

applies to this Green's function. But I would like also to point out the singular behaviour at $(x, y) = (x', y')$ that corresponds to the logarithmic singularity of the Poisson equation, even if not obvious (see Linton (1998)). An alternative expression of this Green's function is presented shortly when dealing with the 2-dim. Helmholtz equation in polar coordinates. Then the logarithmic singularity in the source point becomes more obvious.

Let us finally consider the eigenvalue problem of the finite string with fixed ends at $x = 0$ and $x = L$, as already announced in the foregoing section. It represents the showpiece of the Fourier analysis and is defined by the homogeneous equation

$$\frac{d^2\psi(x)}{dx^2} + k^2 \cdot \psi(x) = 0 \tag{3.273}$$

together with the homogeneous Dirichlet conditions

$$\psi(x = 0) = \psi(x = L) = 0\,. \tag{3.274}$$

The corresponding temporal problem was already considered in Sect. 2.6. Equations (3.242) and (3.243) are the normalized eigenfunctions and eigenvalues. The Green's function of the 1-dim. Helmholtz equation

$$G_{xx}(x, x') + k^2 \cdot G(x, x') = -\delta(x - x') \tag{3.275}$$

subject to the conditions (3.274) and to the Reciprocity condition (3.4) may therefore be represented by the bilinear expansion

$$G(x, x') = \sum_{n=1}^{\infty} \frac{\varphi_n(x) \cdot \varphi_n(x')}{k_n^2 - k^2} \tag{3.276}$$

with its characteristic poles at $k = k_n$, in close analogy to (2.287).

$$\delta(x - x') = \sum_{n=1}^{\infty} \varphi_n(x) \cdot \varphi_n(x') \tag{3.277}$$

is the corresponding bilinear expansion of Dirac's delta function. And, as also discussed in Sect. 2.6, if expanding the source $\rho(x)$ in terms of the same eigenfunctions we can consider

$$\psi(x) = \int_0^L \delta(x' - x) \cdot \rho(x')\, dx' \tag{3.278}$$

with $\delta(x - x')$ according to (3.277) as the "source picture" of the Fourier series.

3.5.2 Green's Functions of the Two- and Three-Dimensional Helmholtz Equation

The 2-dim. Helmholtz equation for the Green's function in polar coordinates is given by

$$G_{RR}^{(2)}(R) \; + \; \frac{1}{R} \cdot G_{R}^{(2)}(R) \; + \; k^2 \, G^{(2)}(R) \; = \; -2 \cdot \delta_p(R) \tag{3.279}$$

if the source point is located in the origin of the coordinate system. To derive the free-space Green's function of the infinite region requires the fulfillment of the 2-dim. radiation condition (see Sommerfeld (1949))

$$\lim_{R \to \infty} \sqrt{R} \cdot \left(\frac{\partial G^{(2)}(R)}{\partial R} \; - \; i \, k \, G^{(2)}(R) \right) \; = \; 0 \; . \tag{3.280}$$

As already done in connection with the Poisson equations of higher dimensions *ansatz*

$$G^{(2)}(R) \; = \; F(R) \cdot H(R) \tag{3.281}$$

is used to solve this equation. The general solution of the unknown function $F(R)$ can be quickly obtained if looking at expressions (3.64)/(3.66) and (3.179) we derived already for the 1-dim. Klein-Gordon- and the 2-dim. Poisson equation. Regarding (3.179) we must only add the term $k^2 \, F(R)$ to get the homogeneous differential equation related to the 2-dim. Helmholtz equation. The resulting expression becomes identical with (3.64) if replacing a by k and v by R. But now we have to choose the Hankel function of first kind and zeroth order (instead of Bessel's function!) as the only solution of Bessel's differential equation that is in correspondence with the radiation condition (3.280) (see Abramowitz and Stegun (1984), relation 9.2.3, for example). We thus have

$$F(R) \; = \; C \cdot H_0^{(1)}(kR) \; . \tag{3.282}$$

The unknown constant C can again be determined from condition (3.174) of the unit source in two dimensions, and if replacing $+1$ on the right-hand side by -1. Taking additionally the relations

$$H_0^{(1)}(z) \; = \; J_0(z) \; + \; i \, Y_0(z) \; , \tag{3.283}$$

$$\left[\frac{dH_0^{(1)}(z)}{dz} \right]_{z \to 0} \; = \; -i \; [Y_1(z)]_{z \to 0} \; , \tag{3.284}$$

and

$$[Y_1(z)]_{z\to 0} \;=\; -\frac{2}{\pi z} \tag{3.285}$$

into account (see Abramowitz and Stegun (1984), relation 9.1.9 therein) results in

$$C \;=\; \frac{i}{4}\,. \tag{3.286}$$

We thus get finally

$$G^{(2)}(R) \;=\; \frac{i}{4}\cdot H_0^{(1)}(kR)\cdot H(R) \tag{3.287}$$

for the free-space Green's function of the 2-dim. Helmholtz equation in an infinite region subject to the radiation condition (3.280). In so doing, we have proved (3.226) true. Looking at relation 9.1.89 in Abramowitz and Stegun (1984), for example, we can also discover the logarithmic singularity of $H_0^{(1)}(z)$ if $z \to 0$, as mentioned before.

As also discussed in Sect. 3.5.1, solving the problem of a perpendicularly incident plane wave scattered on a periodic grid requires a Green's function of the 2-dim. Helmholtz equation that is in correspondence with the periodicity condition (3.263). Equation (3.271) is one possible expression. Based on (3.287) and by use of Green's theorem it was shown in Twersky (1956) that an alternative expression is given by

$$G(x,y;x',y') \;=\; \frac{i}{4}\cdot\sum_{n=-\infty}^{\infty} H_0^{(1)}(kr_n)\,, \tag{3.288}$$

where

$$r_n \;=\; \sqrt{(x-x'-nL)^2 \;+\; (y-y')^2}\,. \tag{3.289}$$

But this expression is quite slowly converging, which is why it is not used very often (Linton 1998). The generalization to the case of an oblique incident plane wave on a periodic grid can also be found in this reference.

The free-space Green's function of the 3-dim. Helmholtz equation

$$G^{(3)}_{RR}(R) \;+\; \frac{2}{R}\cdot G^{(3)}_{R}(R) \;+\; k^2\,G^{(3)}(R) \;=\; -\delta_s(R)\,, \tag{3.290}$$

of the infinite region subject to the 3-dim. radiation condition (see Sommerfeld (1949))

$$\lim_{R\to\infty} R\cdot\left(\frac{\partial G^{(3)}(R)}{\partial R} \;-\; i\,k\,G^{(3)}(R)\right) \;=\; 0 \tag{3.291}$$

is of special importance for the scattering problems we intend to consider in the next chapter. Looking back to the derivation of the Green's function of the 3-dim. Poisson equation (see Sect. 3.3.3) tells us that the unknown function $F(R)$ in *ansatz* (3.281) must now be a solution of the homogeneous equation

$$F_{RR}(R) + \frac{2}{R} \cdot F_R(R) + k^2 \cdot F(R) = 0 \tag{3.292}$$

Its general solution reads

$$F(R) = C_1 \cdot \frac{e^{ikR}}{R} + C_2 \cdot \frac{e^{-ikR}}{R} . \tag{3.293}$$

But only the first term

$$F(R) = C_1 \cdot \frac{e^{ikR}}{R} \tag{3.294}$$

of the right-hand side remains because of (3.291). The constant C_1

$$C_1 = \frac{1}{4\pi} \tag{3.295}$$

results from condition (3.175) of the unit source, where $+1$ on the right-hand side must again be replaced by -1. Thus we have

$$G^{(3)}(R) = \frac{e^{ikR}}{4\pi R} \cdot H(R) \tag{3.296}$$

as the free-space Green's function of the Helmholtz equation in an infinite region subject to radiation condition (3.291). Moving the source point away from the origin of the coordinate system results in

$$G^{(3)}(\mathbf{r}, \mathbf{r}') = \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} . \tag{3.297}$$

The Green's function (3.192) of the 3-dim. Poisson equation follows from $k = 0$, and after multiplication of (3.296) by –1—a consequence of the different signs of the inhomogeneities.

Chapter 4
Green's Functions and Plane Wave Scattering

Traversing slit one, or traversing slit two, that is the question

4.1 General Aspects

It is not an exaggeration to say that scattering processes are of basic importance in physics. They are used in different fields of physics to gain information about the objects of interest and the interaction processes these objects may undergo. We became already acquainted with scattering of a point mass on a rigid sphere and the Kepler problem in the second chapter, and with d'Alembert's solution in the presence of a fixed boundary and a discontinuity in the foregoing chapter. Now we are going to consider another scattering process—scattering of a plane wave on different obstacles characterized by their geometry and material properties. On the one hand, this is aimed at seeing the Green's function of the 3-dim. Helmholtz equation in action. On the other hand, dealing with this problem will allow us to illustrate once again some of the aspects discussed in the Prologue from a more abstract point of view. The experiences I have gained over the years when dealing with electromagnetic wave scattering on nonspherical objects by using Green's functions was in fact an essential trigger to write this book.

As already mentioned at the beginning of Sect. 2.7, in a scattering experiment the information is gained by comparing the asymptotic free states before and after the scattering process. In what follows we start from the assumption of a steady state situation with a time dependence given by $exp(-i\omega t)$. The scattering process itself is assumed to be a local process in space. The incident plane wave represents the asymptotic free state before the scattering process. The scattered field in the nonlocal far field of the scattering object represents the asymptotic free state after the scattering process. But both these asymptotic free states are abstract quantities, at first, and appropriately measurable quantities like intensities and differential or total cross-sections have to be defined. All the scattering processes we intend to consider in this section are well-known from the literature and analytically solvable. The reader who may be interested in more realistic scattering scenarios which can be solved only by a considerable numerical effort is referred to our book (Rother and Kahnert 2013). Green's functions form again the methodical backbone of this book.

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Regarding the scattering problem of electromagnetic waves we have actually to take the vector character of these fields into account. This would force us to solve the vector-wave equation instead of the Helmholtz equation, in general. And all the corresponding Green's functions would become dyadic quantities. But for the reason of simplicity, in this chapter we intend to consider only such cases that allow for a decomposition of Maxwell's equations into two independent systems each of which is related to a scalar quantity governed by the Helmholtz equation and appropriate boundary conditions. In so doing, we provide at once a solution of the scattering problem of acoustic waves.

Figure 4.1 shows the general configuration of a scattering experiment that is of our interest in what follows. The finite volume of the scatterer is enclosed by its boundary surface S. The outer space Γ, on the other hand, is enclosed by this surface and the spherical surface S_∞ of the nonlocal far field. This space is physically characterized by the constant k. The local source $\rho(\mathbf{r})$ generates the primary incident field $\psi_0(\mathbf{r})$. This field interacts with an ideal metallic or acoustically soft scatterer. As a result of this interaction process a scattered field $\psi_s(\mathbf{r})$ is generated that superposes the primary incident field. The volume inside the scatterer is assumed to be free of fields. The primary incident field is a solution of the inhomogeneous Helmholtz equation

$$\left(\nabla^2 + k^2\right) \psi_0(\mathbf{r}) = -\rho(\mathbf{r}) \tag{4.1}$$

in Γ while the scattered field solves the corresponding homogeneous equation. Green's theorem for any two functions $\psi(\mathbf{r})$ and $\phi(\mathbf{r})$ defined within any volume

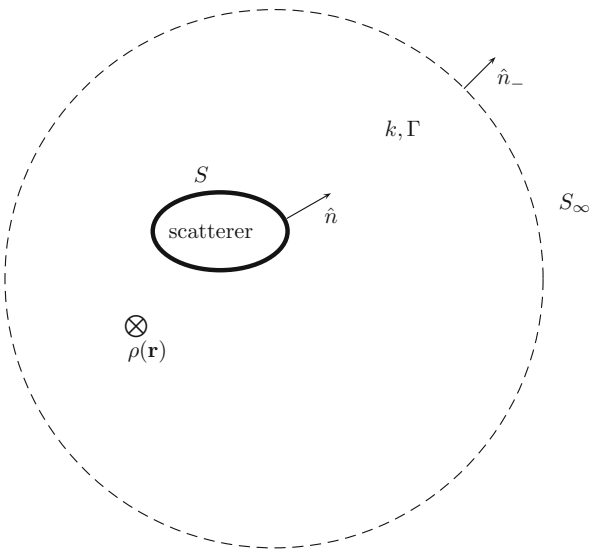

Fig. 4.1 General configuration of a scattering experiment

Γ enclosed by the surface $\partial\Gamma$ is given by

$$\int_{\Gamma} \left[\psi(\mathbf{r}) \cdot \nabla^2\phi(\mathbf{r}) - \phi(\mathbf{r}) \cdot \nabla^2\psi(\mathbf{r})\right] dV(\mathbf{r}) = \oint_{\partial\Gamma} \left[\psi(\mathbf{r}) \cdot \frac{\partial\phi(\mathbf{r})}{\partial\hat{n}} - \phi(\mathbf{r}) \cdot \frac{\partial\psi(\mathbf{r})}{\partial\hat{n}}\right] dS(\mathbf{r}) \,. \tag{4.2}$$

The radiation condition (3.291) must hold on the nonlocal surface S_∞ for any primary incident field generated by a local source, for the scattered field, and for the free-space Green's function of the 3-dim. Helmholtz equation, as already discussed in the foregoing chapter. If identifying $\psi(\mathbf{r})$ with the total field

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \psi_s(\mathbf{r}) \,, \tag{4.3}$$

$\phi(\mathbf{r})$ with the free-space Green's function (3.297) of the 3-dim. Helmholtz equation,

$$\phi(\mathbf{r}) = G^{(3)}(\mathbf{r}, \mathbf{r}') \,, \tag{4.4}$$

and if taking its Reciprocity into account we get from Green's theorem

$$\psi(\mathbf{r}) = \int_{\Gamma} G^{(3)}(\mathbf{r}, \mathbf{r}') \cdot \rho(\mathbf{r}')\, dV(\mathbf{r}') - \oint_{S} \left[\psi(\mathbf{r}') \cdot \frac{\partial G^{(3)}(\mathbf{r}, \mathbf{r}')}{\partial\hat{n}'} - G^{(3)}(\mathbf{r}, \mathbf{r}') \cdot \frac{\partial\psi(\mathbf{r}')}{\partial\hat{n}'}\right] dS(\mathbf{r}') \,. \tag{4.5}$$

The normal derivative at the scatterer surface is defined by

$$\frac{\partial f(\mathbf{r})}{\partial\hat{n}} := \hat{n} \cdot \nabla f(\mathbf{r}) \,. \tag{4.6}$$

It is important to note that the gradient operation in expression $\partial\psi(\mathbf{r}')/\partial\hat{n}'$ must initially be applied to the field outside the boundary surface of the scatterer. The transition to the scatterer surface is performed only afterwards. The first term on the right-hand side of (4.5) just provides the primary incident field ψ_0. The second term represents the scattered field ψ_s. It was moreover assumed that the scattered field has no influence on the local source ρ.

$$\psi(\mathbf{r}) = 0 \quad ; \, \mathbf{r} \in S \tag{4.7}$$

is the boundary condition we additionally require for the total field at the scatterer surface. With this homogeneous Dirichlet condition we are able to describe the scattering process of an electric or acoustic field on an ideal metallic or acoustically soft object. But regarding the electromagnetic case boundary condition (4.7) holds

only for fields with a certain polarization. It can therefore only be applied if Maxwell's equations can be splitted into two scalar Helmholtz equations each of which is related to a certain polarization. In contrast to (4.7) the homogeneous von Neumann boundary condition

$$\frac{\partial \psi(\mathbf{r})}{\partial \hat{n}} = 0 \quad ; \; \mathbf{r} \in S \tag{4.8}$$

applies to the field with the respective other polarization. This boundary condition is related in acoustics to the scattering problem of an acoustically hard object. But in what follows we will restrict the considerations to the problems described by the homogeneous Dirichlet condition. Applying this condition to (4.5) by shifting the observation point $\mathbf{r}$ toward the surface S provides

$$-\psi_0(\mathbf{r}) = \mathrm{pv} \oint_S \frac{\partial \psi(\mathbf{r}')}{\partial \hat{n}'} \cdot G^{(3)}(\mathbf{r}, \mathbf{r}') \, dS(\mathbf{r}') \quad ; \; \mathbf{r} \in S \, , \tag{4.9}$$

where "pv" in front of the integral denotes again the "principal value" integration. The necessity of such an integration results from the singular behaviour of the Green's function (3.297) of the 3-dim. Helmholtz equation if $\mathbf{r} = \mathbf{r}'$. It is defined as follows:

$$\mathrm{pv} \oint_S G^{(3)}(\mathbf{r}, \mathbf{r}') \cdot f(\mathbf{r}') \, dS(\mathbf{r}') := \lim_{S_\delta \to 0} \int_{S - S_\delta} G^{(3)}(\mathbf{x}, \bar{\mathbf{x}}) \cdot f(\mathbf{r}') \, dS(\mathbf{r}') \, . \tag{4.10}$$

S_δ denotes a small surface element that encloses the singular point. It is excluded from the surface integral since it does not contribute to this integral in the limit $\lim_{S_\delta \to 0}$. To be more specific we consider the following decomposition of the surface integral:

$$\begin{aligned} \oint_S G^{(3)}(\mathbf{r}, \mathbf{r}') \cdot f(\mathbf{r}') \, dS(\mathbf{r}') &= \int_{S - S_\delta} G^{(3)}(\mathbf{x}, \bar{\mathbf{x}}) \cdot f(\mathbf{r}') \, dS(\mathbf{r}') + \\ &\int_{S_\delta} G^{(3)}(\mathbf{r}, \mathbf{r}') \cdot f(\mathbf{r}') \, dS(\mathbf{r}') \quad ; \; \mathbf{r} \in S \, . \end{aligned} \tag{4.11}$$

It can then be shown that for any sufficiently smooth function $f(\mathbf{r})$ with no singularities along the surface S

$$\lim_{S_\delta \to 0} \int_{S_\delta} G^{(3)}(\mathbf{r}, \mathbf{r}') \cdot f(\mathbf{r}') \, dS(\mathbf{r}') \to 0 \quad ; \; \mathbf{r} \in S \, , \tag{4.12}$$

holds. To prove this, let us consider the surface integral

$$\int_{S_\delta} G^{(3)}(\mathbf{r}, \mathbf{r}') \cdot f(\mathbf{r}') \, dS(\mathbf{r}') \quad ; \; \mathbf{r} \in S \, . \tag{4.13}$$

Since S_δ is a small surface element the Green's function (3.297) can be replaced by its static approximation

$$G^{(3)}(\mathbf{r}, \mathbf{r}') \;\approx\; \frac{1}{4\pi |\mathbf{r} - \mathbf{r}'|} \;. \tag{4.14}$$

S_δ can furthermore be assumed w.l.o.g. to represent a surface patch with a circular boundary, and with the z-axis of the coordinate system going through the center of the boundary circle (compare Fig. 4.2). The observation point $\mathbf{r}$ is placed in the center of the circle in distance a from the origin of the coordinate system. $|\mathbf{r}| = |\mathbf{r}'| = a$ is assumed to be constant across the small surface element S_δ. In spherical coordinates we have

$$dS(\mathbf{r}') \;=\; a^2 \, \sin\theta' \, \mathrm{d}\theta' \, \mathrm{d}\phi' \;, \tag{4.15}$$

and

$$|\mathbf{r} - \mathbf{r}'| \;\approx\; \sqrt{2} \cdot a \cdot \left(1 - \cos\theta'\right)^{\frac{1}{2}} \;. \tag{4.16}$$

Together with 2π, that results from the integration with respect to ϕ', we thus get the approximate expression

$$\int_{S_\delta} \frac{f(\mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|} \, dS(\mathbf{r}') \;\approx\; \frac{f(a)}{2\sqrt{2}} \cdot a \cdot \int_0^{\theta'_\delta} \frac{\sin\theta'}{(1 - \cos\theta')^{\frac{1}{2}}} \, d\theta' \;. \tag{4.17}$$

In so doing, we have moreover replaced the sufficiently smooth function $f(\mathbf{r}')$ by its value in point $(r = a, \theta = 0°, \phi = 0°)$ everywhere across S_δ. Since the possible angles θ' are very small on S_δ it is sufficient to approximate $\cos\theta'$ by the first two

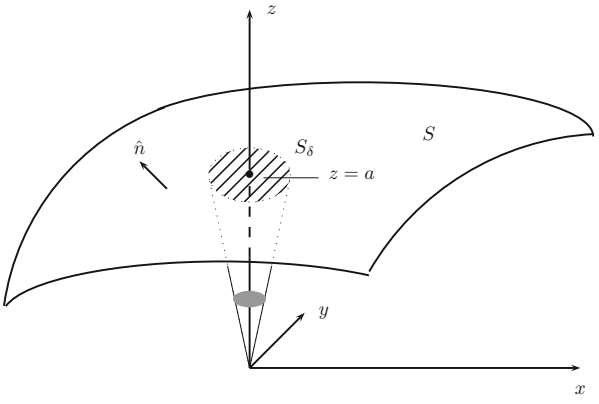

Fig. 4.2 Geometrical configuration to calculate the contribution of the surface integral (4.13)

terms of its Taylor series (i.e., by $1 - \theta'^2/2$) and $\sin\theta'$ by θ'. This gives finally

$$\int_{S_\delta} \frac{f(\mathbf{r}')}{4\pi|\mathbf{r}-\mathbf{r}'|}\, dS(\mathbf{r}') \;\approx\; \frac{f(a)}{2}\cdot a\cdot\theta'_\delta\,. \tag{4.18}$$

This vanishes indeed if $\theta'_\delta \to 0$. Now we can continue with expression (4.9). The normal derivative on the right-hand side is defined as the induced surface current j_s. This results in the well-known integral equation

$$-\,\psi_0(\mathbf{r}) \;=\; \mathrm{pv}\oint_S j_s(\mathbf{r}')\cdot G^{(3)}(\mathbf{r},\mathbf{r}')\, dS(\mathbf{r}') \quad ;\; \mathbf{r}\in S \tag{4.19}$$

to calculate the unknown surface current. The total field outside the scatterer is then given by

$$\psi(\mathbf{r}) \;=\; \int_\Gamma G^{(3)}(\mathbf{r},\mathbf{r}')\cdot\rho(\mathbf{r}')\, dV(\mathbf{r}') \;+\; \oint_S G^{(3)}(\mathbf{r},\mathbf{r}')\cdot j_s(\mathbf{r}')\, dS(\mathbf{r}')\,. \tag{4.20}$$

This is another example of what I formally called the "generalized understanding of Huygens' principle" in the Prologue—the replacement of the interaction of a scalar plane wave with an ideal metallic or acoustically soft obstacle by an equivalent source called "induced surface current". When dealing with the scattering problem of an ideal metallic sphere later on we will become acquainted with an alternative approach that avoids the singularity problem of the Green's function considered above. But the derivation of Eq. (4.19) has revealed moreover that the field quantities $\psi(\mathbf{r}')$ and $\partial\psi(\mathbf{r}')/\partial\hat{n}'$ are not independent of each other. They are linked by an inhomogeneous Fredholm integral equation of the second kind (Maue's integral equation) at the scatterer surface. That is, the scattering problem is already uniquely solvable if only one of these quantities is given! A more detailed discussion of this aspect can be found in Hönl et al. (1961). Even if this book exists only in German, it is highly recommended for those readers who intend to go further into scattering problems.

Starting from Eq. (4.5) it is straightforward to derive the classical Huygens' principle. In so doing, it is assumed that the primary source ρ as well as the scatterer are confined within the volume bounded by the surface S_ρ (see Fig. 4.3). We ask for the field in the source-free region bounded by S_ρ and S_∞. The first term on the right-hand side of (4.5) vanishes and it remains

$$\psi(\mathbf{r}) \;=\; -\oint_{S_\rho}\left[\psi(\mathbf{r}')\cdot\frac{\partial G^{(3)}(\mathbf{r},\mathbf{r}')}{\partial\hat{n}'} \;-\; G^{(3)}(\mathbf{r},\mathbf{r}')\cdot\frac{\partial\psi(\mathbf{r}')}{\partial\hat{n}'}\right] dS(\mathbf{r}')\,. \tag{4.21}$$

That is, the field in the source-free region is known if its behaviour along the boundary surface S_ρ is known. But it should be emphasized once again that $\psi(\mathbf{r}')$ and $\partial\psi(\mathbf{r}')/\partial\hat{n}'$ are related by an integral equation. The boundary surface S_ρ divides the region Γ into a region with a source and a source-free region, and it can be

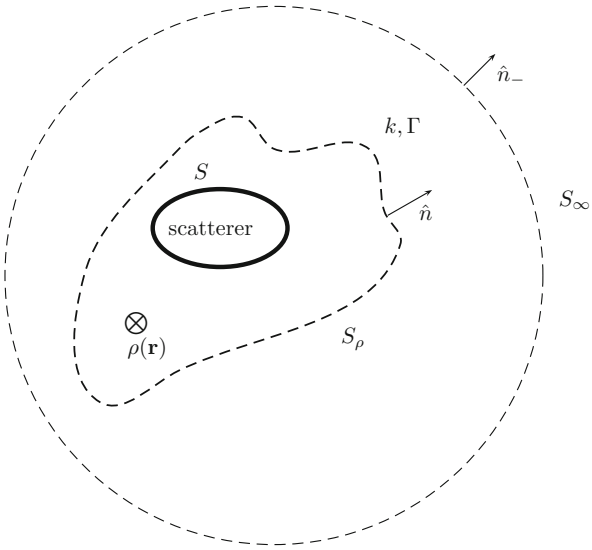

Fig. 4.3 Scattering configuration to discuss Huygens' principle

chosen in such a way that it fits into the physical situation under consideration. We face this problem when solving the scattering of a plane wave on the double-slit. But before we will come to this example, let us look briefly at the somehow strange nature of the object "plane wave".

$$\psi_0(x,t) \;=\; E_0 \cdot e^{\,i(kx-\omega t)} \tag{4.22}$$

represents such an object that is traveling with an amplitude E_0 along the positive x-axis. We will omit the time dependency in what follows. The remaining space dependent part is obviously a solution of the 1-dim., homogeneous Helmholtz equation

$$\frac{d^2\psi_0(x)}{dx^2} \;+\; k^2 \cdot \psi_0(x) \;=\; 0\,. \tag{4.23}$$

In contrast to the Green's function (3.262) the radiation condition (3.259) does not applies to $\psi_0(x)$. That is, the object "scalar plane wave"—characterized by the wave number k and amplitude E_0—exists without any source, and, therefore, must be given a priori in corresponding scattering experiments. But this is in contrast to our concept formulated in the Prologue. There we have required that any state of an object must be related to a source/cause to express the basic principle of Causality. And in any real scattering experiment the primary incident plane wave will be generated in fact by a certain real source (a widespread LASER beam, an antenna, etc.). And if we intend to express such a plane wave by the first term on the right-hand side of (4.5) a source is a necessary prerequisite. To see how we can relate a source to such a plane wave let us consider the far field approximation of the

3-dim. Green's function (3.297) if a unit source is located on the negative x-axis but at a very large distance from the origin of the coordinate system. That is, we have

$$\mathbf{r}' \;=\; (-x_b', 0, 0) \quad ;\; x_b' >> x, y, z \;, \tag{4.24}$$

where $\mathbf{r} = (x, y, z)$ are the coordinates of the observation point located close to the origin of the coordinate system. The denominator of (3.297) can then be replaced by x_b'. But the phase term $|\mathbf{r} - \mathbf{r}'|$ must be approximated more precisely by

$$|\mathbf{r} - \mathbf{r}'| \;=\; \sqrt{r^2 + r'^2 - 2\mathbf{r}\mathbf{r}'} \;\approx\; x \,+\, x_b' \tag{4.25}$$

if the angle between source and observation point is close to 180^0. This happens if the observation point is located close to the positive x-axis—a situation we will consider in the double-slit experiment. The Green's function reads therefore

$$G^{(3)}(\mathbf{r}, \mathbf{r}') \;\approx\; \frac{e^{\,ikx_b'}}{4\pi x_b'} \cdot e^{\,ikx} \;. \tag{4.26}$$

This is nothing but a plane wave traveling along the positive x-axis with an amplitude given by

$$\frac{e^{\,ikx_b'}}{4\pi x_b'} \;. \tag{4.27}$$

The space dependent part of the plane wave (4.22) follows from the integral representation

$$\psi_0(x) \;=\; \int G^{(3)}(\mathbf{r}, \mathbf{r}') \cdot \rho(\mathbf{r}')\, dx'\, dy'\, dz' \;, \tag{4.28}$$

with the approximation (4.26) of the Green's function and the source

$$\rho(x') \;=\; 4\pi x_b'\, e^{\,-ikx_b'}\, E_0 \;\cdot \delta(x' + x_b')\, \delta(y')\, \delta(z') \;. \tag{4.29}$$

4.2 Double-Slit Experiments

4.2.1 Classical Double-Slit Experiment

This experiment was elected in 2002 as one the most beautiful experiments of physics by the "Physics World" journal. It was first accomplished by T. Young in the nineteenth century to demonstrate the wave nature of light. But it plays also a major role in the discussion regarding the epistemological consequences of Quantum Mechanics. Figure 4.4 shows the experimental setup. Two slits with the

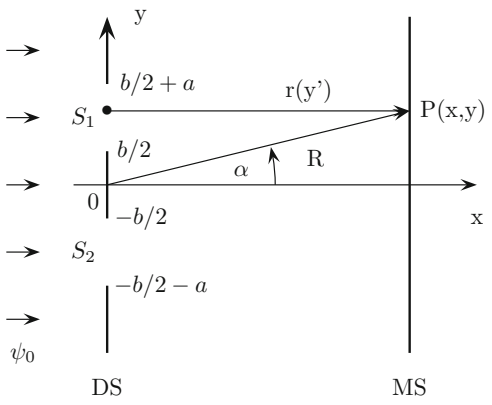

Fig. 4.4 Scattering of a scalar plane wave (ψ_0) perpendicularly incident from the left on a double-slit (DS). The measurement screen (MS) is placed in the far field behind the double-slit. Both slits S_1 and S_2 are symmetrically placed with respect to the x-axis, infinitely extended into the z-direction, and characterized by the same width a

same width a and at a center distance of $a + b$ in an ideal metallic screen are placed symmetrically with respect to the x-axis. The ideal metallic screen itself is stretched across the whole y-z-plane. A scalar plane wave

$$\psi_0(x) \;=\; E_0 \cdot e^{\,ikx} \tag{4.30}$$

is perpendicularly incident on the double-slit from the left. The configuration does not change along the z-direction if the plane wave (4.30) is generated by a line source located along the z-direction on the left-hand side of—but far away from the double slit. This allows us to neglect the z-dependence and to restrict the scattering problem to the x-y-plane only. The ideal metallic screen separates the source region of the incident plane wave generated by the source (4.29) on its left-hand side from the source-free region on its right-hand side. The field in the source-free region on the right-hand side can be calculated from the field distribution in the plane of the screen, according to Huygens' principle (4.21). Within the framework of the Kirchhoff approximation it is assumed that ψ as well as its normal derivative $\partial\psi/\partial\hat{n}'$ are nonzero and identical with the corresponding quantities of the incident plane wave only in the slits. The Kirchhoff approximation is not without controversy and raises the issue of its applicability. A detailed analysis of this aspect can be found in Hönl et al. (1961). It seems intuitively comprehensible from the point of view of the Geometric Optics, i.e., if the slit width a is large compared to the wavelength of the incident field, and if neglecting diffraction effects. On the other hand, we have already mentioned that the two quantities ψ and $\partial\psi/\partial\hat{n}'$ along the ideal metallic screen are not independent of each other and related by an integral equation. The situation becomes even more complicate by the sharp edges of the slits. This requires the formulation of additional edge conditions. These conditions have to take into account that a sharp edge may act as a passive scatterer but not as an additional source of energy. In a rigorous theory the scattering problem becomes only then uniquely solvable. And it can indeed be shown that the Kirchhoff approximation fails near the edges. However, regarding a perpendicularly incident plane wave, and

if only looking for the solution in the far field behind the slits and in near forward direction (i.e., for relatively small angles α) the theoretical results obtained with the Kirchhoff approximation are in good correspondence with the experiments. The following considerations are therefore restricted to this situation but from the point of view of Green's functions. The obtained solution is the well-known Fraunhofer diffraction on a double-slit.

Starting from (4.21) and the Kirchhoff approximation we get the following expression for the field in the source-free region behind the screen:

$$\psi(\mathbf{r}) \;=\; -E_0 \int_{\frac{b}{2}+a}^{-\frac{b}{2}-a} \left[e^{ikx'} \cdot \frac{\partial G^{(3)}(\mathbf{r},\mathbf{r}')}{\partial x'} \;-\; G^{(3)}(\mathbf{r},\mathbf{r}') \cdot \frac{\partial e^{ikx'}}{\partial x'} \right]_{x'=0} dy' \;, \tag{4.31}$$

where $\mathbf{r} = (x, y)$, $R = \sqrt{x^2 + y^2}$, $\mathbf{r}' = (x', y')$,

$$G^{(3)}(\mathbf{r},\mathbf{r}') \;=\; \frac{e^{ikg(x',y')}}{4\pi g(x',y')} \;, \tag{4.32}$$

and

$$g(x',y') \;=\; \sqrt{(x-x')^2 \;+\; (y-y')^2} \;. \tag{4.33}$$

The normal derivative of the Green's function in the far field approximation (the derivation with respect to x') is given by

$$\left[\frac{\partial G^{(3)}(\mathbf{r},\mathbf{r}')}{\partial x'} \right]_{x'=0} \;\approx\; -ik \cdot \frac{e^{ikg(x',y')}}{4\pi R} \;. \tag{4.34}$$

In so doing, it was assumed that $x >> y$ holds. The contribution of the term $1/g^2(x', y')$ was neglected accordingly. $g(x', y') \approx R$ was used to approximate the denominator. Regarding the phase term—in order to consider the y-dependence of the observation point $P(x, y)$ on the measurement screen—$g(x', y')$ is approximated by

$$g(x',y') \;\approx\; R \;-\; \frac{y \cdot y'}{R} \;=\; R \;-\; y' \cdot \sin\alpha \;=\; r(y') \tag{4.35}$$

(see Fig. 4.4). Using these approximations we can decompose (4.31) into the two slit integrals

$$\psi(\alpha) \;=\; \psi_1(\alpha) \;+\; \psi_2(\alpha) \;= f(\alpha) \cdot E_0 \cdot \frac{e^{ikR}}{R} \;=$$

$$\frac{ik}{2\pi} \cdot \left[\int_{b/2}^{b/2+a} e^{-iky' \sin\alpha}\, dy' \;+\; \int_{-b/2-a}^{-b/2} e^{-iky' \sin\alpha}\, dy' \right] \cdot E_0 \cdot \frac{e^{ikR}}{R} \tag{4.36}$$

(see Elmore and Heald (1985), for example), where

$$f(\alpha) \;=\; \frac{ik}{2\pi}\cdot\left[\int_{b/2}^{b/2+a} e^{-iky'\sin\alpha}\,dy' \;+\; \int_{-b/2-a}^{-b/2} e^{-iky'\sin\alpha}\,dy'\right]. \tag{4.37}$$

We will denote this quantity as the α-dependent Fraunhofer approximation of the scattering amplitude of the double-slit. It should also be mentioned at this point that instead of starting with the 3-dim. Green's function $G^{(3)}(\mathbf{r},\mathbf{r}')$ and reducing it to the 2-dim. situation one can also start with the 2-dim. Green's function

$$G^{(2)}(\mathbf{r},\mathbf{r}') \;=\; \frac{i}{4}\cdot H_0^{(1)}(k|\mathbf{r}-\mathbf{r}'|)\,. \tag{4.38}$$

The far field behaviour of the Hankel function produces the same slit integrals. But regarding the dependence on R we then have $e^{ikR}/\sqrt{R}$ instead of e^{ikR}/R, as it must be to fit into the 2-dim. radiation condition. However, the characteristic interference pattern of the intensity of the double-slit in the far field agrees in both cases since it is essentially a consequence of the superposition of the two slit integrals. Introducing the two impressed sources

$$\rho_1(y') = 2\,i\,k\,E_0\cdot H\left(y'-\frac{b}{2}\right)\cdot H\left(\frac{b}{2}+a-y'\right) \tag{4.39}$$

$$\rho_2(y') = 2\,i\,k\,E_0\cdot H\left(-y'-\frac{b}{2}\right)\cdot H\left(\frac{b}{2}+a+y'\right) \tag{4.40}$$

which represent the interaction contributions of the slits allows us moreover to express $\psi(\alpha)$ by our pivotal relation

$$\psi(\alpha) \;=\; \int_{-\infty}^{\infty} G(y,y')\cdot\rho(y')\,dy'\,, \tag{4.41}$$

where we have to use

$$G(y,y') \;=\; \frac{e^{ikr(y')}}{4\pi R} \tag{4.42}$$

with $r(y')$ according to (4.35), and if applying the source

$$\rho(y') \;=\; \rho_1(y') \;+\; \rho_2(y')\,. \tag{4.43}$$

The integrals in (4.37) result in the following contributions of each single slit S_1 and S_2 to the scattering amplitude (4.37):

$$f_1(\alpha) \;=\; \frac{ika}{2\pi}\cdot\frac{\sin\Gamma_a}{\Gamma_a}\cdot e^{-i\,\Gamma_+} \tag{4.44}$$

and

$$f_2(\alpha) \;=\; \frac{ika}{2\pi} \cdot \frac{\sin \Gamma_a}{\Gamma_a} \cdot e^{+i\,\Gamma_+} \;, \tag{4.45}$$

where

$$\Gamma_+ = \Gamma_a \;+\; \Gamma_b \tag{4.46}$$

$$\Gamma_{a/b} = \frac{k \cdot a/b}{2} \cdot \sin\alpha \;. \tag{4.47}$$

The superposition of these two contributions provides finally the scattering amplitude

$$f(\alpha) \;= f_1(\alpha) \;+ f_2(\alpha) \;=\; \frac{ika}{\pi} \cdot \frac{\sin \Gamma_a}{\Gamma_a} \cdot \cos \Gamma_+ \tag{4.48}$$

of the double-slit. The α-dependent intensity of the double-slit is calculated from

$$I_{DS}(\alpha) \;=\; |f(\alpha)|^2 \;. \tag{4.49}$$

We thus get the characteristic expression

$$I_{DS}(\alpha) \;=\; \left(\frac{ka}{\pi}\right)^2 \cdot \frac{\sin^2 \Gamma_a}{\Gamma_a^2} \cdot \cos^2 \Gamma_+ \;=\; 4 \cdot I_S(\alpha) \cdot \cos^2 \Gamma_+ \tag{4.50}$$

for the double-slit, where

$$I_{S_1}(\alpha) \;=\; I_{S_2}(\alpha) \;=\; I_S(\alpha) \;=\; \left(\frac{ka}{2\pi}\right)^2 \cdot \frac{\sin^2 \Gamma_a}{\Gamma_a^2} \tag{4.51}$$

are the corresponding intensities of the single slits. When dealing with plane wave scattering on a spherical object at the end of this chapter we will derive the so-called "optical theorem". It relates the total extinction cross-section—a quantity that is identical with the total scattering cross-section if there is no absorption—to the scattering amplitude in forward direction by the relation

$$\sigma_{ext} \;=\; \frac{4\pi}{k} \cdot Im\{f(0)\} \;. \tag{4.52}$$

This theorem enjoys a quite interesting history (see Newton (1976)) and is of some importance not only in classical physics but also in Quantum Mechanics. We will use it later on to discuss the "extinction paradox". To get a first impression of this paradox already at this point let us apply (4.52) to the scattering amplitudes (4.44)

and (4.48) of the single- and double-slit. This gives

$$\sigma_{ext}^{(S)}(\alpha = 0) \;=\; 2\,a \tag{4.53}$$

and

$$\sigma_{ext}^{(DS)}(\alpha = 0) \;=\; 4\,a\,, \tag{4.54}$$

respectively. It is just twice of the respective geometrical slit width! However, from the point of view of the Geometric Optics (i.e., if the slit width is large compared to the wavelength of the incident plane wave so that this plane wave is replaced by a bundle of noninteracting rays) one would expect that the total extinction- or scattering cross-section equals the geometrical slit width. The total cross-sections, on the other hand, is usually calculated from the integration over all possible scattering angles $\alpha \in [-\pi/2, \pi/2]$. It is therefore questionable to apply (4.44) and (4.48) to this approach since these two expressions have been derived by assuming small angles α only. It takes a less approximate scattering theory to be more accurate. That (4.53) and (4.54) are independent of the wavelength of the incident field and the slit width may serve as an indication that these results must be considered with some caution. But it was quite interesting for me to see that they agree already with what is known from a more rigorous but also more sophisticated theory, as it will be discussed at the very end of this chapter.

Expression (4.51) for the single slit is often used in Quantum Mechanics to discuss the uncertainty relation of position and momentum (see Burkhardt and Leventhal (2008), for example). In so doing, it is assumed that describing scattering of quantum particles on a single slit requires already a fallback to a methodology known from classical wave scattering. Regarding (4.51) the maximum of the intensity is at $\Gamma_a(\alpha = 0) = 0$, and the first minimum is at $\Gamma_a = \pi$. This allows one to determine the uncertainty of the momentum $\triangle p_y$ in y-direction if the wavelength of the incident plane wave determines the momentum of the quantum particle in x-direction before the scattering process according to the de-Broglie relation. The uncertainty of the position $\triangle y$, on the other hand, is identical with the slit width. The angular dependent intensity (4.51) itself—after appropriate normalization—can be interpreted as the probability that a quantum object perpendicularly incident on a single slit will be scattered at an angle of α into the direction of the measurement screen.

But there is another aspect I want to emphasize at this place. Figures similar to the one presented in Fig. 4.5 are frequently utilized in discussions regarding the principle of complementarity or the wave-particle dualism in Quantum Mechanics. I do not want to step into this discussion but to point to a problem that is related to this figure, and that is often ignored in its interpretation. We first note that, while the interference pattern $I_{DS}(\alpha)$ of plane wave scattering on a double-slit is depicted correctly and in agreement with (4.50) this does not holds for the intensity distribution $I_{S_1}(\alpha)$ or $I_{S_2}(\alpha)$ according to (4.51) if one of the two slits is closed.

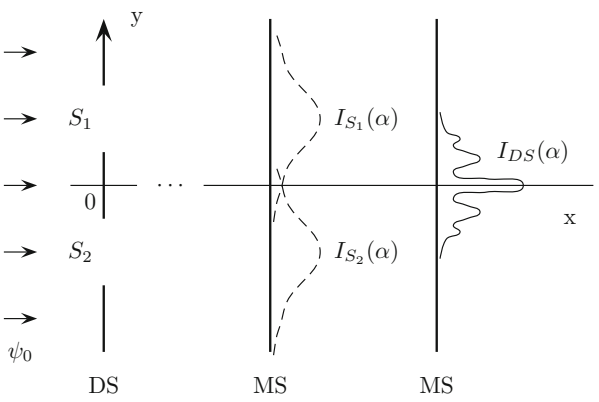

Fig. 4.5 Representation of the results of plane wave- or quantum particle scattering on a double-slit that can frequently be found in the literature. The intensity distribution $I_{DS}(\alpha)$ if both slits are open is correctly depicted. But the intensity distributions $I_{S_1}(\alpha)$ if slit S_2 is closed, and $I_{S_2}(\alpha)$ if slit S_1 is closed are incorrect and not in agreement with (4.51)

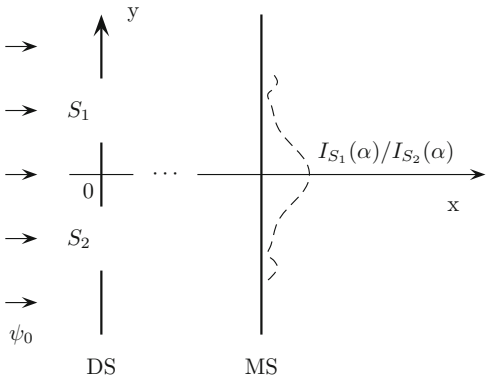

Fig. 4.6 Correct representation of the intensity distributions of plane wave scattering on a single slit according to (4.51), i.e., if either slit S_1 or S_2 is closed in the double-slit experiment

This representation suggests that it would be possible to decide in a corresponding scattering experiment with a primary incident plane wave and by just looking at the intensity distribution on the measurement screen in the far field whether slit S_1 or slit S_2 is closed. But this is impossible as one can see from the expressions (4.44), (4.45), and (4.51). A local shift of a single slit along the y-axis appears in the far field only as a contribution in the phase term Γ_+. It is therefore washed out if calculating the intensity. Its maximum value can always be found in the forward direction at $\alpha = 0$, as represented in Fig. 4.6. That is, from the intensity measurement in the far field we are only able to find out whether two slits were open or if one slit was closed. On the other hand, if using classical particles instead of a plane wave in the double-slit experiment, then we will indeed observe a frequency distribution on the measurement screen that agrees with the intensities represented in Fig. 4.5 if either slit S_1 or S_2 is closed. But now the frequency distribution does not agrees with the intensity distribution for both slits open. That is, now we are able to decide whether slit S_1 or S_2 was closed or if both slits were open. As a consequence we may state that scattering on a single slit will already allow us to distinguish between the particle- or wave nature of the objects used in this experiment. By the way, a first

real double-slit experiment in Quantum Mechanics with electrons was performed in 1961 by C. Jönsson (see Jönsson (1961)). Especially Fig. 7 in this paper shows the typical frequency distribution of the Fraunhofer diffraction.

Exercise: Development of a computer program for the single- and double-slit experiment. Use this program to show that the intensity of the double-slit in forward direction is always 4-times the intensity of the single slit. What happens if the intensities of several double-slits with different slit distances but with the same slit width are averaged? Compare the result of this averaging process with the sum of the intensities of the two single slits! What happens if more and more slits with identical slit width and distances are added? For an initial program see Appendix A.1.

4.2.2 Interaction of a Linearly Polarized Plane Wave with a Polarizing Filter

The following discussion is aimed at a preparation of the description of the modified double-slit experiment that is performed with a linearly polarized plane wave, and that uses polarizing filters to cover the two slits. It can be considered as the classical analog to the quantum eraser. But we will also benefit from the following discussion in the next chapter, when deriving the Green's function that can be related to Bell's experiments. The interaction of a linearly polarized plane wave with a polarizing filter is the only situation where we abandon the restriction to scalar waves. It is our main goal here to demonstrate that

- there is an equivalence between a basis transformation and an interaction that rotates the plane of linear polarization of a plane wave. This issue is re-addressed at the end of this chapter to describe plane wave scattering on a sphere.
- the basis transformation can be described by use of an "intensity operator" that is the classical analog to the statistical operator known from Quantum Mechanics. This intensity operator contains already "negative weights" comparable to the "negative quasi-probabilities" known from Quantum Optics.

A linearly polarized plane wave traveling along the positive x-axis and with an unit amplitude vector oscillating in the plane that forms an angle of 45° with the positive z-axis can be expressed according to

$$|\psi\rangle \;=\; |\psi_1\rangle \;+\; |\psi_2\rangle \;=\; \frac{e^{ikx}}{\sqrt{2}} \cdot |y\rangle \;+\; \frac{e^{ikx}}{\sqrt{2}} \cdot |z\rangle \tag{4.55}$$

by the superposition of two scalar subfields (see Fig. 4.7). The unit vectors $|z\rangle$ and $|y\rangle$ given by

$$|z\rangle = (1, 0) \tag{4.56}$$

$$|y\rangle = (0, 1) \tag{4.57}$$

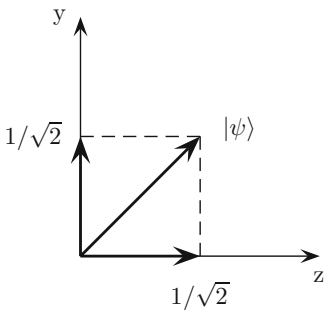

Fig. 4.7 Representation of a linearly polarized plane wave $|\psi\rangle$ as a superposition of two disjoint subfields which are orthogonal among each other

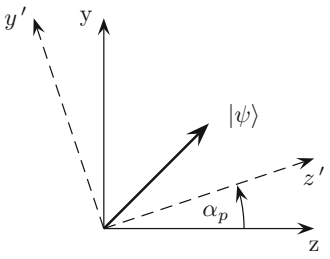

Fig. 4.8 Representation of the field (4.55) if the coordinate system is rotated by an angle α_p

are the basis vectors of the considered coordinate system. The two subfields $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthogonal among each other. Moreover, since they do not contain common basis vectors we will call these subfields being **disjoint**. The intensity of this linearly polarized plane wave is given by the scalar product

$$I = \langle\psi|\psi\rangle = 1 \,. \tag{4.58}$$

It is identical with the sum of the intensities $I_y = I_z = 1/2$ of the subfields. That there is no interference contribution from this superposition is a consequence of the disjoint character of the two subfields. The intensity I_y of the subfield $|\psi_1\rangle = e^{ikx}/\sqrt{2} \cdot |y\rangle$ can be measured by using a polarizing filter with its forward direction in parallel to the y-axis. The intensity I_z of the other subfield can be measured accordingly but not at the same time.

Next, let us rotate the coordinate system by an angle α_p in a mathematical positive sense (see Fig. 4.8). It is then our goal to express the field (4.55) by the new basis vectors $|y'\rangle$ and $|z'\rangle$. To this end, we first note that the new and old basis vectors are related by

$$\begin{pmatrix} |y'\rangle \\ |z'\rangle \end{pmatrix} = \mathbf{R}_{\alpha_p} \cdot \begin{pmatrix} |y\rangle \\ |z\rangle \end{pmatrix} \,, \tag{4.59}$$

where

$$\mathbf{R}_{\alpha_p} = \begin{pmatrix} \cos\alpha_p & -\sin\alpha_p \\ \sin\alpha_p & \cos\alpha_p \end{pmatrix} , \tag{4.60}$$

is the matrix of rotation. Please, note that the elements of the column vectors on the left- and right-hand side of (4.59) are just the new and old basis vectors. We thus have

$$|y'\rangle = (-\sin\alpha_p, \cos\alpha_p) \tag{4.61}$$

$$|z'\rangle = (\cos\alpha_p, \sin\alpha_p) . \tag{4.62}$$

The inverse of this transformation reads

$$\begin{pmatrix} |y\rangle \\ |z\rangle \end{pmatrix} = \mathbf{R}_{\alpha_p}^{-1} \cdot \begin{pmatrix} |y'\rangle \\ |z'\rangle \end{pmatrix} , \tag{4.63}$$

where

$$\mathbf{R}_{\alpha_p}^{-1} = \begin{pmatrix} \cos\alpha_p & \sin\alpha_p \\ -\sin\alpha_p & \cos\alpha_p \end{pmatrix} \tag{4.64}$$

is the inverse of the matrix of rotation. The matrix of rotation is a unitary matrix since

$$\mathbf{R}_{\alpha_p}^{-1} \cdot \mathbf{R}_{\alpha_p} = \mathbf{R}_{\alpha_p}^{tp} \cdot \mathbf{R}_{\alpha_p} = \mathbf{E} \tag{4.65}$$

holds. Applying (4.63) to the subfields of (4.55) results in the new subfields

$$|\psi_1'\rangle = \frac{e^{ikx}}{\sqrt{2}} \cdot \left(\cos\alpha_p \cdot |y'\rangle + \sin\alpha_p \cdot |z'\rangle\right) \tag{4.66}$$

and

$$|\psi_2'\rangle = \frac{e^{ikx}}{\sqrt{2}} \cdot \left(-\sin\alpha_p \cdot |y'\rangle + \cos\alpha_p \cdot |z'\rangle\right) . \tag{4.67}$$

These subfields are still orthogonal among each other but from the same 2-dim. space represented by the basis vectors $|y'\rangle$ and $|z'\rangle$. We will therefore call the new subfields (4.66) and (4.67) being **nondisjoint** because they do have basis vectors in common. The superposition of the new subfields provides the representation

$$|\psi\rangle = \frac{e^{ikx}}{\sqrt{2}} \cdot \left[\left(\cos\alpha_p - \sin\alpha_p\right) \cdot |y'\rangle + \left(\cos\alpha_p + \sin\alpha_p\right) \cdot |z'\rangle\right] \tag{4.68}$$

of (4.55) in the rotated coordinate system. Since $|y'\rangle$ and $|z'\rangle$ are orthogonal unit vectors the total intensity is again given by sum of the intensities of the respective components, i.e., we have

$$I = \langle\psi|\psi\rangle = I_{y'} + I_{z'} = 1 , \tag{4.69}$$

where

$$I_{y'} = \frac{1}{2}\left(1 - 2\cos\alpha_p \sin\alpha_p\right) \tag{4.70}$$

and

$$I_{z'} = \frac{1}{2}\left(1 + 2\cos\alpha_p \sin\alpha_p\right) . \tag{4.71}$$

Please, note the characteristic interference term "$2\cos\alpha_p \sin\alpha_p$" in these expressions that results from the superposition of the contributions from the new basis vectors $|y'\rangle$ and $|z'\rangle$ in (4.66) and (4.67). But the contributions of this interference term are obviously balanced in such a way that the total intensity is preserved.

Next, let us introduce an "intensity operator" $\hat{\mathbf{I}}$ by

$$\hat{\mathbf{I}} := I_0 \cdot \sum_{i=1}^{4} p_i \cdot |\phi_i\rangle\langle\phi_i| \tag{4.72}$$

with weights p_i given by

$$p_1 = p_2 = \frac{1}{2} \tag{4.73}$$

$$p_3 = -p_4 = \cos\alpha_p \cdot \sin\alpha_p , \tag{4.74}$$

the total intensity I_0, and vectors

$$|\phi_1\rangle = \cos\alpha_p \cdot |y'\rangle + \sin\alpha_p \cdot |z'\rangle = c_{y'} \cdot |y'\rangle + c_{z'} \cdot |z'\rangle \tag{4.75}$$

$$|\phi_2\rangle = -\sin\alpha_p \cdot |y'\rangle + \cos\alpha_p \cdot |z'\rangle = d_{y'} \cdot |y'\rangle + d_{z'} \cdot |z'\rangle \tag{4.76}$$

$$|\phi_3\rangle = |z'\rangle \tag{4.77}$$

$$|\phi_4\rangle = |y'\rangle . \tag{4.78}$$

These vectors are normalized to unity,

$$\langle\phi_i|\phi_i\rangle = 1 ; \quad i = 1, \cdots, 4 . \tag{4.79}$$

But only $|\phi_1\rangle$ and $|\phi_2\rangle$ as well as $|\phi_3\rangle$ and $|\phi_4\rangle$ are orthogonal among each other. The sum of the weights gives unity,

$$\sum_{i=1}^{4} p_i \;=\; 1\;. \tag{4.80}$$

Moreover, p_3 and p_4 compensate each other, i.e. we have a negative weight (weight p_4) in (4.72). This expresses the fact that the interference term does not contribute to the total intensity I_0. On the other hand, $|\phi_3\rangle$ and $|\phi_4\rangle$ are responsible for a redistribution of the total intensity to the intensities of the single components according to (4.70) and (4.71). The weights p_3 and p_4 are obtained from the amplitude functions of the vectors $|\phi_1\rangle$ and $|\phi_2\rangle$ in the following way:

$$p_3 = c_{z'} \cdot d_{z'} \tag{4.81}$$

$$p_4 = c_{y'} \cdot d_{y'}\;. \tag{4.82}$$

It is a consequence of the conservation of the total intensity of the field in the original and in the rotated coordinate system. The intensities $I_{y'}$ and $I_{z'}$ of the components can then be calculated from this intensity operator according to

$$I_{y'} = \langle y'|\,\hat{\mathbf{I}}\,|y'\rangle \tag{4.83}$$

$$I_{z'} = \langle z'|\,\hat{\mathbf{I}}\,|z'\rangle\;. \tag{4.84}$$

This is in close analogy to the calculation of probabilities from the statistical operator in Quantum Mechanics.

One may ask why I was going to complicate the simple issue of a coordinate transformation in this way? Simply because I wanted to demonstrate the applicability of a formalism known from Quantum Mechanics to this classical situation. As a consequence of the superposition of the two subfields (4.66) and (4.67) and the resulting interference terms we could observe a negative weight in the intensity operator that can be related to this classical situation. This can be compared to the appearance of "negative quasi-probabilities" known from the Wigner functions and the Glauber-Sudarshan equation in Quantum Optics. Now, let us assume that there is a polarizing filter fixed to the y-axis and with a forward direction in parallel to this axis. After rotating the coordinate system by an angle of α_p about the x-axis we can calculate the intensity behind the filter simply from (4.83). Figure 4.9 shows three different positions. Case (a) results in the intensity $I_{y'} = 1/2$, case (b) in $I_{y'} = 1$, and case (c) in $I_{y'} = 0$. These intensities are obviously asymmetric with respect to the two cases (b) and (c), i.e. with respect to the rotation by $\alpha_p = \pi/4$ or $\alpha_p = -\pi/4$ of the coordinate system with the polarizing filter fixed to the y-axis. On the other hand, if we consider the primary field

$$|\psi\rangle \;=\; |y\rangle \tag{4.85}$$

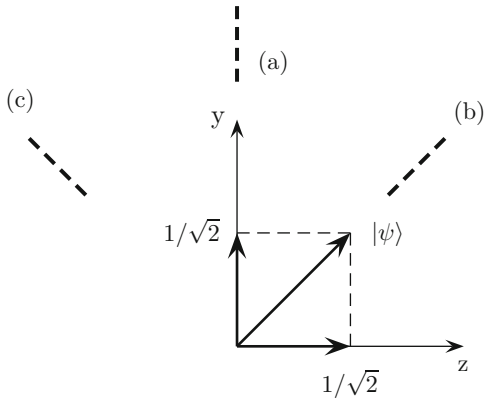

Fig. 4.9 Interaction of the linearly polarized plane wave of Fig. 4.7 with a polarizing filter in three different positions. (**a**): polarizing filter in position $\alpha_p = 0$, (**b**): polarizing filter in position $\alpha_p = -\pi/4$, (**c**): polarizing filter in position $\alpha_p = \pi/4$

the intensity operator becomes simply

$$\hat{\mathbf{I}} = |\phi_1\rangle\langle\phi_1| \,. \tag{4.86}$$

Thus we get the following intensities for the three positions depicted in Fig. 4.9: $I_{y'} = 1$ in case (a), and $I_{y'} = 1/2$ in both the cases (b) and (c). This now symmetric behaviour is due to the fact that (4.85) reads in the rotated coordinate system

$$|\psi\rangle = \cos\alpha_p \cdot |y'\rangle + \sin\alpha_p \cdot |z'\rangle \,. \tag{4.87}$$

The original y-component of the primary field is reduced to $\cos\alpha_p$, and, correspondingly, its intensity reduces to $I_{y'} = \cos^2\alpha_p$. With such measurements we are able to determine the state of linear polarization of the primary field, for example. If the polarizing filter is fixed to the z-axis we can proceed in a similar way by employing (4.84) instead of (4.83). The generalization of the intensity operator to a linearly polarized plane wave $|\psi\rangle$ given in the original coordinate system by

$$|\psi\rangle = \sin\alpha \cdot |y\rangle + \cos\alpha \cdot |z\rangle \tag{4.88}$$

is obtained if replacing the weights (4.73) and (4.74) by the new weights

$$p_1 = \sin^2\alpha \tag{4.89}$$

$$p_2 = \cos^2\alpha \tag{4.90}$$

$$p_3 = -p_4 = 2 \cdot \cos\alpha \cdot \sin\alpha \cdot \cos\alpha_p \cdot \sin\alpha_p \,. \tag{4.91}$$

The weights considered before and (4.86) are special cases of $\alpha = \pi/4$ and $\alpha = \pi/2$. And, moreover, we can state that the following two processes are equivalent with respect to the intensity measurement behind the polarizing filter: We can either rotate the coordinate system by an angle of $+\alpha_p$ while holding the primary field

fixed, or, equivalently, we can actively rotate the plane of polarization of the primary field (4.55) by an angle of $-\alpha_p$ while the coordinate system is fixed. In other words: The rotation of the plane of polarization of a linearly polarized plane wave by a certain interaction process (with $\lambda/2$-wave plates, for example) can be described by a corresponding basis transformation.

To conclude this discussion we will consider the transformation (4.68) of the linearly polarized plane wave (4.55) from a different point of view. We ask for the relation between the new coefficients

$$c_{z'} = \frac{1}{\sqrt{2}} \cdot \left(\cos\alpha_p + \sin\alpha_p\right) \tag{4.92}$$

$$c_{y'} = \frac{1}{\sqrt{2}} \cdot \left(\cos\alpha_p - \sin\alpha_p\right) \tag{4.93}$$

with respect to the basis vectors $|z'\rangle$ and $|y'\rangle$, and the old coefficients

$$c_z = c_y = \frac{1}{\sqrt{2}} \tag{4.94}$$

with respect to the basis vectors $|z\rangle$ and $|y\rangle$. This relation is established by the T-matrix we introduced already in Sect. 2.6. Its elements are again calculated from the scalar products of the old and new unit vectors (4.56)/(4.57) and (4.61)/(4.62) according to

$$\mathbf{T} := \begin{pmatrix} \langle z'|z\rangle & \langle z'|y\rangle \\ \langle y'|z\rangle & \langle y'|y\rangle \end{pmatrix} . \tag{4.95}$$

It is identical with (4.64), i.e., with the inverse of the matrix of rotation. Then we have

$$\begin{pmatrix} c_y \\ c_z \end{pmatrix} = \mathbf{T} \cdot \begin{pmatrix} c_{y'} \\ c_{z'} \end{pmatrix} . \tag{4.96}$$

Calculating

$$\left(c_y, c_z\right) \cdot \begin{pmatrix} c_y \\ c_z \end{pmatrix} = \left(c_{y'}, c_{z'}\right) \cdot \mathbf{T}^{\mathbf{tp}} \cdot \mathbf{T} \cdot \begin{pmatrix} c_{y'} \\ c_{z'} \end{pmatrix} \tag{4.97}$$

we get the relation

$$c_y^2 + c_z^2 = c_{y'}^2 + c_{z'}^2 , \tag{4.98}$$

where we used the unitarity relation (4.65). This is nothing but the expression of the conservation of the total intensity for this transformation. But instead of the T-matrix

we can also introduce the so-called S-matrix

$$\mathbf{S} = \mathbf{E} + 2 \cdot \mathbf{W} . \tag{4.99}$$

The "interaction matrix" $\mathbf{W}$ therein is given by

$$\mathbf{W} = \frac{1}{2} \cdot (\mathbf{T} - \mathbf{E}) . \tag{4.100}$$

In the simple situation considered here the S-matrix is nothing but the T-matrix. It relates also the old and new coefficients according to

$$\begin{pmatrix} c_y \\ c_z \end{pmatrix} = \mathbf{S} \cdot \begin{pmatrix} c_{y'} \\ c_{z'} \end{pmatrix} . \tag{4.101}$$

But the S-matrix is more appropriate if taking up the interaction position, i.e. the position of an active rotation of the primary field (4.55) by an additional mechanism. If the interaction matrix $\mathbf{W}$ vanishes, then there is no additional rotation of the primary plane wave, and the new coefficients are just the old coefficients. We will face all these matrices in more complex situations later on.

4.2.3 *Modified Double-Slit Experiment*

The classical double-slit experiment considered before is now modified as follows (see Fig. 4.10): Slit S_1 is covered with a polarizing filter with its forward direction in parallel to the y-axis. Slit S_2, on the other hand, is covered with a polarizing filter with its forward direction in parallel to the z-axis. The plane of linear polarization of the incident plane wave has a slope of 45° with respect to the positive z-axis,

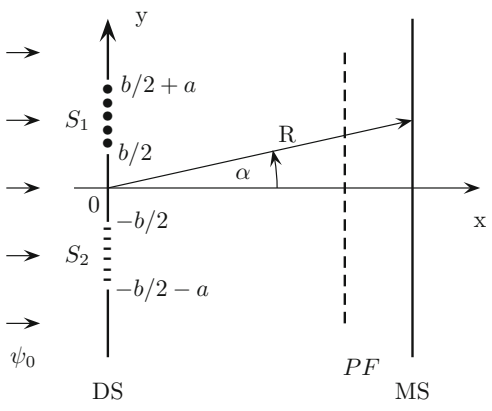

Fig. 4.10 Modified double-slit experiment. Geometry as in Fig. 4.4 but now with two additional polarizing filters masking the two slits. The polarizing filters are oriented perpendicularly to each other

as already shown in Fig. 4.7. As mentioned at the beginning of this section, this modified double-slit experiment makes it necessary to take the polarization of the primary plane wave into account by separating the vectorial problem into two scalar problems. However, in the far field and since looking at the intensity distribution close to the forward direction the results of both these separate problems agree quite well with the scalar result of the Fraunhofer diffraction (see Hönl et al. (1961)). This will allow us to consider the polarization in a quite simple manner. Regarding the above mentioned modification we would therefore get an intensity pattern on the measurement screen in the far field behind the double-slit that corresponds with the intensity pattern caused by a scalar plane wave just interacting with a single slit of width a. This is due to the fact that the subfields behind the slits are disjoint. According to (4.44) and (4.45), these subfields are given in the far field by

$$|\psi_1(\alpha)\rangle \;=\; f_1(\alpha)\,\frac{E_0}{\sqrt{2}}\,\frac{e^{\,ikR}}{R}\cdot|y\rangle \;=\; E_0\,\frac{e^{\,ikR}}{R}\cdot|f_1(\alpha)\rangle \tag{4.102}$$

and

$$|\psi_2(\alpha)\rangle \;=\; f_2(\alpha)\,\frac{E_0}{\sqrt{2}}\,\frac{e^{\,ikR}}{R}\cdot|z\rangle \;=\; E_0\,\frac{e^{\,ikR}}{R}\cdot|f_2(\alpha)\rangle\;. \tag{4.103}$$

Thus we get for the total field

$$|\psi(\alpha)\rangle \;=\; E_0\,\frac{e^{\,ikR}}{R}\cdot\left(|f_1(\alpha)\rangle \;+\; |f_2(\alpha)\rangle\right) \;=\; E_0\,\frac{e^{\,ikR}}{R}\cdot|f(\alpha)\rangle\;. \tag{4.104}$$

The total angularly dependent intensity pattern (4.51) follows immediately from the scalar product $\langle f(\alpha)|f(\alpha)\rangle$, and if taking the orthonormality of the unit vectors $|y\rangle$ and $|z\rangle$ into account.

In the next step, let us place an additional polarizing filter PF between the double-slit and the measurement screen (see Fig. 4.10). If this filter is oriented with its forward direction in parallel to the y-axis the intensity (4.51) is reduced to $I_s(\alpha)/2$. But we know also that only the part of the primary incident plane wave that was traversing slit S_1 is responsible for this intensity pattern. Similarly, if PF is oriented with its forward direction in parallel to the z-axis, the same intensity pattern $I_s(\alpha)/2$ is then produced by the part of the primary incident plane wave that was traversing slit S_2. In this way we have lost the characteristic interference pattern of the double-slit. But the situation changes if we rotate filter PF by an arbitrary angle α_p. To describe the situation behind PF we can use the transformation of the field (4.55) if rotating the coordinate system. In conjunction with (4.63) we get for the amplitude functions

$$|f_1'(\alpha)\rangle \;=\; \frac{ika}{2\pi\sqrt{2}}\cdot\frac{\sin\Gamma_a}{\Gamma_a}\cdot e^{\,-i\,\Gamma_+}\cdot\left(\cos\alpha_p\cdot|y'\rangle \;+\; \sin\alpha_p\cdot|z'\rangle\right) \tag{4.105}$$

and

$$|f_2'(\alpha)\rangle \;=\; \frac{ika}{2\pi\sqrt{2}} \cdot \frac{\sin\Gamma_a}{\Gamma_a} \cdot e^{i\Gamma_+} \cdot \left(-\sin\alpha_p \cdot |y'\rangle \;+\; \cos\alpha_p \cdot |z'\rangle\right) . \tag{4.106}$$

The superposition provides

$$\begin{aligned} |f'(\alpha)\rangle \;=\; \frac{ika}{2\pi\sqrt{2}} \cdot \frac{\sin\Gamma_a}{\Gamma_a} \cdot \Big[&\left(\cos\alpha_p \cdot e^{-i\Gamma_+} \;-\; \sin\alpha_p \cdot e^{i\Gamma_+}\right) \cdot |y'\rangle \\ &+\; \left(\cos\alpha_p \cdot e^{i\Gamma_+} \;+\; \sin\alpha_p \cdot e^{-i\Gamma_+}\right) \cdot |z'\rangle\Big] . \end{aligned} \tag{4.107}$$

Regarding our experiment, from field (4.107) we need only the z'-component since it is in parallel with the forward direction of the filter *PF*. It is therefore given by

$$|f_{z'}(\alpha)\rangle \;=\; \frac{ika}{2\pi\sqrt{2}} \cdot \frac{\sin\Gamma_a}{\Gamma_a} \cdot \left(\cos\alpha_p \cdot e^{i\Gamma_+} \;+\; \sin\alpha_p \cdot e^{-i\Gamma_+}\right) \cdot |z'\rangle . \tag{4.108}$$

If choosing $\alpha_p = 45°$ this becomes

$$|f_{z'}(\alpha)\rangle \;=\; \frac{ika}{2\pi} \cdot \frac{\sin\Gamma_a}{\Gamma_a} \cdot \cos\Gamma_+ \cdot |z'\rangle . \tag{4.109}$$

Calculating the intensity from the scalar product gives

$$\langle f_{z'}(\alpha)|f_{z'}(\alpha)\rangle \;=\; I_S(\alpha) \cdot \cos^2\Gamma_+ . \tag{4.110}$$

This corresponds to the characteristic interference pattern (4.50) of the double-slit with an intensity reduced to $1/4$. With this specific orientation of the polarizing filter *PF* we have "erased" the scattering behaviour of a single slit, so to speak. But we can also observe another well-known effect. If choosing an angle $\alpha_p = -45°$ instead of $\alpha_p = 45°$ of the polarizing filter *PF* we get for the intensity

$$\langle f_{z'}(\alpha)|f_{z'}(\alpha)\rangle \;=\; I_S(\alpha) \cdot \sin^2\Gamma_+ \;=\; I_S(\alpha) \cdot \cos^2\left(\frac{\pi}{2} + \Gamma_+\right) , \tag{4.111}$$

i.e., a shift of $\pi/2$ of the characteristic interference pattern is observed.

4.3 Eigensolutions of the Three-Dimensional Helmholtz Equation in Spherical Coordinates

In preparation for the scattering problem of a scalar plane wave on a spherical object we have to become acquainted with the eigensolutions of the 3-dim. Helmholtz equation and with some of their properties. The relations between the Cartesian and

Table 4.1 Relations between the unit vectors in Cartesian and spherical coordinates

	$\hat{x}$	$\hat{y}$	$\hat{z}$
$\hat{r}$	$\sin\theta\cos\phi$	$\sin\theta\sin\phi$	$\cos\theta$
$\hat{\theta}$	$\cos\theta\cos\phi$	$\cos\theta\sin\phi$	$-\sin\theta$
$\hat{\phi}$	$-\sin\phi$	$\cos\phi$	0

spherical coordinates are given by (3.165). The corresponding relations between the unit vectors of both coordinate systems can be taken from Table 4.1. The homogeneous Helmholtz equation reads

$$\left(\nabla^2 + k^2\right)\psi(k, r, \theta, \phi) \;=\; 0 \tag{4.112}$$

with the Laplace operator given by

$$\nabla^2 \;=\; \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{4.113}$$

in spherical coordinates. The boundary surface element is given by (4.15) if S in Fig. 4.1 is the boundary surface of a sphere with radius $r = a$. The unit vector $\hat{n}$ is in this case identical with the unit vector $\hat{r}$. Application of the Bernoulli ansatz

$$\psi(k, \mathbf{r}) \;=\; \psi(k, r, \theta, \phi) \;=\; R(r)\cdot\Theta(\theta)\cdot\Phi(\phi) \tag{4.114}$$

for the unknown function $\psi(r, \theta, \phi)$ results in a separation of the Helmholtz equation in spherical coordinates. Using (4.114) in (4.112), and if introducing the at first arbitrary separation constants α and β converts the original Helmholtz equation into the three ordinary differential equations

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\beta}{r^2}\right] r\cdot R(r) = 0 \tag{4.115}$$

$$\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right) + \beta - \frac{\alpha}{\sin^2\theta}\right]\Theta(\theta) = 0 \tag{4.116}$$

$$\left[\frac{d^2}{d\phi^2} + \alpha\right]\Phi(\phi) = 0\,. \tag{4.117}$$

of second order. Each of these ordinary differential equations provides two linearly independent solutions. But regarding the scattering problem we are only interested in the following eigensolutions:

$$\zeta_{l,n}(k, \mathbf{r}) = j_n(kr)\cdot Y_{l,n}(\theta, \phi) \tag{4.118}$$

$$\varphi_{l,n}(k, \mathbf{r}) = h_n^{(1)}(kr)\cdot Y_{l,n}(\theta, \phi) \tag{4.119}$$

$$\chi_{l,n}(k, \mathbf{r}) = h_n^{(2)}(kr)\cdot Y_{l,n}(\theta, \phi)\;. \tag{4.120}$$

$Y_{l,n}(\theta,\phi)$ are the spherical harmonics

$$Y_{l,n}(\theta,\phi) := \sqrt{\frac{2n+1}{4\pi}\frac{(n-l)!}{(n+l)!}} \cdot P_n^l(\cos\theta)\, e^{il\phi} \tag{4.121}$$

normalized to unity. They obey the orthogonality relation

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta\; Y^*_{l',n'}(\theta,\phi)\, Y_{l,n}(\theta,\phi) \;=\; \delta_{ll'}\delta_{nn'} \tag{4.122}$$

as well as the following relations:

$$Y^*_{l,n}(\theta,\phi) \;=\; (-1)^l \cdot Y_{-l,n}(\theta,\phi) \tag{4.123}$$

and

$$Y_{l,n}(\pi-\theta,\phi\pm\pi) \;=\; (-1)^n \cdot Y_{l,n}(\theta,\phi)\;. \tag{4.124}$$

$Y^*_{l,n}$ denotes the conjugate-complex of $Y_{l,n}$. The completeness relation is given by

$$\sum_{n=0}^{\infty}\sum_{l=-n}^{n} Y^*_{l,n}(\theta,\phi)\cdot Y_{l,n}(\theta',\phi') \;=\; \delta(\cos\theta-\cos\theta')\cdot\delta(\phi-\phi')\;. \tag{4.125}$$

Index n is restricted to the natural numbers $n = 0, 1, 2, \ldots \infty$, and index l takes the integer numbers $l = -n, -n+1, \ldots, n-1, n$. These indices are related to the separation constants α and β by $n(n+1) = \beta$ and $l^2 = \alpha$. j_n in (4.118), $h_n^{(1)}$ in (4.119), and $h_n^{(2)}$ in (4.120) are the spherical Bessel functions, the spherical Hankel functions of first kind, and the spherical Hankel functions of second kind, respectively. All these functions are possible solutions of equation (4.115) and are related to the corresponding functions with fractional orders according to

$$j_n(kr) = \sqrt{\frac{\pi}{2kr}} \cdot J_{n+1/2}(kr) \tag{4.126}$$

$$h_n^{(1)}(kr) = \sqrt{\frac{\pi}{2kr}} \cdot H^{(1)}_{n+1/2}(kr) \tag{4.127}$$

$$h_n^{(2)}(kr) = \sqrt{\frac{\pi}{2kr}} \cdot H^{(2)}_{n+1/2}(kr)\;. \tag{4.128}$$

The functions $P_n^l(\cos\theta)$ in (4.121) are the associated Legendre polynomials. They form one of the two linearly independent solutions of the ordinary differential equation (4.116). At the elevation angles $\theta = 0$ and $\theta = \pi$ they fulfil the

homogeneous von Neumann condition if $l = 0$ and the homogeneous Dirichlet condition if $l \neq 0$:

$$\frac{d}{d\theta}P_n^l(1) = \frac{d}{d\theta}P_n^l(-1) = 0\,; \quad l = 0 \tag{4.129}$$

$$P_n^l(1) = P_n^l(-1) = 0\,; \quad l \neq 0\,. \tag{4.130}$$

These functions are moreover orthogonal, i.e.,

$$\int_0^\pi d\theta \sin\theta \cdot P_n^l(\cos\theta)\, P_{n'}^l(\cos\theta) = \frac{2}{2n+1}\frac{(n+l)!}{(n-l)!}\cdot\delta_{nn'} \tag{4.131}$$

holds.

$$P_n^{-l}(\cos\theta) = (-1)^l \cdot \frac{(n-l)!}{(n+l)!}\cdot P_n^l(\cos\theta) \tag{4.132}$$

is the relation between the associated Legendre polynomials with positive and negative index l. The associated Legendre polynomials may be calculated from the conventional Legendre polynomials $P_n(x)$ by use of the relation

$$P_n^l(x) = (-1)^l \cdot (1-x^2)^{l/2} \cdot \frac{d^l P_n(x)}{dx^l} \tag{4.133}$$

and with $P_n(x)$ given by

$$P_n(x) = \frac{1}{2^n n!}\left(\frac{d}{dx}\right)^n (x^2-1)^n\,. \tag{4.134}$$

The functions $e^{il\phi}$ are the solutions the ordinary differential equation (4.117). They are periodic functions with respect to 2π,

$$\Phi(\phi) = \Phi(\phi + 2\pi)\,, \tag{4.135}$$

and comply with the orthogonality relation

$$\int_0^{2\pi} d\phi e^{il\phi} e^{-il'\phi} = 2\pi\delta_{ll'}\,. \tag{4.136}$$

Regarding the scattering solution outside the spherical object we require the fulfillment of Sommerfeld's radiation condition (3.291). A closer look at the

asymptotic behaviour

$$\lim_{r\to\infty} j_n(kr) = \frac{1}{kr}\cdot\sin\left[kr-\frac{n\,\pi}{2}\right] \tag{4.137}$$

$$\lim_{r\to\infty} h_n^{(1)}(kr) = (-i)^{n+1}\cdot\frac{e^{ikr}}{kr} \tag{4.138}$$

$$\lim_{r\to\infty} h_n^{(2)}(kr) = (i)^{n+1}\cdot\frac{e^{-ikr}}{kr} \tag{4.139}$$

of the Bessel- and Hankel functions for large arguments reveals that only the Hankel functions $h_n^{(1)}$ of the first kind are in accordance with this radiation condition. The functions $\varphi_{l,n}(r,\theta,\phi)$ of (4.119) are therefore called "radiating functions" or "radiating solutions" of the Helmholtz equation. However, these functions possess a singularity in the origin of the coordinate system. The functions $\zeta_{l,n}(r,\theta,\phi)$ of (4.118) are the only functions which are regular in this point. The remaining functions $\chi_{l,n}(r,\theta,\phi)$ in (4.120) are called the "incoming solutions". Both types of Hankel functions can be expressed by the combination

$$h_n^{(1)}(kr) \;=\; j_n(kr) \;+\; iy_n(kr) \tag{4.140}$$

$$h_n^{(2)}(kr) \;=\; j_n(kr) \;-\; iy_n(kr) \tag{4.141}$$

of the Bessel and Neumann functions. The Neumann functions $y_n(kr)$ are also possible solutions of the ordinary differential equation (4.115). The regular solutions (4.118) can be described by a superposition of the radiating- and incoming solution according to

$$\zeta_{l,n}(k,\mathbf{r}) \;=\; \frac{1}{2}\cdot\left[\varphi_{l,n}(k,\mathbf{r}) \;+\; \chi_{l,n}(k,\mathbf{r})\right]\;. \tag{4.142}$$

If k in the Helmholtz equation is a real-valued parameter (and only this case is of our interest here and related to nonabsorbing materials), then the Bessel- and Neumann functions are also real-valued quantities. For later purposes we additionally introduce the functions

$$\tilde{\varphi}_{l,n}(k,\mathbf{r}) \;:=\; (-1)^l\cdot\varphi_{-l,n}(k,\mathbf{r}) \tag{4.143}$$

$$\tilde{\chi}_{l,n}(k,\mathbf{r}) \;:=\; (-1)^l\cdot\chi_{-l,n}(k,\mathbf{r})\;. \tag{4.144}$$

$$\tilde{\zeta}_{l,n}(k,\mathbf{r}) \;:=\; (-1)^l\cdot\zeta_{-l,n}(k,\mathbf{r})\;, \tag{4.145}$$

where

$$\tilde{\zeta}_{l,n}(k,\mathbf{r}) \;=\; \zeta_{l,n}^{*}(k,\mathbf{r}) \tag{4.146}$$

holds for a real-valued parameter k.

Using these eigenfunctions will allow us to approximate a function $\psi(k, \mathbf{r})$ by the finite series expansion

$$\psi^{(N)}(k, \mathbf{r}) = \sum_{n=0}^{N} \sum_{l=-n}^{n} a_{l,n}^{(N)} \cdot \varphi_{l,n}(k, \mathbf{r}) \tag{4.147}$$

or by

$$\psi^{(N)}(k, \mathbf{r}) = \sum_{n=0}^{N} \sum_{l=-n}^{n} \tilde{a}_{l,n}^{(N)} \cdot \zeta_{l,n}(k, \mathbf{r}) \tag{4.148}$$

depending on whether the radiation condition or the regularity requirement must be fulfilled by this function. Two examples of such an expansion are of special importance for the scattering problem considered in what follows:

$$\psi_0(k, \mathbf{r}) = E_0 \cdot e^{ikr\cos\theta} \tag{4.149}$$

represents a scalar plane wave $E_0 \cdot e^{ikz}$ in spherical coordinates traveling along the positive z-axis of the Cartesian coordinate system. This plane wave can be approximated by the series expansion

$$\psi_0(k, \mathbf{r}) \approx E_0 \sum_{n=0}^{N} \sum_{l=-n}^{n} c_{l,n} \cdot \zeta_{l,n}(k, \mathbf{r}) \tag{4.150}$$

with expansion coefficients $c_{l,n}$ given by

$$c_{l,n} = \delta_{0l} \cdot i^n \cdot \sqrt{4\pi(2n+1)} \tag{4.151}$$

(see Sommerfeld (1949), for example). Please, note that these coefficients are final (i.e., they are independent of the truncation parameter N), and that only $l = 0$ provides a contribution to this expansion. The second example is the bilinear expansion

$$G^{(3)}(\mathbf{r}, \mathbf{r}') \approx i\,k \cdot \sum_{n=0}^{N} \sum_{l=-n}^{n} \begin{cases} \varphi_{l,n}(k, \mathbf{r}) \cdot \tilde{\zeta}_{l,n}(k, \mathbf{r}') \; ; \; r > r' \\ \\ \zeta_{l,n}(k, \mathbf{r}) \cdot \tilde{\varphi}_{l,n}(k, \mathbf{r}') \; ; \; r < r' \; . \end{cases} \tag{4.152}$$

known for the free-space Green's function (3.297) of the 3-dim. Helmholtz equation (see Morse and Feshbach (1953), for example). For the sake of brevity let us

introduce the shorter notation

$$G^{>}(\mathbf{r},\mathbf{r}') = i\,k\cdot\sum_{n=0}^{N}\sum_{l=-n}^{n}\varphi_{l,n}(k,\mathbf{r})\cdot\tilde{\zeta}_{l,n}(k,\mathbf{r}') \tag{4.153}$$

$$G^{<}(\mathbf{r},\mathbf{r}') = i\,k\cdot\sum_{n=0}^{N}\sum_{l=-n}^{n}\zeta_{l,n}(k,\mathbf{r})\cdot\tilde{\varphi}_{l,n}(k,\mathbf{r}') \tag{4.154}$$

for the upper and lower row of this bilinear expansion. A similar splitting of the Green's function was already applied in (3.117) and (3.121) in conjunction with the d'Alembert solution on a fixed boundary.

Starting from the assumption that $r < r'$ holds we should be able to derive the approximation (4.150) with expansion coefficients (4.151) by use of our pivotal integral relation (4.28) and an appropriate source. In spherical coordinates (4.28) reads

$$\psi_0(k,\mathbf{r}) \;=\; \int_0^{\infty}(r')^2dr'\int_0^{\pi}\sin\theta'd\theta'\int_0^{2\pi}d\phi'\;G^{<}(\mathbf{r},\mathbf{r}')\cdot\rho(k,\mathbf{r}')\;. \tag{4.155}$$

Now, if using (4.154) and the source

$$\rho(k,\mathbf{r}') \;=\; 2\,E_0\cdot\frac{e^{-ikr'_q}}{r'_q}\cdot\delta_{0,l}\cdot\delta_{\theta'}(\theta'-\pi)\cdot\delta(r'-r'_q) \tag{4.156}$$

we get

$$\psi_0(k,\mathbf{r}) \;=\; i\,k\,E_0\,r'_q\,e^{-ikr'_q}\cdot\sum_{n=0}^{N}\sqrt{4\pi(2n+1)}\cdot h_n^{(1)}(k\,r'_q)\cdot(-1)^n\cdot\zeta_{0,n}(k,\mathbf{r})\;. \tag{4.157}$$

This source describes a unit source that is located on the negative z-axis since only $\theta' = \pi$ provides a nonvanishing contribution. Next, if increasing r'_q up to infinity (i.e., if shifting the unit source along the negative z-axis toward the far field), the asymptotic expression (4.138) can be used for the Hankel function $h_n^{(1)}(k\,r'_q)$. This gives

$$\psi_0(k,\mathbf{r}) \;=\; E_0\cdot\sum_{n=0}^{N}\sqrt{4\pi(2n+1)}\cdot i^n\cdot\zeta_{0,n}(k,\mathbf{r}) \tag{4.158}$$

and corresponds indeed with (4.150)/(4.151).

It is sometimes more useful to write down the series expansions (4.147) and (4.148) in a more compact form with only one summation index. This can be accomplished with the index i (that must not be confused with the imaginary unit)

Table 4.2 Relation between the combined summation index i and the original indices n and l

i	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	⋯
n	0	1	1	1	2	2	2	2	2	3	3	3	3	3	3	3	⋯
l	0	−1	0	1	−2	−1	0	1	2	−3	−2	−1	0	1	2	3	⋯

that combines the two indices n and l according to

$$i \;=\; n(n+1)+l\,. \tag{4.159}$$

Table 4.2 illustrates the relation (4.159) explicitly. Using this index we can rewrite (4.147) and (4.148) into

$$\psi^{(N)}(k,\mathbf{r}) \;=\; \sum_{i=0}^{N} a_i^{(N)} \cdot \varphi_i(k,\mathbf{r}) \tag{4.160}$$

and

$$\psi^{(N)}(k,\mathbf{r}) \;=\; \sum_{i=0}^{N} \tilde{a}_i^{(N)} \cdot \zeta_i(k,\mathbf{r})\,. \tag{4.161}$$

The two indices n and l can conversely be recalculated from the relations

$$n(i) = nint\left[\frac{1}{2}\left(-1+\sqrt{1+4i}\right)\right] \tag{4.162}$$

$$l(i) = i - n(i)\cdot[n(i)+1] \tag{4.163}$$

with $nint(a)$ being the integer number closest to the real number a. Equation (4.162) can be inferred from the solution of (4.159) if $l = 0$. Next, if $n(i)$ has been determined for a given i, then (4.163) provides the corresponding $l(i)$ in a unique way.

And, finally, the following orthogonality relations for the eigensolutions $\varphi_i(a,\theta,\phi)$ and $\zeta_i(a,\theta,\phi)$ on the surface of a sphere with radius $r = a$ are of importance for our purposes:

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta a^2 \sin\theta\; \varphi_i^*(a,\theta,\phi)\cdot\varphi_j(a,\theta,\phi) \;=\; a^2\cdot c_i^{(\varphi,\varphi)}\cdot\delta_{ij} \tag{4.164}$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta a^2 \sin\theta\; \varphi_i^*(a,\theta,\phi)\cdot\zeta_j(a,\theta,\phi) \;=\; a^2\cdot c_i^{(\varphi,\zeta)}\cdot\delta_{ij} \tag{4.165}$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta a^2 \sin\theta \; \zeta_i^*(a,\theta,\phi) \cdot \zeta_j(a,\theta,\phi) \; = \; a^2 \cdot c_i^{(\zeta,\zeta)} \cdot \delta_{ij} \tag{4.166}$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta a^2 \sin\theta \; \zeta_i^*(a,\theta,\phi) \cdot \varphi_j(a,\theta,\phi) \; = \; a^2 \cdot c_i^{(\zeta,\varphi)} \cdot \delta_{ij} \; . \tag{4.167}$$

The normalization constants c_i therein are given by the expressions

$$c_i^{(\varphi,\varphi)} = \left(h_{n(i)}^{(1)}(ka)\right)^* \cdot h_{n(i)}^{(1)}(ka) \tag{4.168}$$

$$c_i^{(\varphi,\zeta)} = \left(h_{n(i)}^{(1)}(ka)\right)^* \cdot j_{n(i)}(ka) \tag{4.169}$$

$$c_i^{(\zeta,\zeta)} = j_{n(i)}^*(ka) \cdot j_{n(i)}(ka) \tag{4.170}$$

$$c_i^{(\zeta,\varphi)} = j_{n(i)}^*(ka) \cdot h_{n(i)}^{(1)}(ka) \; . \tag{4.171}$$

4.4 Scattering on a Sphere

4.4.1 Green's Function, Interaction Matrix, and T-Matrix

Now we are prepared to solve the following scattering problem: ψ denotes the total field in region Γ outside a spherical obstacle with boundary surface S. Due to the linearity of the Helmholtz equation the total field is represented by the sum of a primary incident field ψ_0 and a scattered field ψ_s, as given in Eq. (4.3). The latter is generated by the interaction of the primary incident field with the spherical obstacle. The origin of the coordinate system is assumed to be identical with the center of the spherical scatterer. The primary incident field is a solution of the inhomogeneous Helmholtz equation (4.1) with $\rho(\mathbf{r})$ being an impressed source that generates a plane wave. Regarding the total field we require the fulfillment of the homogeneous Dirichlet condition (4.7) at the spherical surface S. The inhomogeneous Dirichlet condition

$$\psi_s(\mathbf{r}) \; = \; -\psi_0(\mathbf{r}) \quad ; \; \mathbf{r} \in S \tag{4.172}$$

may be used alternatively for the scattered field which is a solution of the homogeneous Helmholtz equation subject to the radiation condition. If the impressed source of the primary incident field is located at a finite distance from the scatterer, then the radiation condition must be required for the total field. This scattering problem is uniquely solvable. For example, if ψ_0 is known we can first use the integral equation (4.19) to determine the induced surface current j_s. The total field outside the sphere may then be calculated from (4.20). But we will choose a different

approach in what follows by relating a Green's function—let us denote it with G_Γ—to this scattering problem. $G_\Gamma(\mathbf{r},\mathbf{r}')$ is only defined in Γ. It is a solution of the inhomogeneous Helmholtz equation

$$(\nabla^2 + k^2)\, G_\Gamma(\mathbf{r},\mathbf{r}') \;=\; -\,\delta(\mathbf{r}-\mathbf{r}')\;. \tag{4.173}$$

subject to the radiation condition (3.291) and the homogeneous Dirichlet condition

$$G_\Gamma(\mathbf{r},\mathbf{r}') \;=\; 0 \quad ;\; \mathbf{r}\in S \tag{4.174}$$

at the surface of the spherical scatterer. Using this Green's function together with the scattering problem defined before in (4.5) results once more in our pivotal integral relation

$$\psi(\mathbf{r}) \;=\; \int_\Gamma G_\Gamma(\mathbf{r},\mathbf{r}')\cdot\rho(\mathbf{r}')\,dV(\mathbf{r}') \tag{4.175}$$

for the total field in region Γ outside the spherical scatterer. To determine G_Γ we choose the following *ansatz*:

$$\begin{aligned} G_\Gamma(\mathbf{r},\mathbf{r}') \;=\; G^{(3)}(\mathbf{r},\mathbf{r}') \;+\; G_s(\mathbf{r},\mathbf{r}') \;=\; G^{(3)}(\mathbf{r},\mathbf{r}') \;+\; \\ \oint_S G^{>}(\mathbf{r},\bar{\mathbf{r}})\cdot W_S(\bar{\mathbf{r}},\tilde{\mathbf{r}})\cdot G^{<}(\tilde{\mathbf{r}},\mathbf{r}')\,dS(\bar{\mathbf{r}})\,dS(\tilde{\mathbf{r}})\;. \end{aligned} \tag{4.176}$$

The second term on the right-hand side represents the scattering contribution and should be perceived as the defining equation for the so far unknown "interaction operator" W_S. $G^{(3)}$, on the other hand, represents the free-space Green's function (3.297). The Green's functions $G^{>}$ and $G^{<}$ in the surface integral are the respective contributions of the free-space Green's function according to (4.152)–(4.154). The upper symbols ">" and "<" indicate that $\mathbf{r} > \bar{\mathbf{r}}$ and $\tilde{\mathbf{r}} < \mathbf{r}'$ hold generally in Γ. Using (4.153) and (4.154) in *ansatz* (4.176) gives

$$G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}') \;=\; G^{(3)}(\mathbf{r},\mathbf{r}') \;+\; i\,k\cdot\sum_{i,k=0}^{N}\,[W_S]_{i,k}\cdot\varphi_i(k,\mathbf{r})\cdot\tilde{\varphi}_k(k,\mathbf{r}')\;, \tag{4.177}$$

where $[W_S]_{i,k}$ are the still unknown matrix elements of the interaction operator defined by the surface integral

$$[W_S]_{i,k} \;:=\; i\,k\cdot\oint_S \tilde{\zeta}_i(k,\bar{\mathbf{r}})\cdot W_S(\bar{\mathbf{r}},\tilde{\mathbf{r}})\cdot\zeta_k(k,\tilde{\mathbf{r}})\,dS(\bar{\mathbf{r}})\,dS(\tilde{\mathbf{r}}) \tag{4.178}$$

(please, note again that the imaginary unit "i" and wavenumber "k" in front of the integral must not be confused with the indices "i" and "k" of the summation). The thus approximated Green's function $G_\Gamma^{(N)}$ is a solution of the inhomogeneous

Helmholtz equation (4.173) subject to Sommerfeld's radiation condition. The unknown matrix elements of the interaction operator can now be determined by application of the additional condition (4.174). Using (4.177) in (4.174), shifting the observation point $\mathbf{r}$ toward the spherical surface S, and if replacing w.l.o.g. $G^{(3)}$ in (4.177) by $G^{<}(\mathbf{r}, \mathbf{r}')$ results in the equation

$$-\sum_{i,k=0}^{N} [W_S]_{i,k} \cdot \varphi_i(a,\theta,\phi) \cdot \tilde{\varphi}_k(k,\mathbf{r}') = \sum_{k=0}^{N} \zeta_k(a,\theta,\phi) \cdot \tilde{\varphi}_k(k,\mathbf{r}') \; . \tag{4.179}$$

This equation describes the interaction of an at first arbitrary, primary incident field ψ_0 with an ideal metallic or acoustically soft sphere on the level of Green's functions.

The countably infinite number of functions $\zeta_i(a,\theta,\phi)$ and $\varphi_i(a,\theta,\phi)$ form an orthogonal and even a complete system in a normed function space with a scalar product defined by

$$\langle f|g\rangle := \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \, a^2 \, \sin\theta \, f^*(a,\theta,\phi) \cdot g(a,\theta,\phi) \; . \tag{4.180}$$

$f(a,\theta,\phi)$ and $g(a,\theta,\phi)$ are any two functions on the spherical surface. To simplify the calculation of the matrix elements of the interaction operator from (4.179) let us make the following arrangement: $\vec{\zeta}(a,\theta,\phi)$ denotes a $(N+1)$-dimensional vector with functions $\zeta_i(a,\theta,\phi)$, $i = 0,\cdots,N$ as its components. Correspondingly, $\vec{\varphi}(a,\theta,\phi)$ represents a $(N+1)$-dimensional vector with functions $\varphi_i(a,\theta,\phi)$, $i = 0,\cdots,N$ as its components. Using the matrix-vector notation, expression "$-\sum_{i=0}^{N} [W_S]_{i,k} \cdot \varphi_i(a,\theta,\phi)$" on the left-hand side of (4.179) can then be rewritten into

$$\vec{f}^{\,tp}(a,\theta,\phi) = -\sum_{i=0}^{N} [W_S]_{i,k} \cdot \varphi_i(a,\theta,\phi) = -\mathbf{W_S^{tp}} \cdot \vec{\varphi}^{\,tp}(a,\theta,\phi) \tag{4.181}$$

or

$$\vec{f}(a,\theta,\phi) = -\vec{\varphi}(a,\theta,\phi) \cdot \mathbf{W_S} \tag{4.182}$$

with $\mathbf{W_S}$ representing the interaction matrix with elements $[W_S]_{i,k}$. Dyadic multiplication of this expression from the left by the column vector $\vec{\zeta}^*(a,\theta,\phi)$ and subsequent integration according to (4.180) results in

$$\mathbf{W_S} = -\mathbf{A^{-1}} \cdot \mathbf{B} \; , \tag{4.183}$$

where the elements of the two matrices **A** and **B** are given by the scalar products

$$[A]_{i,k} = \langle \zeta_i(a,\theta,\phi) | \varphi_k(a,\theta,\phi) \rangle \tag{4.184}$$

$$[B]_{i,k} = \langle \zeta_i(a,\theta,\phi) | f_k(a,\theta,\phi) \rangle \ . \tag{4.185}$$

Equation (4.179) is obviously fulfilled if

$$\vec{f}(a,\theta,\phi) = \vec{\zeta}(a,\theta,\phi) \ . \tag{4.186}$$

Performing the corresponding replacement in matrix **B** we then have

$$[B]_{i,k} = \langle \zeta_i(a,\theta,\phi) | \zeta_k(a,\theta,\phi) \rangle \ . \tag{4.187}$$

Since matrix **A** is already known we are now able to calculate the interaction matrix. Taking the orthogonality relations (4.166) and (4.167) into account we get

$$[A]_{i,k} = \delta_{i,k} \cdot \frac{1}{a^2} \cdot j^*_{n(i)}(ka) \cdot h^{(1)}_{n(i)}(ka) \tag{4.188}$$

and

$$[B]_{i,k} = \delta_{i,k} \cdot \frac{1}{a^2} \cdot j^*_{n(i)}(ka) \cdot j_{n(i)}(ka) \ . \tag{4.189}$$

And, finally, we end up with the Green's function

$$G^{(N)}_{\Gamma}(\mathbf{r},\mathbf{r}') = G^{(3)}(\mathbf{r},\mathbf{r}') - i\,k \cdot \sum_{i=0}^{N} \frac{j_{n(i)}(ka)}{h^{(1)}_{n(i)}(ka)} \cdot \varphi_i(k,\mathbf{r}) \cdot \tilde{\varphi}_i(k,\mathbf{r}') \ . \tag{4.190}$$

Please, note again that we have to differ between the imaginary unit "i" in front of the sum and the combined summation index "i" !

To test Reciprocity if interchanging $\mathbf{r}$ and $\mathbf{r}'$ in (4.190) it is sufficient to look at the scattering part $G^{(N)}_s(\mathbf{r},\mathbf{r}')$ on the right-hand side. Regarding the free-space Green's function $G^{(3)}(\mathbf{r},\mathbf{r}')$ we know already the fulfillment of this condition. To this end, let us resolve the summation on the right-hand side of (4.190) according to

$$G^{(N)}_s(\mathbf{r},\mathbf{r}') = -i\,k \cdot \sum_{l=-n}^{n} \sum_{n=0}^{n_{max}} \frac{j_n(ka)}{h^{(1)}_n(ka)} \cdot \varphi_{l,n}(k,\mathbf{r}) \cdot (-1)^l \cdot \varphi_{-l,n}(k,\mathbf{r}') \tag{4.191}$$

by taking (4.143) into account. We then replace the summation index l by $-l$. This is nothing but a rearrangement of the initial summation. This gives

$$G_s^{(N)}(\mathbf{r},\mathbf{r}') = -ik \cdot \sum_{l=-n}^{n} \sum_{n=0}^{n_{max}} \frac{j_n(ka)}{h_n^{(1)}(ka)} \cdot \varphi_{-l,n}(k,\mathbf{r}) \cdot (-1)^l \cdot \varphi_{l,n}(k,\mathbf{r}') = G_s^{(N)}(\mathbf{r}',\mathbf{r}) \tag{4.192}$$

which proves Reciprocity. Regarding scattering on a spherical obstacle Reciprocity holds obviously for any single expansion term in the derived approximation of the corresponding Green's function. This is a consequence of the fact that the interaction matrix $\mathbf{W_S}$ is a diagonal matrix for this special geometry. For plane wave scattering on a spherical scatterer it is clear from the very beginning that interchanging source and observation point does not results in a different scattering configuration. But this becomes less obvious for a nonspherical geometry of the scatterer. In this case the interaction matrix $\mathbf{W_S}$ becomes a full matrix, and Reciprocity can be tested only numerically. A possible test configuration for a spheroidal particle is shown in Fig. 4.11. Similar configurations represent appropriate criteria to estimate the accuracy of scattering results for a nonspherical scatterer obtained with a certain numerical method, as demonstrated with several examples in Rother and Kahnert (2013), especially in Chap. 8 therein.

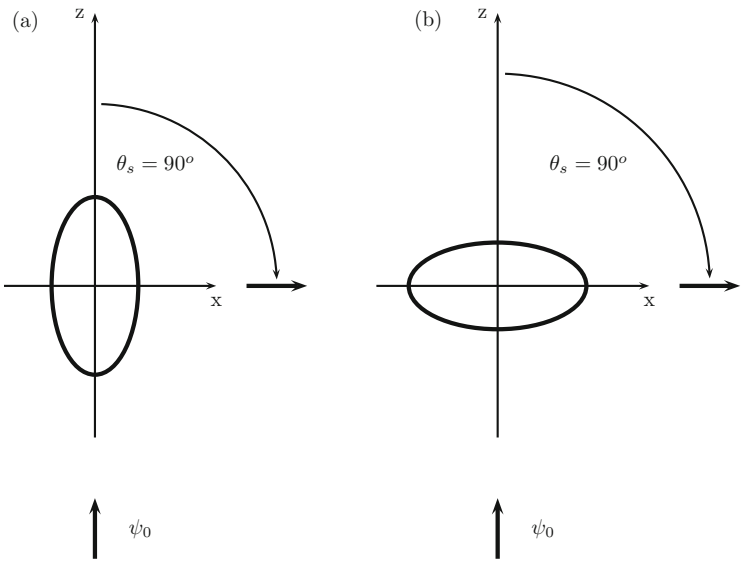

Fig. 4.11 Configuration of a numerical or experimental test of the Reciprocity if a spheroidal scatterer in two different orientations is considered. Both orientations must provide the same differential scattering cross-section at a scattering angle of $\theta_s = 90°$

Using (4.190) in (4.175) provides the scattering solution in a form that represents an alternative to expression (4.20), as already mentioned subsequent to the latter. It makes therefore sense to consider (4.20) as the "source picture" and (4.175)/(4.190) as the "interaction picture" of scattering. Although both pictures should provide identical results they may differ considerably in their numerical realization. A more detailed consideration of the differences between both pictures can again be found in Rother and Kahnert (2013), Chap. 5 therein. Here we will mention only one aspect in this context. Regarding the above discussed interaction formulation there exist a straightforward way to treat scattering on obstacles with only a slight deviation from a spherical geometry.

To this end, let us go back to expression (4.183) but before its multiplication by $\mathbf{A^{-1}}$. From (4.182) it follows

$$\mathbf{A} \cdot \mathbf{W_S} \;=\; -\mathbf{B}\;. \tag{4.193}$$

In case of a nonspherical scattering geometry both matrices **A** and **B** are no longer diagonal- but full matrices. The necessary inversion of matrix **A** can become a numerically challenging task. However, if the geometry deviates only slightly from a nonspherical one the following iteration scheme can be applied with benefit: First we calculate the elements of both matrices according to (4.184) and (4.185) but now with surface integrals over the nonspherical surface of the scatterer. Next, we calculate the diagonal matrix $\mathbf{A_0}$ of the corresponding volume-equivalent spherical scatterer. Equation (4.193) can then be rewritten into

$$(\mathbf{A_D} \;+\; \mathbf{A_0}) \cdot \mathbf{W_S} \;=\; -\mathbf{B} \tag{4.194}$$

with the difference matrix $\mathbf{A_D}$ given by

$$\mathbf{A_D} \;=\; \mathbf{A} \;-\; \mathbf{A_0}\;. \tag{4.195}$$

This can be treated further to give

$$\mathbf{A_0} \cdot \mathbf{W_S} \;=\; -\mathbf{B} \;-\; \mathbf{A_D} \cdot \mathbf{W_S}\;, \tag{4.196}$$

and, after multiplication by $\mathbf{A_0^{-1}}$,

$$\mathbf{W_S} \;=\; -\mathbf{A_0^{-1}} \cdot \mathbf{B} \;-\; \mathbf{A_0^{-1}} \cdot \mathbf{A_D} \cdot \mathbf{W_S}\;. \tag{4.197}$$

This last equation looks like the algebraic version of a Lippmann-Schwinger equation for the interaction matrix and can be solved iteratively by inversion of the diagonal matrix $\mathbf{A_0}$ only. But this inversion produces no additional difficulties.

$$\mathbf{W_S^{(0)}} \;=\; -\mathbf{A_0^{-1}} \cdot \mathbf{B} \tag{4.198}$$

is its lowest, and

$$\mathbf{W_S^{(1)}} = -\mathbf{A_0^{-1}} \cdot \mathbf{B} - \mathbf{A_0^{-1}} \cdot \mathbf{A_D} \cdot \mathbf{W_S^{(0)}} \tag{4.199}$$

its first iteration.

Another possibility to derive a Lippmann-Schwinger equation which is more in agreement with that one considered in the second chapter of this book is offered with Green's theorem (4.2) if used with

$$\psi(\mathbf{r}) = G_\Gamma(\mathbf{r}, \mathbf{r}') \tag{4.200}$$

and the free-space Green's function

$$\phi(\mathbf{r}) = G^{(3)}(\mathbf{r}, \mathbf{r}') \, . \tag{4.201}$$

This gives

$$G_\Gamma(\mathbf{r}, \mathbf{r}') = G^{(3)}(\mathbf{r}, \mathbf{r}') + \oint_S G^{(3)}(\mathbf{r}, \bar{\mathbf{r}}) \cdot \frac{\partial G_\Gamma(\mathbf{r}, \bar{\mathbf{r}})}{\partial \hat{\bar{n}}'} \, dS(\bar{\mathbf{r}}) \tag{4.202}$$

if taking the boundary condition (4.174) and the Reciprocity into account. G_Γ in the surface integral over the nonspherical surface of the scatterer on the right-hand side can again be replaced in a first iteration by the free-space Green's function $G^{(3)}$.

Next we want to demonstrate the strong relation between the interaction matrix $\mathbf{W_S}$ and a T-matrix that can be introduced to describe the basis transformation of the primary incident plane wave. For this purpose let us rewrite the expansion (4.150) with coefficients (4.151) once again but in a shorter notation, and if restricted to the surface of a spherical scatterer with radius $r = a$ only. This restriction is due to the fact that the regular and radiating eigenfunctions of the Helmholtz equation form a basis on this surface. The shorter notation is obtained by using the scalar multiplication of the two "vectors" $\vec{c}$ and $\vec{\zeta}$ to represent the expansion of the plane wave,

$$\psi_0(a, \theta, \phi) = E_0 \cdot \vec{c} \cdot \vec{\zeta}^{\,tp}(a, \theta, \phi) \, . \tag{4.203}$$

The components of $\vec{c}$ are just the expansion coefficients according to (4.151). In a further step we want to express this expansion by the new basis functions $\varphi_i(a, \theta, \phi)$ which form the components of $\vec{\varphi}$. The transformation between these basis functions may be expressed by

$$\vec{\zeta}(a, \theta, \phi) = \vec{\varphi}(a, \theta, \phi) \cdot \mathbf{T} \, , \tag{4.204}$$

thus introducing the corresponding T-matrix. Looking at (4.182) and (4.186), we see that this matrix is identical with the negative interaction matrix,

$$\mathbf{T} \;=\; -\,\mathbf{W_S}\;. \tag{4.205}$$

The expansion of the primary incident plane wave on the spherical surface in terms of the radiating eigenfunctions reads therefore

$$\psi_0(a,\theta,\phi) \;=\; E_0 \cdot \vec{d} \cdot \vec{\varphi}^{\,tp}(a,\theta,\phi)\;, \tag{4.206}$$

where the new expansion coefficients d_i—the components of vector $\vec{d}$—are calculated from the old expansion coefficients c_i according to

$$\vec{d}^{\,tp} \;=\; \mathbf{T} \cdot \vec{c}^{\,tp}\;. \tag{4.207}$$

The T-matrix transforms once again the "old" expansion coefficients c_i into the "new" expansion coefficients d_i. It is of some interest here since we are now able to present immediately the scattering solution. Since condition (4.172) must hold at the surface of the scatterer we have at first

$$\psi_s(a,\theta,\phi) \;=\; -E_0 \cdot \vec{d} \cdot \vec{\varphi}^{\,tp}(a,\theta,\phi) \tag{4.208}$$

for the scattered field at this surface. However, that this expansion can be continued into the outer region Γ of the spherical scatterer, i.e., that

$$\psi_s(k,\mathbf{r}) \;=\; -E_0 \cdot \vec{d} \cdot \vec{\varphi}^{\,tp}(k,\mathbf{r})\;; \quad \mathbf{r} \in \Gamma \tag{4.209}$$

holds, was proven in Rother and Kahnert (2013). Relation (4.205) emphasizes once again the equivalence of a basis transformation and an interaction process.

4.4.2 S-Matrix

The S-matrix or "scattering matrix" was originally and independently introduced by (Wheeler 1937) and (Heisenberg 1943) in Quantum Mechanics. It was utilized only later on also in the theory of electromagnetic wave scattering (Saxon 1955). The unitarity property of this matrix is of our special interest in what follows since it can be related to the energy conservation of scattering processes. In so doing, let us go back to equation (4.204) where we replace $\vec{\zeta}(a,\theta,\phi)$ by relation (4.142) and the T-matrix by the negative interaction matrix $\mathbf{W_S}$. Thus we get

$$\vec{\chi}(a,\theta,\phi) \;=\; -\vec{\varphi}(a,\theta,\phi) \;-\; 2 \cdot \vec{\varphi}(a,\theta,\phi) \cdot \mathbf{W_S} \tag{4.210}$$

or

$$\vec{\chi}(a,\theta,\phi) \;=\; -\vec{\varphi}(a,\theta,\phi)\cdot\;\mathbf{S} \tag{4.211}$$

if introducing the S-matrix by

$$\mathbf{S} \;:=\; \mathbf{E} \;+\; 2\cdot\mathbf{W_S}\;. \tag{4.212}$$

In contrast to the T-matrix, the S-matrix relates the radiating and incoming eigensolutions at the spherical surface. With the definition of the scalar product

$$\left(\vec{u},\vec{v}\right)_S \;:=\; \sum_{i=0}^{N}\langle u_i(a,\theta,\phi)|v_i(a,\theta,\phi)\rangle\;, \tag{4.213}$$

where $\langle\cdot\,|\,\cdot\rangle$ is defined according to (4.180) at the spherical surface, and if assuming a real-valued k we see that

$$\left(\vec{\chi},\vec{\chi}\right)_S \;=\; \left(\vec{\varphi},\vec{\varphi}\right)_S\;. \tag{4.214}$$

This is a consequence of (4.140) and (4.141). Using relation (4.211) on the left-hand side of this identity provides

$$\left(\vec{\varphi},\vec{\varphi}\cdot\mathbf{S}^{\dagger}\cdot\mathbf{S}\right)_S \;=\; \left(\vec{\varphi},\vec{\varphi}\right)_S\;. \tag{4.215}$$

This proves the unitarity

$$\mathbf{S}^{\dagger}\cdot\mathbf{S} \;=\; \mathbf{E} \tag{4.216}$$

of the S-matrix for a real-valued parameter k. Please, note that $\mathbf{S}^{\dagger}$ represents the conjugate-complex and transpose of matrix S.

The unitarity property of the S-matrix for a real-valued parameter k is at first a mere mathematical property. But exactly this mathematical property can be used with benefit to express our physical experience of energy conservation regarding scattering processes on nonabsorbing obstacles if imbedded in a nonabsorbing environment. The energy conservation is usually expressed by the condition

$$\oint_{S_\infty}\left[\frac{\partial\psi^*(\mathbf{r})}{\partial r}\cdot\psi(\mathbf{r}) \;-\; \frac{\partial\psi(\mathbf{r})}{\partial r}\cdot\psi^*(\mathbf{r})\right]dS(\mathbf{r}) \;=\; 0 \tag{4.217}$$

that must hold for the total field $\psi \;=\; \psi_0 + \psi_s$ in the far field (see Morse and Feshbach (1953), Chap. 9 therein, for example). Regarding our initially formulated scattering problem this condition states that the energy flux produced by the incident and scattered field through the surface S_∞ in the far field is balanced if there are no sources and no absorption in region Γ. The assumption of no sources in Γ in

connection with a plane wave as the primary incident field results in a somewhat strange situation. We have already discussed how an impressed source must be choosen within the Green's function formalism to generate such a plane wave at the location of the scatterer. The impressed source (4.29) must be located in the far field of the scatterer. However, in order to avoid a conflict with (4.217) and the necessary assumption of no sources in Γ (i.e., no sources between the scatterer surface S and the surface S_∞ of the far field) this impressed source must yet be shifted behind the far field—whatever this means! This situation emphasizes once again the strange and quite artificial nature of the object "plane wave" if not considered as a priori existing. It is hard to understand, on the other hand, that the question of energy conservation should be restricted to the energy flux through S_∞ in the far field. One may also expect the conservation of energy across the surface S_a for the scattering configuration depicted in Fig. 4.12 which is a more realistic one and not restricted to a primary incident plane wave. And, moreover, the question of energy conservation should be decoupled from the nature of the source and solely related to the Green's function.

To find an answer to these questions we define the following functional at the boundary surface S_a with its outward directed unit normal vector $\hat{n}_a$:

$$\{f(\mathbf{r}), g(\mathbf{r})\}_{S_a} := \oint_{S_a} \left\{ \frac{\partial f^*(\mathbf{r})}{\partial \hat{n}_a} \cdot g(\mathbf{r}) - \frac{\partial g(\mathbf{r})}{\partial \hat{n}_a} \cdot f^*(\mathbf{r}) \right\} dS(\mathbf{r}) \,. \tag{4.218}$$

This definition is choosen in close analogy to (4.217). Let us further assume for simplicity that S_a is the surface of a sphere enclosing the scatterer. If applied to the

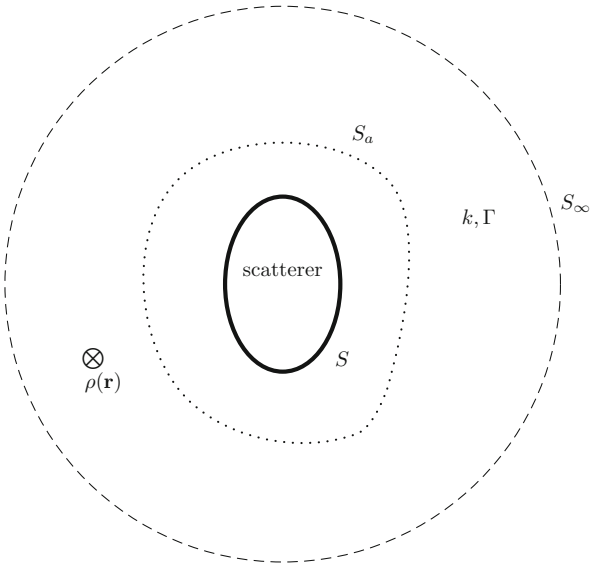

Fig. 4.12 Scattering configuration to prove energy conservation

eigensolutions of the Helmholtz equation we obtain for a real-valued parameter k

$$\left\{\varphi_i(k,\mathbf{r}),\varphi_j(k,\mathbf{r})\right\}_{S_a} \;=\; \left\{\chi_i(k,\mathbf{r}),\chi_j(k,\mathbf{r})\right\}_{S_a} \;= \\ \left\{\chi_i(k,\mathbf{r}),\varphi_j(k,\mathbf{r})\right\}_{S_a} \;=\; 0 \tag{4.219}$$

if $i \neq j$, and

$$\{\chi_i(k,\mathbf{r}),\varphi_i(k,\mathbf{r})\}_{S_a} \;=\; \{\varphi_i(k,\mathbf{r}),\chi_i(k,\mathbf{r})\}_{S_a} \;=\; 0 \tag{4.220}$$

as well as

$$\{\chi_i(k,\mathbf{r}),\chi_i(k,\mathbf{r})\}_{S_a} \;=\; -\,\{\varphi_i(k,\mathbf{r}),\varphi_i(k,\mathbf{r})\}_{S_a} \;=\; c \tag{4.221}$$

for all $i = 0,\cdots,N$. c in the last expression is a constant that does not depend on the index "i". These identities can be proven by application of Green's theorem in the region enclosed by S_a and S_∞, and if taking the far field behaviour of the Hankel functions and their orthogonality relation on a spherical surface into account. But in contrast to (4.2) the additional surface integral over the surface S_∞ in the far field must now be considered since the radiation condition does not apply to some of these functions or to some of the conjugate-complex functions! The analysis, even if not complicate, is quite tedious for which reason we leave it to the interested reader to practice Green's theorem. Alternatively, one may look in our book (Rother and Kahnert 2013). Now, let us go back to the Green's function (4.177) with the matrix elements of the interaction matrix assumed to be known. Assuming moreover that $\mathbf{r} < \mathbf{r}'$ always holds (and exactly this situation is required to prove energy conservation), and if taking (4.142) and (4.212) into account provides

$$G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}') \;=\; i\,k\cdot\sum_{i,k=0}^{N}\frac{1}{2}\cdot\left\{\delta_{i,k}\cdot\chi_i(k,\mathbf{r}) \;+\; [S]_{i,k}\cdot\varphi_i(k,\mathbf{r})\right\}\cdot\tilde{\varphi}_k(k,\mathbf{r}')\;. \tag{4.222}$$

$[S]_{i,k}$ therein are the corresponding matrix elements of the S-matrix according to (4.212). Employing the shorter matrix-vector notation this approximation reads

$$G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}') \;=\; \frac{i\,k}{2}\cdot\left[\vec{\chi}(k,\mathbf{r})\cdot\mathbf{E} \;+\; \vec{\varphi}(k,\mathbf{r})\cdot\mathbf{S}\right]\cdot\vec{\tilde{\varphi}}^{\,tp}(k,\mathbf{r}')\;. \tag{4.223}$$

It can be used in the functional (4.218) since $\mathbf{r} < \mathbf{r}'$ always holds at the scatterer surface. Then, from (4.219)–(4.221) we get

$$\left\{G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}'),G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}')\right\}_{S_a} \;=\; \frac{k^2\,c}{4}\sum_{i,k,q=0}^{N}\left[\delta_{i,k}\cdot\delta_{i,q} \;- \right. \\ \left.\left[S^*\right]_{i,k}\cdot[S]_{i,q}\right]\cdot\tilde{\varphi}_k^{\,*}(k,\mathbf{r}')\cdot\tilde{\varphi}_q(k_0,\mathbf{r}') \tag{4.224}$$

or

$$\left\{G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}'),G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}')\right\}_{S_a} = \frac{k^2\,c}{4}\cdot\vec{\tilde{\varphi}}^{\,*}(k,\mathbf{r}')\cdot\left[\mathbf{E}-\mathbf{S}^\dagger\cdot\mathbf{S}\right]\cdot\vec{\tilde{\varphi}}^{\,tp}(k,\mathbf{r}') \tag{4.225}$$

if using again the shorter matrix-vector notation. Since the absence of absorption is characterized by a real-valued parameter k

$$\left\{G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}'),G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}')\right\}_{S_a} = 0 \tag{4.226}$$

follows from the unitarity (4.216) of the S-matrix. This expresses energy conservation with respect to the closed boundary surface S_a. The interaction matrix $\mathbf{W_S}$ is identical zero if no scatterer exists. $G_\Gamma^{(N)}(\mathbf{r},\mathbf{r}')$ becomes then identical with the free-space Green's function $G^{(3)}(\mathbf{r},\mathbf{r}')$, and we have $\mathbf{S}=\mathbf{E}$.

$$\left\{G^<(\mathbf{r},\mathbf{r}'),G^<(\mathbf{r},\mathbf{r}')\right\}_{S_a} = 0 \tag{4.227}$$

holds therefore for the part $G^<$ of the free-space Green's function as long as the primary impressed source is located outside the region enclosed by S_a. And, finally, since the $\mathbf{r}$- and $\mathbf{r}'$-dependence are decoupled in the considered approximation of the Green's function the same expressions of energy conservation apply to the primary incident field $\psi_0(k,\mathbf{r})$ and the total field $\psi(k,\mathbf{r})$. It should be also noted that the spherical geometry of the scatterer was not a precondition for the derivation of (4.226).

4.4.3 Scattering Phase and Optical Theorem

We will now turn our attention toward the scattered field of the initially formulated scattering problem on an ideal metallic or acoustically soft sphere if the impressed source of the primary incident field is given by (4.156). It is moreover assumed that the location r_q' of this source is shifted on the z-axis to $-\infty$ toward the far field. This source, since applied to $G^<$ of the free-space Green's function on the right-hand side of (4.190), generates the plane wave (4.158) as the primary incident field ψ_0. On the other hand, application of this source to the scattering part of (4.190) (that is the second part on the right-hand side of this equation) results in the approximation

$$\psi_s^{(N)}(k,\mathbf{r}) = -E_0\cdot\sum_{n=0}^{N}\frac{j_n(ka)}{h_n^{(1)}(ka)}\cdot(2n+1)\cdot i^n\cdot P_n(\cos\theta)\cdot h_n^{(1)}(kr) \tag{4.228}$$

for the scattered field ψ_s. Please, note that the summation index "n" is not the combined summation index, due to the $\delta_{0,l}$ term in (4.156). The term "$-j_n(ka)/h_n^{(1)}(ka)$"

are just the matrix elements of the diagonal interaction matrix $\mathbf{W_S}$. Taking relation (4.212) between the W_S—and S-matrix into account, and since

$$j_n(ka) \;=\; \frac{1}{2}\cdot\left[h_n^{(1)}(ka) \;+\; h_n^{(2)}(ka)\right] \tag{4.229}$$

follows from (4.140) and (4.141) we may write

$$\psi_s^{(N)}(k,\mathbf{r}) \;=\; E_0\cdot\sum_{n=0}^{N}\frac{(2n+1)}{2}\left([S]_n \;-\; 1\right)\cdot i^n\cdot P_n(\cos\theta)\cdot h_n^{(1)}(kr) \tag{4.230}$$

instead of (4.228).

$$[S]_n \;=\; -\frac{h_n^{(2)}(ka)}{h_n^{(1)}(ka)} \tag{4.231}$$

are the diagonal elements of the S-matrix. We choose $E_0 = 1$ for simplicity and denote the product ka of wave number and radius $r = a$ of the sphere with β. β is an important parameter in scattering theory called the "size parameter". It describes the ratio of a characteristic dimension of the scatterer and the wave length of the primary incident plane wave. The elements of the S-matrix can be expressed as pure phase terms. Using (4.140) and (4.141) it follows

$$[S]_n \;=\; e^{\,2i\,\delta_n} \tag{4.232}$$

with δ_n being the real-valued scattering phase given by

$$\tan\delta_n \;=\; \frac{j_n(\beta)}{y_n(\beta)} \tag{4.233}$$

(just a hint: use $e^{\,2i\delta_n} = e^{\,i\delta_n}/e^{-i\delta_n}$ in (4.231) in order to derive this relation!). Instead of (4.230) we then may write

$$\psi_s^{(N)}(k,\mathbf{r}) \;=\; \sum_{n=0}^{N}(2n+1)\cdot i^{n+1}\cdot e^{\,i\,\delta_n}\cdot\sin\delta_n\cdot P_n(\cos\theta)\cdot h_n^{(1)}(kr)\;. \tag{4.234}$$

If shifting the observation point r into the far field

$$\lim_{r\to\infty}\left[\psi_s^{(N)}(k,\mathbf{r})\right] \;=\; f(\theta)\cdot\frac{e^{\,ikr}}{r} \tag{4.235}$$

follows from (4.138), where

$$f(\theta) \;=\; \frac{1}{k} \cdot \sum_{n=0}^{N} (2n+1) \cdot e^{\,i\,\delta_n} \cdot \sin\delta_n \cdot P_n(\cos\theta) \tag{4.236}$$

represents the scattering amplitude function.

To get a clearer understanding of the importance of the scattering phase δ_n we decompose the primary incident plane wave (4.158) into

$$\psi_0^{(N)}(k,\mathbf{r}) \;=\; \psi_0^{(i,N)}(k,\mathbf{r}) \;+\; \psi_0^{(r,N)}(k,\mathbf{r}) \;, \tag{4.237}$$

where

$$\psi_0^{(i,N)}(k,\mathbf{r}) \;=\; \sum_{n=0}^{N} \frac{(2n+1)}{2} \cdot e^{\,in\pi/2} \cdot P_n(\cos\theta) \cdot h_n^{(2)}(kr) \tag{4.238}$$

is the incoming part. On the other hand,

$$\psi_0^{(r,N)}(k,\mathbf{r}) \;=\; \sum_{n=0}^{N} \frac{(2n+1)}{2} \cdot e^{\,in\pi/2} \cdot P_n(\cos\theta) \cdot h_n^{(1)}(kr) \tag{4.239}$$

represents the outgoing- or radiating part. (4.118) and (4.229) as well as identity $i^n = e^{\,in\pi/2}$ was used for this decomposition. If we add the radiating part (4.239) of the incident plane wave to the scattered field (4.234) we thus get the radiating part of the total field,

$$\psi^{(r,N)}(k,\mathbf{r}) \;=\; \sum_{n=0}^{N} \frac{(2n+1)}{2} \cdot e^{\,i(n\pi/2+2\,\delta_n)} \cdot P_n(\cos\theta) \cdot h_n^{(1)}(kr) \;. \tag{4.240}$$

It differs from the radiating part of the primary incident plane wave by the scattering phase term $2\,\delta_n$.

Whereas the differential scattering cross-section is given by the square of the scattering amplitude function (4.236) in the far field, the total scattering cross-section σ_{tot} is defined by the solid angle integral over this quantity, i.e., by

$$\sigma_{tot} \;:=\; \int f^*(\theta) \cdot f(\theta) \cdot \sin\theta \; d\theta \, d\phi \;. \tag{4.241}$$

Due to the orthogonality relation (4.131) of the Legendre polynomials this gives

$$\sigma_{tot} \;=\; \frac{4\,\pi}{k^2} \cdot \sum_{n=0}^{N} (2n+1) \cdot sin^2\delta_n \;. \tag{4.242}$$

On the other hand, if $\theta = 0°$ is choosen in (4.236) (this corresponds to the forward direction of the incident plane wave) and since $P_n(1) = 1$, we have

$$Im\{f(0)\} = \frac{1}{k} \cdot \sum_{n=0}^{N} (2n+1) \cdot sin^2\delta_n \,. \tag{4.243}$$

Comparing this with (4.242) provides the well-known "optical theorem"

$$\sigma_{tot} = \frac{4\pi}{k} \cdot Im\{f(0)\} \tag{4.244}$$

we mentioned already in conjunction with the double-slit experiment. The above given derivation of this theorem is restricted to a spherical scattering geometry. However, a more general derivation that avoids this restriction can be found, for example, in Morse and Feshbach (1953) for the scalar case, and in Saxon (1955) and Rother and Kahnert (2013) for the case of electromagnetic wave scattering.

4.4.4 Extinction Paradox

Which basic approach can be used to solve a certain scattering problem is mainly dependent on the above introduced size parameter β. Regarding electromagnetic wave scattering, and if the dimension of the scatterer is small compared to the wavelength of the primary incident plane wave—this corresponds to a small size parameter $\beta \leq 1$—the quite simple Rayleigh approximation that is characterized by the scattering behaviour of a dipole can be applied with benefit. But this approximation is less sensitive to the geometry of the scatterer. In other words, looking at the resulting differential scattering cross-sections provides only little information about its geometry. The situation changes if $\beta > 1$. Now we have to solve the Helmholtz equation without any physical simplifications, as it was discussed so far in this chapter. Due to the necessary application of the boundary condition at the scatterer surface the geometry of the scatterer has an important influence on its scattering behaviour. However, the Rayleigh approximation is contained as a limiting situation in this rigorous approach. The situation changes again for very large size parameters, i.e., if the dimension of the scatterer is very large compared to the wavelength of the incident plane wave. One possible approach is the Geometric Optics approximation that neglects diffraction since replacing the incoming plane wave by a bundle of noninteracting rays which propagate according to the laws of transmission and reflection. But even if very large size parameters are considered the diffraction effects are of importance in some situations and result in essential (and measurable!) differences in the scattering behaviour if compared to the Geometric Optics approach. This will be demonstrated in what follows with the so-called "extinction paradox".

Starting point is the far field approximation (4.235) of the scattered field with the scattering amplitude function (4.236) rewritten into

$$f(\beta,\theta) \;=\; \frac{1}{2\,i\,k}\cdot\sum_{n=0}^{N}(2n+1)\cdot([S(\beta)]_n \;-\; 1)\cdot P_n(\cos\theta) \tag{4.245}$$

by use of the matrix elements (4.232) of the S-matrix. Increasing the size parameter β makes it necessary to take an increasing number of expansion terms in this approximation into account. It was shown by Nussenzveig in an impressive way that the resulting problems for very large size parameters can be bypassed by using the Watson transformation or Poisson's summation formula (see Nussenzveig (1965)). This allows one to derive simple analytical expressions in this limiting situation. However, these simple analytical expressions are obtained only by walking the long and bumpy road through the analytical landscape of complex analysis. This is one of the reasons why this method has not been gained much attention. The fact that our recent computational possibilities and numerical procedures allow an easy treatment of (4.245) even for size parameters of $\beta = 20000$ and beyond may be another reason. But in what follows we will go back to the method of Nussenzveig and discuss—not in detail but the two essential steps for very large size parameters—the derivation of the extinction paradox. Compared to the brut force approach of a numerical computation this analysis has the advantage of revealing the differences between wave- and ray optics and the underlying physics much more clearly.

Due to (4.127) and (4.128), we first note that we may write

$$[S]_n \;=\; -\frac{H^{(2)}_{n+1/2}(\beta)}{H^{(1)}_{n+1/2}(\beta)} \tag{4.246}$$

instead of (4.231). Application of Poisson's summation formula

$$\sum_{n=0}^{\infty} f(n+1/2) \;=\; \sum_{m=-\infty}^{\infty}(-1)^m\int_0^{\infty} f(\lambda)\cdot e^{\,2im\pi\lambda}\,d\lambda \tag{4.247}$$

to (4.245) results in

$$f(\beta,\theta) \;=\; \sum_{m=-\infty}^{\infty}(-1)^m\int_0^{\infty} f(\lambda,\beta)\cdot P_{\lambda-1/2}(\cos\theta)\cdot e^{\,2im\pi\lambda}\cdot\lambda\,d\lambda\;, \tag{4.248}$$

where

$$f(\lambda,\beta) \;=\; \frac{i}{k}\cdot[1 \;-\; S(\lambda,\beta)] \tag{4.249}$$

and

$$S(\lambda, \beta) \;=\; -\frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)} \,. \tag{4.250}$$

For our purpose, the evaluation of the integral requires a detailed consideration of its integrand in the complex λ-plane at large size parameters β. To this end we have to take note of the following problem that has a major impact on the analysis: The scattering angle θ is in the range of $[0, \pi]$. But the Legendre functions $P_\lambda(\cos\theta)$ are singular if $\theta = \pi$, and the Legendre functions $P_\lambda(-\cos\theta)$ are singular if $\theta = 0$. Only for nonnegative and integer numbers of λ we obtain the conventional Legendre polynomials which are nonsingular in $\theta = 0, \pi$. As it was shown by Nussenzveig, it is advantageous to consider the two regions

- near forward direction: $\theta \leq \beta^{-1/3}$
- $\theta < \beta^{-1/3} \leq \pi$

with respect to the scattering angle θ separately. Equations (4.248)–(4.250) can be used in the near forward region. In the other region we have to make use of the identity

$$P_\lambda(\cos\theta) \;=\; Q_\lambda^{(1)}(\cos\theta) \;+\; Q_\lambda^{(2)}(\cos\theta) \,, \tag{4.251}$$

where

$$Q_\lambda^{(1,2)}(\cos\theta) \;=\; \frac{1}{2} \cdot \left[P_\lambda(\cos\theta) \pm \frac{2i}{\pi} Q_\lambda(\cos\theta) \right] \,. \tag{4.252}$$

The upper or lower sign in front of the second term in the square brackets on the right-hand side applies if $Q_\lambda^{(1)}$ or $Q_\lambda^{(2)}$ is considered. Beside P_λ, Q_λ represents a second linear independent solution of (4.116). Let us discuss the near forward region first.

By means of an ingenious (and breathtaking, according to my mind) manipulation Nussenzveig was able to split (4.248) into contributions of different parts. In the far field and if $\theta \to 0$ the largest of these contributions agrees with the well-known Fraunhofer diffraction of a circular aperture. The other parts describe the transition into the so-called Fock region and result in an expansion in terms of $(1/\beta)^\alpha$, $\alpha > 0$. But since it is our goal to calculate the total scattering cross-section by use of the optical theorem (4.244), it is sufficient to look at the Fraunhofer contribution only. This results from (4.248) if only $m = 0$ is considered and if $S(\lambda, \beta)$ is neglected, i.e., from

$$f(\beta >> 1, \theta \to 0) \;=\; \frac{i}{k} \int_0^\beta P_{\lambda - 1/2}(\cos\theta) \cdot \lambda \; d\lambda \,. \tag{4.253}$$

Substituting $x = \lambda\,\theta$ and if taking the expansion

$$P_{\lambda-1/2}(\cos\theta) \;\approx\; \left(\frac{\theta}{\sin\theta}\right)^{1/2} \cdot J_0(2\theta) \;+\; \cdots \tag{4.254}$$

into account (see Nussenzveig (1965), Eq. (C.11) therein) gives

$$f(\beta >> 1, \theta \to 0) \;=\; \frac{i}{k} \cdot \left(\frac{\theta}{\sin\theta}\right)^{1/2} \cdot \frac{1}{\theta^2} \cdot \int_0^{\beta\,\theta} x \cdot J_0(x)\; dx\;. \tag{4.255}$$

From

$$\int_a^b x^{-n+1} \cdot J_n(x)\; dx \;=\; -\left[x^{-n+1} \cdot J_{n-1}(x)\right]_a^b\;, \tag{4.256}$$

(as can be proven by means of integration by parts) and identity

$$J_{-n}(x) \;=\; (-1)^n \cdot J_n(x) \tag{4.257}$$

it follows

$$f(\beta >> 1, \theta \to 0) \;=\; i \cdot \beta\, a \cdot \left(\frac{\theta}{\sin\theta}\right)^{1/2} \cdot \frac{J_1(\beta\,\theta)}{\beta\,\theta}\;. \tag{4.258}$$

This results in the Fraunhofer diffraction of a circular aperture for very small scattering angles θ and if $\sin\theta$ is correspondingly approximated by θ. Finally, from L'Hospital's rule we get for the scattering amplitude function in the limit $\theta = 0$

$$f(\beta >> 1, \theta = 0) \;=\; \frac{i\,k\,a^2}{2} \tag{4.259}$$

(just to remember: $\beta = ka$). Using this result in the optical theorem (4.244) provides the total scattering cross-section

$$\sigma_{tot} \;=\; 2\,\pi\,a^2\;. \tag{4.260}$$

This is twice the geometrical cross-section of the circular aperture with radius $r = a$ one would get from the Geometric Optics approach. This approach obviously fails in the near forward direction even at very large size parameters.

The contribution from the second region, on the other hand, can in fact be identified with the Geometric Optics result if very large size parameters are considered. This was also demonstrated by Nussenzveig. The corresponding contribution results again only from the term $m = 0$ of (4.248), from relation (4.251) if taking only $Q_\lambda^{(1)}$ into account, and, moreover, if only the contribution $S(\lambda, \beta)$ of the scattering

amplitude function $f(\lambda, \beta)$ is considered. We thus get

$$f_r(\beta, \theta) \;=\; -\frac{i}{k} \int_0^\infty S(\lambda, \beta) \cdot Q^{(1)}_{\lambda - 1/2}(\cos\theta) \cdot \lambda \; d\lambda \; . \tag{4.261}$$

The estimation of this integral by use of the stationary phase approximation at the dominant point

$$\bar{\lambda} \;=\; \beta \cdot \cos\frac{\theta}{2} \tag{4.262}$$

on the positive and real-valued λ-axis requires a considerable analytical effort regarding the deformation of the path of integration in the complex λ-plane and the behaviour of Bessel's functions at infinity. We do not want to go into the details of this sophisticated analysis performed by Nussenzveig. The final result is given by

$$f_r(\beta, \theta) \;=\; -\frac{a}{2} \cdot e^{-2i\beta \sin\frac{\theta}{2}} \; . \tag{4.263}$$

The subindex "r" indicates that this represents the reflective part of the solution in the far field of this region. The differential scattering cross-section $d\sigma/d\Omega$—the square of the scattering amplitude function—reads

$$\frac{d\sigma}{d\Omega} \;=\; \frac{a^2}{4} \tag{4.264}$$

and is identical with expression (2.393) that was already derived in Chap. 2 for particle scattering on a rigid sphere. The dominant point (4.262) can directly be compared to the impact parameter (2.391). The different behaviour for large size parameters in the two regions can also be seen from Fig. 4.13. On the one hand, there is the nearly constant part from the backward direction up to the near forward direction that can be related to reflection only. The shift of this contribution toward the forward direction for an increasing size parameter β can also be observed! The strong increase of the contribution of the other part near and in forward direction is responsible for the doubling of the total cross section and cannot be explained by the Geometric Optics approach.

Exercise: Development of a computer program for the scattering amplitude function that results from (4.228) and the far field approximation (4.138). Calculate the differential scattering cross-section that is the square of this function. Use this program to demonstrate the extinction paradox and its dependence on the size parameter β, as it is demonstrated in Fig. 4.13. Modify this program to consider scattering of a plane wave on a acoustically hard sphere. Hint: This requires only a small change in (4.228) since the homogeneous Dirichlet

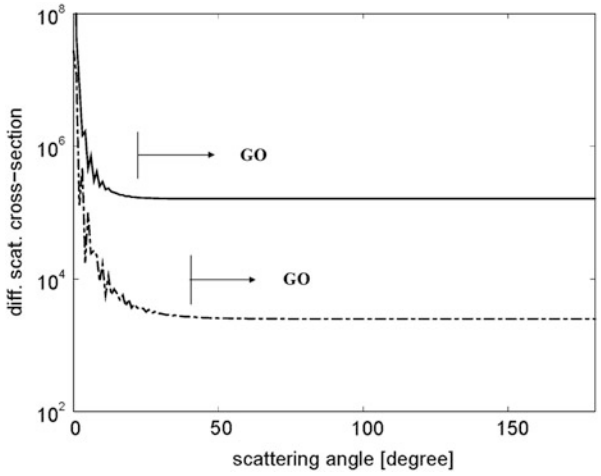

Fig. 4.13 Differential scattering cross-section for two different size parameters. Results are numerically obtained from (4.245). *Dot-dashed line*: $\beta = 100$, *full line*: $\beta = 800$

condition must be replaced by the homogeneous von Neumann condition at the spherical surface of the scatterer! Compare the different scattering behaviour of acoustically soft and hard spheres. For an initial program see Appendix A.2.

Chapter 5
Probability Experiments and Green's Functions in Classical Event Spaces

Maybe God is not playing dice. But the devil will most likely do it

It was already mentioned in Sect. 1.3 that in contrast to Quantum Mechanics probabilities are of less conceptual importance in classical physics. In this chapter I will therefore propose an abstract probability state concept in two- and four-dimensional but classical event spaces which can be related to special stochastic sources and interactions. The classical event spaces are introduced independent of whether the corresponding events are generated by classical or quantum objects. Related Schrödinger-like equations and their Green's functions are also introduced. In so doing, it will be demonstrated that well-known concepts from Quantum Mechanics can be applied with benefit also to special probability experiments with classical particles, and that entanglement does not belong exclusively to the realm of Quantum Mechanics (see the quotation of Schrödinger in Sect. 1.3). But I want to emphasize that **this chapter is not concerned with Quantum Mechanics**. It rather provides a phenomenological point of view on the probability experiments which can be traced back to stochastic but impressed sources and to stochastic interactions. As discussed in the Prologue of this book, we are not interested in an analysis of the stochastic nature of the impressed sources. They are simply accepted to exist. But it is our goal in what follows to find out if we are able to bring these sources and the resulting probabilities measured in corresponding experiments into agreement, and if this can be accomplished by use of a corresponding Green's function formalism.

In Chap. 2, in conjunction with the temporal boundary value problem and based on the bilinear expansion of Dirac's delta function, the "source picture" of the Fourier series was already introduced and discussed. In what follows, it is discussed once again but as a result of the required time independence of the probabilities related to the events of the considered event spaces.

A quite instructive class room experiment is introduced and discussed from the point of view of the developed formalism in the second section of this chapter. This experiment can be considered to represent the classical analog to the quantum mechanical Bell's experiment. It will allow us to discuss the different outcome of

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both experiments from a point of view that differs from the conventional discussion one can find in the corresponding literature. The Clauser-Horne-Shimony-Holt-inequality (CHSH-inequality) is of special importance in this context (see Clauser et al. (1969)). Comparing these two experiments allows moreover an interesting interpretation of the so-called "negative quasi-probabilities" known from the Wigner functions and the Glauber-Sudarshan equation in Quantum Optics, for example. The epistemological meaning of such probabilities is a further objective that is still under discussion in Quantum Mechanics.

5.1 Probability Experiments in a Two-Dimensional Event Space

5.1.1 Probability States and Green's Function

We start from the assumption that we are able to relate characteristic states of certain classical or quantum objects by use of an appropriate experimental setup to two classical events—let us say to a "click" or "not a click" of a detector. That is, "click" and "not a click" are the two possible events one may observe in a single experimental step. Alternatively, a lamp may be "switched on", or it remains "switched off". A probability can be related to each of these events if a multitude of identical experimental steps are performed. We consider these probabilities as the measurable quantities of the corresponding probability experiment. The following simple examples are to put the idea across:

- When a coin is flipped, the result is either a head or tail. A detector produces a click if the head is detected. There will be no click otherwise.
- When a marble is blindly drawn from a box that contains a number of white and black marbles, its colour is either white or black. A detector produces a click if the colour white is detected. There will be no click otherwise.
- When an electron is traversing an inhomogeneous magnetic field, it is either deflected up or down. A detector produces a click if an upward deflection is detected. There will be no click otherwise. This is the well-known Stern-Gerlach experiment mentioned in the Prologue.
- When a linearly polarized photon hits upon a polarizing filter that is arbitrarily oriented with respect to the plane of polarization of the incoming photon, the photon is either allowed to pass through, or it is blocked out. A detector produces a click if the photon is allowed to pass through. There will be no click otherwise.
- An example of a stochastic momentum source acting on a classical point mass of mass m with two possible momenta is shown in Fig. 5.1. Detector D produces a click if momentum p_a is detected. There will be no click if momentum p_b is detected.

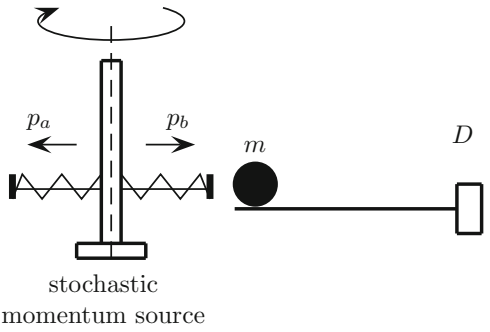

Fig. 5.1 Experimental setup of a stochastic momentum source acting like a wheel of Fortune on a classical point mass m with two possible momenta p_a and p_b

We say that the detector produces a "click"—let us relate the value $\lambda_1 = +1$ to this event—if it is in the state

$$| \varphi_1 \rangle \; = \; (1, 0) \; . \tag{5.1}$$

And we say that the detector produces "not a click"—let us relate the value $\lambda_2 = -1$ to this event—if it is in the state

$$| \varphi_2 \rangle \; = \; (0, 1) \; . \tag{5.2}$$

The two values $\lambda_{1/2} = \pm 1$ and the two vectors $|\varphi_{1/2}\rangle$ are the eigenvalues and eigenvectors of Paulis' spin matrix

$$\mathbf{\Sigma} \; = \; \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \; = \; \sum_{i=1}^{2} \lambda_i \cdot | \, \varphi_i \rangle \langle \varphi_i \, | \tag{5.3}$$

(see Eq. (1.5) in Sect. 1.3), and the related eigenvalue problem reads

$$\mathbf{\Sigma} \circ | \, \varphi_i \rangle \; - \; \lambda_i \cdot | \, \varphi_i \rangle \; = | \, 0 \rangle \; ; \quad i = 1, 2 \; . \tag{5.4}$$

$$\langle \varphi_i \, | \, \varphi_j \rangle \; = \; \delta_{i,j} \quad i, j = 1, 2 \tag{5.5}$$

holds for the eigenvectors. They form a basis in this 2-dim. event space. It should therefore be possible to completely characterize every probability experiment in this space by the abstract probability state vector

$$| \, \psi \rangle \; = \; c_1 \cdot | \, \varphi_1 \rangle \; + \; c_2 \cdot | \, \varphi_2 \rangle \; , \tag{5.6}$$

where c_1 and c_2 are the probability amplitudes related to the two possible events. These amplitudes are given by the square root of the measured probabilities c_1^2 and c_2^2 of detecting a "click" and "not a click" in the considered probability experiment. This is the experimental point of view. Contrary, once we have derived the probability state (5.6) of a certain experiment from theoretical considerations on

the level of the abstract states—and this is exactly what we intend to do later on in this chapter—the corresponding probabilities are obtained by the scalar product of the projections

$$| \psi_n\rangle \; = | \varphi_n\rangle\langle\varphi_n \mid \psi\rangle \; ; \quad n = 1, 2 \; . \tag{5.7}$$

That is, we have

$$\langle\psi_n \mid \psi_n\rangle \; = \; c_n^2 \; ; \quad n = 1, 2 \; , \tag{5.8}$$

as well-known from Quantum Mechanics. The probabilities derived in this way from theoretical considerations are justified only by their agreement with the measured probabilities in a corresponding experiment, of course.

Next, we intend to relate this procedure to a Green's function formalism. To this end, let us consider the Schrödinger-like equation

$$- \, i\, a \cdot \frac{d}{dt} \mid \psi(t)\rangle \; + \; \mathbf{\Sigma} \circ \mid \psi(t)\rangle \; = \; - \; \mid \rho(t)\rangle \tag{5.9}$$

with matrix $\mathbf{\Sigma}$ given by (5.3). For the moment constant a as well as the state $\mid \rho(t)\rangle$ of a primary impressed, stochastic source will be left unspecified. Here it is our main goal to relate a certain probability state (5.6) via our pivotal relation (2.16), i.e., by

$$\mid \psi(t)\rangle \; = \; \int_{t_0'}^{t^+} \mathbf{G}(t, t') \circ \mid \rho(t')\rangle \, dt' \; , \tag{5.10}$$

to a given primary source. $\mathbf{G}(t, t')$ represents the Green's function we are looking for. $t' = t_0'$ is the assumed lower limit of the initial time, and $t \geq t_0'$ is the observation time. The handling of the time dependence will be discussed shortly. The Green's function satisfies the equation

$$- \, i\, a \cdot \frac{d\mathbf{G}(t, t')}{dt} \; + \; \mathbf{\Sigma} \; \circ \mathbf{G}(t, t') \; = \; - \mathbf{D_1} \cdot \delta(t - t') \; , \tag{5.11}$$

where $\mathbf{D_1}$ on the right-hand side represents the unit dyad (unit operator)

$$\mathbf{D_1} \; = \; \sum_{n=1}^{2} \; \mid \varphi_n\rangle\langle\varphi_n \mid \; . \tag{5.12}$$

To demonstrate that this Green's function will provide us indeed with a solution of Eq. (5.9), let us insert (5.10) into Eq. (5.9). This gives

$$\left[- \, i\, a \cdot \frac{d\mathbf{G}(t, t')}{dt} \; + \; \mathbf{\Sigma} \; \circ \mathbf{G}(t, t') \right] \circ \mid \rho(t')\rangle \; = \; - \; \mid \rho(t)\rangle \; . \tag{5.13}$$

Expanding the primary impressed, stochastic source on both sides according to

$$| \rho(t)\rangle \; = \; \sum_{n=1}^{2} \rho_n(t) \cdot | \varphi_n\rangle \tag{5.14}$$

with yet not specified coefficients $\rho_n(t)$, and if taking the property

$$f(t) \cdot \delta(t - t') \; = f(t') \tag{5.15}$$

of Dirac's delta function and identity

$$\mathbf{D_1} \circ | \rho(t')\rangle \; = | \rho(t')\rangle \tag{5.16}$$

on the right-hand side of (5.13) into account results in Eq. (5.11). This equation can be solved with the Fourier transform method by employing

$$\mathbf{G}(t, t') \; = \; \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, \mathbf{G}(\omega) \cdot e^{\,-i\omega(t-t')} \tag{5.17}$$

and

$$\delta(t - t') \; = \; \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, e^{\,-i\omega(t-t')} \tag{5.18}$$

with respect to time, as already done in Sect. 3.4.3. Expanding the Fourier transform of the Green's function in terms of the dyadic products of the eigenvectors $| \varphi_1\rangle$ and $| \varphi_2\rangle$ gives

$$\mathbf{G}(\omega) \; = \; \frac{1}{a} \cdot \sum_{n=1}^{2} \frac{| \varphi_n\rangle\langle\varphi_n |}{\omega - \frac{\lambda_n}{a}} \; , \tag{5.19}$$

where λ_n are the corresponding eigenvalues ± 1. Inserting this expression into (5.17) and applying the residual theorem provides the Green's function

$$\mathbf{G}(t, t') \; = \; \frac{i}{a} \sum_{n=1}^{2} e^{\,-\frac{i}{a}\lambda_n \cdot (t-t')} \cdot | \varphi_n\rangle\langle\varphi_n | = \\ \frac{i}{a} \cdot \sum_{n=1}^{2} | \varphi_n(t)\rangle\langle\varphi_n(t') | \; , \tag{5.20}$$

where

$$| \varphi_n(t)\rangle \; = \; e^{\,-\frac{i}{a}\lambda_n \cdot t} \cdot | \varphi_n\rangle \; . \tag{5.21}$$

Please, consider that $\langle \varphi_n(t) \mid$ denotes the conjugate-complex of $\mid \varphi_n(t) \rangle$. Comparable expressions are known from Quantum Mechanics, as we will see in the final chapter. Next we introduce the primary impressed source

$$\mid \rho(t') \rangle \; = \; \frac{a}{i} \cdot \delta(t' - t'_0) \cdot \sum_{n=1}^{2} c_n \cdot \mid \varphi_n \rangle \tag{5.22}$$

with amplitudes c_n considered to be given. We thus get from (5.20) and (5.10) the time dependent probability state vector

$$\mid \psi(t) \rangle \; = \; \sum_{n=1}^{2} c_n \cdot \mid \varphi_n(t - t'_0) \rangle \; . \tag{5.23}$$

Now we reached the point where we have to discuss the handling of the time dependence.

First I want to emphasize once again that we do not practice Quantum Mechanics in this chapter. Thus, there is no need to go into the details of its sophisticated time concept (for a detailed analysis of the time concept in conventional Quantum Mechanics, see Hilgevoord and Atkinson (2011), for example). However, what the following experiments have in common with Quantum Mechanics are the facts that time is not considered as a continuously varying dynamical variable, and that the probabilities we are interested in are independent of time. The only situation where we have to take the "time-parameter" into account is—beside its usage in the primary impressed source (5.22) that produces a process at a certain "initial time" t'_0, and that results in a single event at a "later time" $t \geq t'_0$—the additional existence of a stochastic interaction process that may affect the probabilities of an experiment. We have therefore to distinguish whether the measurements of the single events are performed after the primary impressed source was acting but before this interaction, or after this interaction. This situation will allow us to proceed in an easy and pragmatic way with the time dependence of the Green's functions and the probability state vectors. Regarding the Green's functions, this can be accomplished simply by multiplication by appropriate Heaviside functions, as already done in Sect. 2.7. This will be employed again in what follows. Regarding the state vector (5.23) there are two options. The easiest way to proceed is to ignore the time dependence in (5.23) since it appears only as a phase term and is washed out if calculating the probabilities according to (5.8) from the now time dependent projections (5.7). Unfortunately, it does not work that way if an additional interaction process is considered, as we will see shortly. We will therefore employ the second option that uses the freedom of choosing the parameter a. Let us therefore introduce the time independent probability state vector by the definition

$$\mid \psi \rangle \; := \; \lim_{a \to \infty} \mid \psi(t) \rangle \; = \; \sum_{n=1}^{2} c_n \cdot \mid \varphi_n \rangle \; . \tag{5.24}$$

The corresponding probabilities are again obtained from (5.7) and (5.8). For example, if $c_1 = c_2 = 1/\sqrt{2}$ is used in the primary impressed source (5.22) we get the probabilities $c_1^2 = c_2^2 = 1/2$. All the 5 initially mentioned examples are possible ways to put such an impressed source into practice.

Before we will discuss a specific interaction process it is of some importance for what follows to mention another aspect in conjunction with the impressed source (5.22). It can be considered to consists of the two parts

$$| \rho(t')\rangle = | \rho_1(t')\rangle + | \rho_2(t')\rangle \ , \tag{5.25}$$

where $| \rho_1(t')\rangle$ and $| \rho_2(t')\rangle$ are given by

$$| \rho_1(t')\rangle = \frac{a}{i} \cdot \delta(t' - t'_0) \cdot c_1 \cdot | \varphi_1\rangle \tag{5.26}$$

and

$$| \rho_2(t')\rangle = \frac{a}{i} \cdot \delta(t' - t'_0) \cdot c_2 \cdot | \varphi_2\rangle \ . \tag{5.27}$$

These two subsources result in the two time independent substates

$$| \psi_1\rangle = c_1 \cdot | \varphi_1\rangle \tag{5.28}$$

and

$$| \psi_2\rangle = c_2 \cdot | \varphi_2\rangle \ . \tag{5.29}$$

The superposition of these substates provides the total probability state

$$| \psi\rangle = | \psi_1\rangle + | \psi_2\rangle \ . \tag{5.30}$$

There is obviously no difference in the resulting probabilities if (5.7) and (5.8) are applied to the total probability state (5.30), or if applied to each substate (5.28) and (5.29) separately. This property differs from that one discussed in conjunction with the intensity distribution of plane wave scattering on a double-slit (see Eqs. (4.41)–(4.51) in Sect. 4.2). It can be explained by the fact that the two subsources as well as the two substates (5.28) and (5.29) are disjoint, i.e., that they do not have any basis vectors in common (see also Sect. 4.2 for the definition of disjoint and nondisjoint vectors). Regarding the above situation this behaviour looks like a triviality. However, we will see in the following experiment with an additional interaction but especially in the next section that this aspect is within the heart of our explanation of the different probabilities measured in the quantum mechanical Bell's experiment and its classical analog. But let me also emphasize the fact that the state (5.30) and the resulting probabilities c_1^2 and c_2^2 are in total agreement with our classical experience of such probability experiments!

5.1.2 Stochastic Interaction

Beside the primary impressed source there may also exist an additional stochastic interaction that takes place at time t_{int}. This interaction may result in a change of the initial probabilities c_1^2 and c_2^2 generated by the primary impressed source. The scheme of the stochastic interaction process that is now of our interest is depicted in Fig. 5.2. It depends on a parameter β. The scheme with corresponding probability amplitudes that fits into this interaction process is shown in Fig. 5.3. To give an idea of how to put such a probability experiment into practice, let us go back to the initially mentioned experiment with black and white marbles. It runs as follows: *The primary impressed, stochastic source is represented by a box B_p that contains one white and one black marble. The stochastic interaction, on the other hand, is represented by two additional boxes B_w and B_b filled with different numbers of black and white marbles. The number of marbles in box B_w is such that we have the probabilities* $\cos^2\beta/\sin^2\beta$ *to draw a white/black marble from this box (if $\beta = \pi/8$, for example, then there are 17 white and three black marbles in this box). Correspondingly, the number of marbles in box B_b is such that we have the probabilities* $\cos^2\beta/\sin^2\beta$ *to draw a black/white marble from this box (if $\beta = \pi/8$, then there are 17 black and three white marbles in this box). Each single experiment is performed in the following way: We draw blindly one marble from box B_p. If this is a white marble we draw another marble blindly from box B_w. Its colour is the result of this single experiment. But if we draw a black marble from box B_p we have to draw another marble blindly from box B_b. The result of this single experiment is then given by the colour of this marble*. The observed probabilities are independent of the parameter β and given by

$$c_1^2 = c_2^2 = \frac{1}{2}\,, \tag{5.31}$$

as the reader may verify by himself (500 single events are sufficient for a fixed parameter β, as me and my family find out at a rainy weekend). That is, this

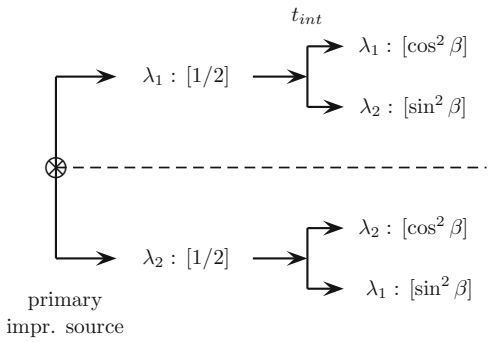

Fig. 5.2 Stochastic interaction at time t_{int}. A primary impressed, stochastic source generates the two probabilities $c_1^2 = c_2^2 = 1/2$ if the two possible events are always detected before t_{int}. After the interaction and depending on the parameter β both events may possibly be observed with different probabilities

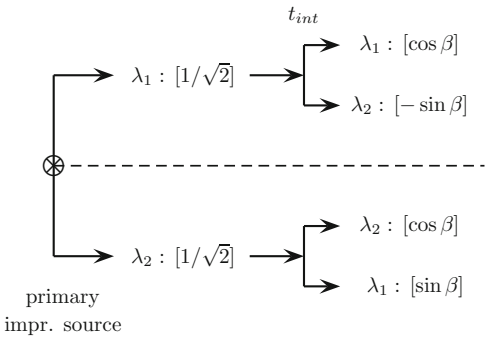

Fig. 5.3 Scheme of β-dependent amplitudes that fits into the stochastic interaction process depicted in Fig. 5.2

experiment does not results in a change of the probabilities generated by the primary impressed source.

But how can this experiment be related to a Green's function formalism? To answer this question we will fall back on our experience that an interaction process can in some situations equivalently be described by a basis transformation. This is what we have already demonstrated in conjunction with the interaction of a linearly polarized plane wave with a polarizing filter, and with plane wave scattering on a sphere. We first note that the two states

$$|\,\tilde{\varphi}_1\rangle \;=\; (\cos\beta, -\sin\beta) \tag{5.32}$$

$$|\,\tilde{\varphi}_2\rangle \;=\; (\sin\beta, \cos\beta) \tag{5.33}$$

form also a basis in the considered 2-dim. event space. Employing the shorter matrix-vector notation introduced in Sect. 4.2 (or, better, matrix-supervector notation since the elements of this supervector are the basis vectors) the relation between the old and new basis vectors may be expressed by

$$(|\,\varphi_1\rangle, |\,\varphi_2\rangle) \;=\; (|\,\tilde{\varphi}_1\rangle, |\,\tilde{\varphi}_2\rangle) \cdot \mathbf{T}_{\boldsymbol{\beta}} \tag{5.34}$$

with the so far unknown transformation matrix $\mathbf{T}_{\boldsymbol{\beta}}$. Dyadic multiplication of this expression by the column vector $(\langle\tilde{\varphi}_1\,|, \langle\tilde{\varphi}_2\,|)^{tp}$ from the left,

$$\begin{pmatrix} \langle\tilde{\varphi}_1\,| \\ \langle\tilde{\varphi}_2\,| \end{pmatrix} \cdot (|\,\varphi_1\rangle, |\,\varphi_2\rangle) \;=\; \begin{pmatrix} \langle\tilde{\varphi}_1\,| \\ \langle\tilde{\varphi}_2\,| \end{pmatrix} \cdot (|\,\tilde{\varphi}_1\rangle, |\,\tilde{\varphi}_2\rangle) \cdot \mathbf{T}_{\boldsymbol{\beta}}\;, \tag{5.35}$$

provides

$$\mathbf{T}_{\boldsymbol{\beta}} \;=\; \begin{pmatrix} \langle\tilde{\varphi}_1\,|\,\varphi_1\rangle & \langle\tilde{\varphi}_1\,|\,\varphi_2\rangle \\ \langle\tilde{\varphi}_2\,|\,\varphi_1\rangle & \langle\tilde{\varphi}_2\,|\,\varphi_2\rangle \end{pmatrix} \;=\; \begin{pmatrix} \cos\beta & -\sin\beta \\ \sin\beta & \cos\beta \end{pmatrix}\;. \tag{5.36}$$

This T-matrix is nothing but the matrix (4.60) of rotation. Furthermore,

$$\mathbf{D_2} \;=\; \sum_{n=1}^{2} |\,\tilde{\varphi}_n\rangle\langle\tilde{\varphi}_n\,| \tag{5.37}$$

represents again a unit dyad (unit operator), and the corresponding Green's function reads

$$\mathbf{G_R}(t,t') \;=\; \frac{i}{a}\cdot\sum_{n=1}^{2} \mid \tilde{\varphi}_n(t)\rangle\langle\tilde{\varphi}_n(t') \mid \;. \tag{5.38}$$

Next,

$$\mathbf{G_t}(t,t') \;=\; \mathbf{G}(t,t')\cdot H(t_{int}-t) \;+\; \mathbf{G_R}(t,\bar{t})\circ\mathbf{W}(\bar{t},\tilde{t})\circ\mathbf{G}(\tilde{t},t')\cdot H(t-t_{int}) \tag{5.39}$$

is used as an *ansatz* for the total Green's function of the considered probability experiment. The Heaviside functions allow us to distinguish whether the single events are measured before or after the interaction process, as already mentioned. $\mathbf{G}(t,t')$ and $\mathbf{G_R}(t,t')$ are given by (5.20) and (5.38). Equation (5.39) can be compared with *ansatz* (4.176) used for the scattering part of the Green's function related to plane wave scattering on a sphere. It should also be perceived as the defining equation for the so far unknown "interaction operator" $\mathbf{W}$. This operator can be determined from the condition

$$\lim_{\epsilon\to 0}\left[\sum_{k=1}^{2}\langle\varphi_k \mid \mathbf{G_t} \mid \varphi_k\rangle\right]_{t=t_{int}-\epsilon} \;=\; \lim_{\epsilon\to 0}\left[\sum_{k=1}^{2}\langle\varphi_k \mid \mathbf{G_t} \mid \varphi_k\rangle\right]_{t=t_{int}+\epsilon} \quad ; \quad \epsilon>0 \tag{5.40}$$

that relates the two parts before and after the interaction, and that guarantees the conservation of the respective sum of probabilities. We thus get

$$\sum_{k,n=1}^{2}\langle\,\varphi_k \mid \varphi_n(t)\rangle\,\langle\,\varphi_n(t') \mid \varphi_k\rangle \;=$$

$$\frac{i}{a}\cdot\sum_{k,n,m=1}^{2}\langle\varphi_k \mid \tilde{\varphi}_n(t)\rangle\,\langle\tilde{\varphi}_n(\bar{t}) \mid \mathbf{W}(\bar{t},\tilde{t}) \mid \varphi_m(\tilde{t})\rangle\,\langle\varphi_m(t') \mid \varphi_k\rangle\;. \tag{5.41}$$

With the definition

$$[W]_{nm}(\bar{t},\tilde{t}) \;:=\; \langle\tilde{\varphi}_n(\bar{t}) \mid \mathbf{W} \mid \varphi_m(\tilde{t})\rangle\;; \quad n,m \;=\; 1,2 \tag{5.42}$$

of the matrix elements of the interaction operator the right-hand side of (5.41) may be rewritten into

$$\frac{i}{a}\cdot\sum_{k,n,m=1}^{2}[W]_{nm}(\bar{t},\tilde{t})\cdot\langle\varphi_k \mid \tilde{\varphi}_n(t)\rangle\cdot\langle\varphi_m(t') \mid \varphi_k\rangle\;. \tag{5.43}$$

Taking relation (5.34) and property (5.15) into account, it follows that Eq. (5.41) holds if the matrix elements of the interaction operator are given by

$$[W]_{nm}(\bar{t},\tilde{t}) \;=\; \frac{a}{i}\cdot e^{\frac{i}{a}\cdot\lambda_n\cdot\bar{t}-\frac{i}{a}\cdot\lambda_m\cdot\tilde{t}}\cdot[T_\beta]_{nm}\cdot\delta(\bar{t}-t_{int})\cdot\delta(\tilde{t}-t_{int})\;;\quad n,m\;=\;1,2\;. \tag{5.44}$$

The total Green's function that fits into the scheme of Fig. 5.3 reads therefore

$$\mathbf{G_t}(t,t') \;=\; \frac{i}{a}\cdot H(t_{int}\;-\;t)\cdot\sum_{n,m=1}^{2}\delta_{nm}\cdot\mid\varphi_n(t)\rangle\langle\varphi_m(t')\mid\;+$$

$$\frac{i}{a}\cdot H(t\;-\;t_{int})\cdot\sum_{n,m=1}^{2}e^{-\frac{i}{a}(\lambda_m-\lambda_n)\cdot t_{int}}\cdot[T_\beta]_{nm}\cdot\mid\tilde{\varphi}_n(t)\rangle\langle\varphi_m(t')\mid\;. \tag{5.45}$$

From (5.10), Green's function (5.45) for observation times $t > t_{int}$, and from the two subsources (5.26) and (5.27) we get the two time dependent substates

$$\mid\psi_1(t)\rangle\;=\;\frac{1}{\sqrt{2}}\cdot\sum_{n=1}^{2}e^{-\frac{i}{a}(\lambda_1-\lambda_n)\cdot t_{int}}\cdot e^{-\frac{i}{a}\lambda_n\cdot t}\cdot e^{\frac{i}{a}\lambda_1\cdot t_0'}\cdot[T_\beta]_{n1}\cdot\mid\tilde{\varphi}_n\rangle \tag{5.46}$$

and

$$\mid\psi_2(t)\rangle\;=\;\frac{1}{\sqrt{2}}\cdot\sum_{n=1}^{2}e^{-\frac{i}{a}(\lambda_2-\lambda_n)\cdot t_{int}}\cdot e^{-\frac{i}{a}\lambda_n\cdot t}\cdot e^{\frac{i}{a}\lambda_2\cdot t_0'}\cdot[T_\beta]_{n2}\cdot\mid\tilde{\varphi}_n\rangle\;. \tag{5.47}$$

Then, from definition (5.24) it follows

$$\mid\psi_1\rangle\;=\;\frac{1}{\sqrt{2}}\cdot\sum_{n=1}^{2}[T_\beta]_{n1}\cdot\mid\tilde{\varphi}_n\rangle\;=$$

$$\frac{1}{\sqrt{2}}\cdot(\cos\beta\cdot\mid\tilde{\varphi}_1\rangle\;+\;\sin\beta\cdot\mid\tilde{\varphi}_2\rangle) \tag{5.48}$$

and

$$\mid\psi_2\rangle\;=\;\frac{1}{\sqrt{2}}\cdot\sum_{n=1}^{2}[T_\beta]_{n2}\cdot\mid\tilde{\varphi}_n\rangle\;=$$

$$\frac{1}{\sqrt{2}}\cdot(-\sin\beta\cdot\mid\tilde{\varphi}_1\rangle\;+\;\cos\beta\cdot\mid\tilde{\varphi}_2\rangle) \tag{5.49}$$

for the corresponding time independent expressions. It is now straightforward to show that we end up with the probabilities (5.31) if the probabilities of each event

are at first calculated separately from the projections

$$| (\psi_{1/2})_n\rangle = | \tilde{\varphi}_n\rangle\langle\tilde{\varphi}_n | \psi_{1/2}\rangle \; ; \quad n = 1, 2 \tag{5.50}$$

of each substate and summed up afterwards. It should also be noted that the probabilities obtained from each substate separately belong to the following modification of the marble experiment: Regarding $| \psi_1\rangle$ we have

$$c_1^2 = \frac{1}{2} \cdot \cos^2 \beta \tag{5.51}$$

and

$$c_2^2 = \frac{1}{2} \cdot \sin^2 \beta \; . \tag{5.52}$$

These are the probabilities for drawing a white (c_1^2) or black marble (c_2^2) from box B_w if a white marble was drawn from the primary box B_p. From $| \psi_2\rangle$ we get on the other hand

$$c_1^2 = \frac{1}{2} \cdot \sin^2 \beta \tag{5.53}$$

and

$$c_2^2 = \frac{1}{2} \cdot \cos^2 \beta \; . \tag{5.54}$$

These are the probabilities for drawing a white (c_1^2) or black marble (c_2^2) from box B_b if a black marble was drawn from the primary box B_p. These probabilities are dependent on the parameter β. But there exists another possibility to calculate probabilities. The superposition of the two substates provides the total state

$$| \psi_t\rangle = \frac{1}{\sqrt{2}} \cdot [(\cos \beta - \sin \beta) \cdot | \tilde{\varphi}_1\rangle + (\cos \beta + \sin \beta) \cdot | \tilde{\varphi}_2\rangle] \; . \tag{5.55}$$

The probabilities are then given by

$$c_1^2 = \frac{1}{2} (1 - 2 \cos \beta \sin \beta) \tag{5.56}$$

and

$$c_2^2 = \frac{1}{2} (1 + 2 \cos \beta \sin \beta) \tag{5.57}$$

which show the characteristic interference term we discovered already in conjunction with the intensities (4.69)–(4.71) in Sect. 4.2. This is a consequence of the fact that both substates are now nondisjoint vectors since they do have basis vectors in common. But these probabilities do not agree with our experimental experience from the marble experiment! One may ask if there exists any probability experiment that would end up with such probabilities? Let us shift the answer to the next section.

5.1.3 An Alternative Description of the Probability Experiments

The whole problem with the time dependence of the probability state vector can be avoided if employing the "source picture" of the Fourier series, as introduced in Sect. 2.6 (see Eqs. (2.297)–(2.299) and the subsequent discussion). Regarding the probability experiments considered in this section this can simply be achieved if replacing our pivotal relation (5.10) by

$$\mid \psi\rangle \; = \; \mathbf{F} \circ \mid \rho\rangle \; , \tag{5.58}$$

and if using

$$\mathbf{F} \; = \; \mathbf{D_1} \cdot H(t_{int} - t) \; + \; \mathbf{D_2} \circ \mathbf{W} \circ \mathbf{D_1} \cdot H(t - t_{int}) \; . \tag{5.59}$$

instead of *ansatz* (5.39) for the Green's function in the presence of the additional stochastic interaction. Let us call $\mathbf{F}$ the "Fourier-operator" since it transfers the Fourier series of the source state into the Fourier series of the probability state. With the exception of the Heaviside functions all quantities in (5.58) and (5.59) are now considered to be independent of time. $\mathbf{D_{1/2}}$ are the unit operators according to (5.12)/(5.37), and $\mathbf{W}$ is again the interaction operator. With the Heaviside function we distinguish again between a "before" and an "after" the interaction. The Fourier operator is identical with the unit operator D_1 before the interaction. Applying condition (5.40) to (5.59) results in

$$\begin{aligned} \mathbf{F} \; = \; H(t_{int} \; - \; t) \cdot \sum_{n,m=1}^{2} \delta_{nm} \cdot \mid \varphi_n\rangle\langle\varphi_m \mid \; + \\ H(t \; - \; t_{int}) \cdot \sum_{n,m=1}^{2} [T_\beta]_{nm} \cdot \mid \tilde{\varphi}_n\rangle\langle\varphi_m \mid \; . \end{aligned} \tag{5.60}$$

$$[W]_{nm} \; = \; [T_\beta]_{nm} \; ; \quad n, m \; = \; 1, 2 \tag{5.61}$$

are now the corresponding matrix elements of the interaction operator. With the impressed source

$$|\,\rho\rangle = |\,\rho_1\rangle + |\,\rho_2\rangle\,, \tag{5.62}$$

where $|\,\rho_1\rangle$ and $|\,\rho_2\rangle$ are given by

$$|\,\rho_1\rangle = c_1 \cdot |\,\varphi_1\rangle \tag{5.63}$$

and

$$|\,\rho_2\rangle = c_2 \cdot |\,\varphi_2\rangle\,, \tag{5.64}$$

and in dependence on whether we have $t < t_{int}$ or $t > t_{int}$ we arrive immediately at (5.28)/(5.29) or (5.48)/(5.49). This is again more than a simple tautological mapping of the source onto the state, as already discussed in Sect. 2.6 in a formal manner.

5.2 Probability Experiments in a Four-Dimensional Event Space

5.2.1 Probability States and Green's Function

The classical events of our interest in this section are still the "click" and "not a click" of a detector. But now we have two detectors placed above and below or on the left- and right-hand side of a primary impressed, stochastic source. To get an idea of the situation let us consider the following modifications of the experiments mentioned at the beginning of Sect. 5.1.1:

- When a coin is flipped, the result is either "head faces up" and "tail faces down" or "tail faces up" and "head faces down". Two detectors are placed above (detector D_A) and below (detector D_B) the coin. A detector produces a click if the head is detected. There will be no click otherwise. The two different pairs of events in a single experimental step are "click of D_A" but "no click of D_B", and "click of D_B" but "no click of D_A".
- An example of a stochastic momentum source acting on two classical point masses of mass m with two possible momenta is shown in Fig. 5.4. A detector produces a click if momentum p_a is detected. There will be no click if momentum p_b is detected. This provides again the two different pairs of events mentioned in the foregoing example.
- Two marbles are blindly drawn from a box that contains a number of white and black marbles. They are placed (also blindly) on the left- and right-hand side of this box. Moreover, a detector is mounted on each side (detector D_A on the left-

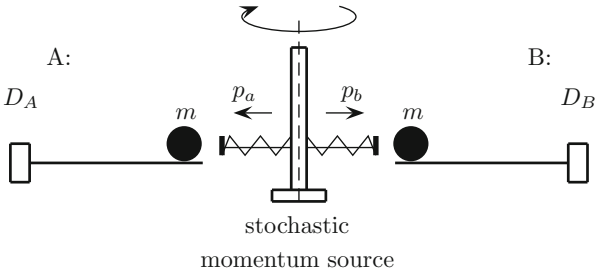

Fig. 5.4 Experimental setup of a stochastic momentum source acting like a wheel of Fortune on two classical point masses of mass m with the two possible momenta p_a and p_b

hand side, and detector D_B on the right-hand side) that produces a click if a white marble is detected. There will be no click otherwise. We thus have in general 4 different pairs of events: "click of D_A" but "no click of D_B", "click of D_B" but "no click of D_A", "click of both detectors", and "no click of both detectors".

- Two electrons are simultaneously emitted from a source into its left- and right-hand side. If each electron is traversing an inhomogeneous magnetic field, it is either deflected up or down. A detector is mounted on each side that produces a click if an upward deflection is detected. There will be no click otherwise. This provides the 4 different pairs of events mentioned in the foregoing example.
- Two linearly polarized photons are simultaneously emitted from a source into its left- and right-hand side. If each photon hits upon a polarizing filter that is arbitrarily oriented with respect to the plane of polarization of the incoming photon, the photon is either allowed to pass through or it is blocked out. A detector on each side produces a click if the photon is allowed to pass through. There will be no click otherwise. This provides the 4 different pairs of events mentioned in the two foregoing examples.

Regarding the last three examples we have in general 4 different pairs of events. These are the combinations of the single events on both sides (side A and B). We say that

- both detectors are in the product state

$$|\,\varphi_1\rangle\,|\,\varphi_1\rangle\,=|\,\varphi_{11}\rangle \tag{5.65}$$

if there are clicks on both sides.

$$\Lambda_{11}\;=\;\lambda_1\cdot\lambda_1 \tag{5.66}$$

is the corresponding product of the eigenvalues.

- both detectors are in the product state

$$|\,\varphi_1\rangle\,|\,\varphi_2\rangle\,=|\,\varphi_{12}\rangle \tag{5.67}$$

if D_A produces a click but not D_B.

$$\Lambda_{12} \;=\; \lambda_1 \cdot \lambda_2 \tag{5.68}$$

is the corresponding product of the eigenvalues.

- both detectors are in the product state

$$|\,\varphi_2\rangle\,|\,\varphi_1\rangle \;=|\,\varphi_{21}\rangle \tag{5.69}$$

if D_B produces a click but not D_A.

$$\Lambda_{21} \;=\; \lambda_2 \cdot \lambda_1 \tag{5.70}$$

is the corresponding product of the eigenvalues.

- both detectors are in the product state

$$|\,\varphi_2\rangle\,|\,\varphi_2\rangle \;=|\,\varphi_{22}\rangle \tag{5.71}$$

if there are no clicks on both sides.

$$\Lambda_{22} \;=\; \lambda_2 \cdot \lambda_2 \tag{5.72}$$

is the corresponding product of the eigenvalues.

The eigenvalues are again $\lambda_1 = 1$ and $\lambda_2 = -1$. These vectors form a basis in the 4-dim. product space. They can be considered to represent the eigenvectors of the dyadic quantity

$$\mathbf{\Sigma} \;=\; \sum_{i,j=1}^{2} \Lambda_{ij} \cdot |\,\varphi_{ij}\rangle\langle\varphi_{ji}\,| \quad . \tag{5.73}$$

The related eigenvalue problem reads

$$\mathbf{\Sigma} \circ |\,\varphi_{ij}\rangle \;-\; \Lambda_{ij} \cdot |\,\varphi_{ij}\rangle \;=|\,0\rangle\;; \quad i,j = 1,2\,. \tag{5.74}$$

Please, note that the scalar product of the two vectors $|f,g\rangle$ and $|p,q\rangle$ in the product space is defined according to

$$\langle g,f\,|\,p,q\rangle \;:=\; \langle f\,|\,p\rangle \cdot \langle g\,|\,q\rangle\,. \tag{5.75}$$

It should therefore again be possible to completely characterize every probability experiment in this product space by the abstract probability state vector

$$|\,\psi\rangle \;=\; \sum_{i,j=1}^{2} c_{ij} \cdot |\,\varphi_{ij}\rangle\,, \tag{5.76}$$

where c_{ij} are now the probability amplitudes related to the four possible pairs of events. The corresponding probabilities are obtained by the scalar product of the projections

$$| \psi_{nm} \rangle = | \varphi_{nm} \rangle \langle \varphi_{mn} | \psi \rangle \; ; \quad n, m = 1, 2 \; . \tag{5.77}$$

That is, we have

$$\langle \psi_{mn} | \psi_{nm} \rangle = c_{nm}^2 \; ; \quad n, m = 1, 2 \; , \tag{5.78}$$

and

$$\sum_{n,m=1}^{2} c_{nm}^2 = 1 \; . \tag{5.79}$$

Next, we intend to relate this procedure again to a Green's function formalism. The Green's function is now a solution of the Schrödinger-like equation

$$- i a \cdot \frac{d\mathbf{G}(t, t')}{dt} + \mathbf{\Sigma} \circ \mathbf{G}(t, t') = - \mathbf{D_1} \cdot \delta(t - t') \tag{5.80}$$

with dyad $\mathbf{\Sigma}$ given by (5.73). $\mathbf{D_1}$ on the right-hand side represents the unit dyad (unit operator)

$$\mathbf{D_1} = \sum_{n,m=1}^{2} | \varphi_{nm} \rangle \langle \varphi_{mn} | \tag{5.81}$$

in this product space. This equation can again be solved with the Fourier transform method by employing (5.17) and (5.18) with respect to time. Expanding the Fourier transform of the Green's function in terms of the dyadic products of the eigenvectors $| \varphi_{nm} \rangle$ gives

$$\mathbf{G}(\omega) = \frac{1}{a} \cdot \sum_{n,m=1}^{2} \frac{| \varphi_{nm} \rangle \langle \varphi_{mn} |}{\omega - \frac{\Lambda_{nm}}{a}} \; , \tag{5.82}$$

Inserting this expression into (5.17) and applying the residual theorem provides now the Green's function

$$\mathbf{G}(t, t') = \frac{i}{a} \sum_{n,m=1}^{2} | \varphi_{nm}(t) \rangle \langle \varphi_{mn}(t') | \; , \tag{5.83}$$

where

$$| \varphi_{nm}(t) \rangle = e^{-\frac{i}{a} \Lambda_{nm} \cdot t} \cdot | \varphi_{nm} \rangle \; , \tag{5.84}$$

and

$$\langle \varphi_{mn}(t) \mid = e^{\frac{i}{a}\Lambda_{nm}\cdot t} \cdot \langle \varphi_{mn} \mid \ . \tag{5.85}$$

Any primary impressed source

$$\mid \rho(t')\rangle \ = \ \frac{a}{i} \cdot \delta(t' - t'_0) \cdot \sum_{i,j=1}^{2} \rho_{ij} \cdot \mid \varphi_{ij}\rangle \tag{5.86}$$

with coefficients ρ_{ij} considered to be given provides the time dependent probability state vector

$$\mid \psi(t)\rangle \ = \ \int_{t'_0}^{t^+} \mathbf{G}(t,t') \circ \mid \rho(t')\rangle \, dt' \ = \ \sum_{i,j=1}^{2} \rho_{ij} \cdot \mid \varphi_{ij}(t - t'_0)\rangle \ . \tag{5.87}$$

Applying definition (5.24) results finally in the corresponding time independent probability state vector

$$\mid \psi\rangle \ = \ \sum_{i,j=1}^{2} \rho_{ij} \cdot \mid \varphi_{ij}\rangle \ . \tag{5.88}$$

As an example, let us now consider the primary impressed source

$$\mid \rho(t')\rangle \ = \mid \rho_1(t')\rangle + \ \mid \rho_2(t')\rangle \ , \tag{5.89}$$

where

$$\mid \rho_1(t')\rangle \ = \ \frac{a}{i} \cdot \delta(t' - t'_0) \cdot \frac{1}{\sqrt{2}} \cdot \mid \varphi_{12}\rangle \tag{5.90}$$

and

$$\mid \rho_2(t')\rangle \ = \ -\frac{a}{i} \cdot \delta(t' - t'_0) \cdot \frac{1}{\sqrt{2}} \mid \varphi_{21}\rangle \ . \tag{5.91}$$

Such a source can be related to the probability experiments with the flipped coin and the momentum source, for example, mentioned at the beginning of this section. The resulting time independent substates are accordingly given by

$$\mid \psi_1\rangle \ = \ \frac{1}{\sqrt{2}} \cdot \mid \varphi_{12}\rangle \tag{5.92}$$

and

$$| \psi_2\rangle \; = \; -\frac{1}{\sqrt{2}} \cdot | \varphi_{21}\rangle \; . \tag{5.93}$$

The superposition of these substates represents again the total state

$$| \psi\rangle \; = | \psi_1\rangle + | \psi_2\rangle \; = \; \frac{1}{\sqrt{2}} \cdot (| \varphi_{12}\rangle - | \varphi_{21}\rangle) \; . \tag{5.94}$$

And, since these substates are disjoint, the resulting probabilities

$$c_{12}^2 \; = \; c_{21}^2 \; = \; 1/2 \tag{5.95}$$

for the two pairs of events are again independent of whether these probabilities are calculated from each substate separately, or if calculated from the total state. Please, note also the minus sign in (5.91) that makes this source differ from that one given in (5.25). But the choice of this sign is of no importance as long as probability experiments with classical objects are considered. However, regarding comparable experiments with quantum objects—these are in particular the quantum mechanical Bell's experiments—the minus sign can frequently be found in the literature to characterize the initial state. I will therefore also use it in what follows. And, finally, I want to emphasize again that the state (5.94) and the resulting probabilities (5.95) are in total agreement with our classical experience of such probability experiments! In view of the discussion regarding the epistemological meaning of entanglement in Quantum Mechanics (see the quotation of Schrödinger mentioned in Sect. 1.3, for example) and the fact that (5.94) represents an entangled state, this aspect seems to me of some importance.

5.2.2 Entangled States and CHSH-Inequality

A general probability state in the 4-dim. product space is given by (5.76) and (5.79). It can be shown that, if condition

$$c_{11} \cdot c_{22} \; = \; c_{12} \cdot c_{21} \tag{5.96}$$

holds for the probability amplitudes, then we are able to resolve (5.76) into the product of the two 2-dim. states

$$| \psi_l\rangle = \sum_{n=1}^{2} c_n \cdot | \varphi_n\rangle \tag{5.97}$$

$$| \psi_r\rangle = \sum_{n=1}^{2} \tilde{c}_n \cdot | \varphi_n\rangle \tag{5.98}$$

related to the left- and right-hand side of the probability experiments. The probability amplitudes are again normalized to unity,

$$\sum_{n=1}^{2} c_n^2 \;=\; \sum_{n=1}^{2} \tilde{c}_n^2 \;=\; 1\;. \tag{5.99}$$

Moreover, if condition (5.96) holds the probabilities and amplitudes are related by

$$c_n^2 = \sum_{m=1}^{2} c_{nm}^2 \quad ;\; n = 1,2\;, \tag{5.100}$$

$$\tilde{c}_n^2 = \sum_{m=1}^{2} c_{mn}^2 \quad ;\; n = 1,2\;, \tag{5.101}$$

and

$$c_{nm} \;=\; c_n \cdot \tilde{c}_m\;. \tag{5.102}$$

On the other hand, if condition (5.96) is violated, we are unable to resolve (5.76) into the product of the two states (5.97) and (5.98). In this case (5.76) is called an "entangled state". Condition (5.96) provides therefore a simple criterion to prove whether a given probability state in the 4-dim. event space is entangled or not. Applied to (5.94), it becomes clear that this is indeed an entangled state. This contradicts the point of view that entanglement belongs exclusively to the realm of Quantum Mechanics. Entangled probability states, even if quite formal, can obviously be used to describe also the results of certain experiments with classical objects in a four-dimensional event space.

Let us now discuss the CHSH-inequality. To this end, we assume that the probability amplitudes $c_{nm}(\alpha,\beta)$ are dependent on the two parameters α and β. How this can be accomplished by an additional interaction will be demonstrated shortly. The corresponding probabilities are still normalized to unity,

$$\sum_{n,m=1}^{2} c_{nm}^2(\alpha,\beta) \;=\; 1\;. \tag{5.103}$$

Once we have determined the probabilities $c_{nm}^2(\alpha,\beta)$, $n,m = 1,2$ related to a fixed parameter set (α,β) of a certain experiment in the 4-dim. event space the following correlation function can be defined:

$$C(\alpha,\beta) \;:=\; c_{11}^2(\alpha,\beta) \;+\; c_{22}^2(\alpha,\beta) \;-\; c_{12}^2(\alpha,\beta) \;-\; c_{21}^2(\alpha,\beta)\;. \tag{5.104}$$

It was shown by J. Clauser, M. Horne, A. Shimony, and R. Holt in Clauser et al. (1969) that the inequality

$$\left|C(\alpha,\beta) - C(\alpha,\beta')\right| + \left|C(\alpha',\beta) + C(\alpha',\beta')\right| \leq 2 \tag{5.105}$$

must hold for any experiment that can be described by a "theory of local realism". Here will left open what precisely a "theory of local realism" means since it is outside the scope of this book. But it is tacitly assumed among most of the physicists that—in contrast to Quantum Mechanics—any theory of classical physics belongs to such a theory. That is, there should exist only quantum mechanical probability experiments which result in a violation of this inequality. And such experiments are indeed possible, as first demonstrated by A. Aspect and co-workers (1982). It would therefore be desirable to have a criterion for proving whether the CHSH-inequality can be violated with a certain probability experiment in our 4-dim. event space or not. Here it is:

Due to definition (5.104) and (5.103)

$$|C(\alpha,\beta)| \leq 1 \tag{5.106}$$

holds for any parameter set (α,β). The difference between the two correlation functions $C(\alpha,\beta)$ and $C(\alpha,\beta')$ may be expressed by

$$\begin{aligned} C(\alpha,\beta) - C(\alpha,\beta') &= C(\alpha,\beta)\cdot\left[1 \pm C(\alpha',\beta')\right] - \\ C(\alpha,\beta')\cdot\left[1 \pm C(\alpha',\beta)\right] &= C(\alpha,\beta) - C(\alpha,\beta') \pm \\ \left[C(\alpha,\beta)\cdot C(\alpha',\beta') - C(\alpha,\beta')\cdot C(\alpha',\beta)\right] &. \end{aligned} \tag{5.107}$$

This is obviously an identity only if

$$C(\alpha,\beta)\cdot C(\alpha',\beta') - C(\alpha,\beta')\cdot C(\alpha',\beta) = 0\,. \tag{5.108}$$

That is, if this condition holds (5.107) represents nothing but adding a "nutritious zero" to the difference of $C(\alpha,\beta)$ and $C(\alpha,\beta')$. Taking the inequality

$$|a-b| \leq |a| + |b| \tag{5.109}$$

into account we thus get from (5.107)

$$\begin{aligned} \left|C(\alpha,\beta) - C(\alpha,\beta')\right| \leq &\left|C(\alpha,\beta)\cdot\left[1 \pm C(\alpha',\beta')\right]\right| + \\ &\left|C(\alpha,\beta')\cdot\left[1 \pm C(\alpha',\beta)\right]\right|\,. \end{aligned} \tag{5.110}$$

The expressions inside the brackets on the right-hand side are always ≥ 0, according to (5.106). We can therefore also write

$$\begin{aligned}\left|C(\alpha,\beta) - C(\alpha,\beta')\right| \leq\ & |C(\alpha,\beta)| \cdot \left[1 \pm C(\alpha',\beta')\right] + \\ & \left|C(\alpha,\beta')\right| \cdot \left[1 \pm C(\alpha',\beta)\right] . \end{aligned} \tag{5.111}$$

From this expression and from (5.106) the inequality

$$\begin{aligned}\left|C(\alpha,\beta) - C(\alpha,\beta')\right| &\leq 2 \pm \left[C(\alpha',\beta') + C(\alpha',\beta)\right] \\ &\leq 2 - \left|C(\alpha',\beta') + C(\alpha',\beta)\right| \end{aligned} \tag{5.112}$$

follows in a straightforward way. But we see also that

$$C(\alpha,\beta) \cdot C(\alpha',\beta') - C(\alpha,\beta') \cdot C(\alpha',\beta) \neq 0 \tag{5.113}$$

is a **necessary condition** to violate the CHSH-inequality!

5.2.3 *Stochastic Interaction*

The scheme of the stochastic interaction process that is of our interest in this 4-dim. event space is depicted in Fig. 5.5. It is an extension of the scheme depicted in Fig. 5.3 to the left-hand side. To give an idea of how to put a corresponding probability experiment with classical objects into practice, let us again fall back to

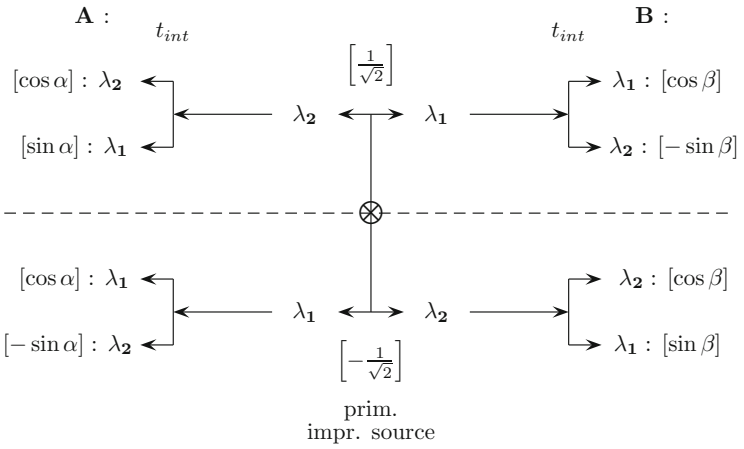

Fig. 5.5 Scheme of a probability experiment with two additional but local interactions at $t = t_{int}$ in a 4-dim. event space. The local interactions on the left- and right-hand side are dependent on the parameters α and β. The related probability amplitudes are given in the square brackets

the marble experiment. It runs as follows: *A box B_p with one white and one black marble represents the primary impressed source that generates the two pairs (white marble, black marble) and (black marble, white marble) on side (A,B), each with a probability of* $1/2$. *Two additional boxes B_w and B_b are filled with 17 white and three black marbles (box B_w), and 17 black and three white marbles (box B_b). These two boxes represent again the local interaction on the right-hand side if* $\beta = \pi/8$. *If there is no additional interaction on the left-hand side we have the parameter configuration* $(\alpha, \beta) = (0, \pi/8)$ *for this experiment. We proceed as follows:*

We draw both marbles blindly from box B_p and put one marble on the left-hand side and the other marble on the right-hand side on our desk. The colour of the marble on the left-hand side is already the result of this side since $\alpha = 0$. *To get the result on the right-hand side requires an additional step. If the primary marble on the right-hand side is white, then we have to draw another marble from box B_w. Its colour is the result on the right-hand side. But if the primary marble on the right-hand side is black, then we have to draw another marble from box B_b. Its colour will then be the result on the right-hand side. We repeat this procedure until we are able to calculate the four probabilities* c_{11}^2 *=(white, white),* c_{22}^2 *=(black, black),* c_{12}^2 *=(white, black), and* c_{21}^2 *=(black, white) related to the colours of the marbles on both sides within a sufficient accuracy (please, remember that a white marble produces a "click", and a black marble produces "not a click" of the respective detector!). The corresponding correlation function* $C(0, \pi/8)$ *is obtained from (5.104).*

If the parameter configuration $(0, 3\pi/8)$ *is chosen, the experiment runs as follows: The first step to get the result on the left-hand side is as before. But, now, if the primary marble on the right-hand side is white, then we have to draw another marble from box B_b. Its colour is the result on the right-hand side. On the other hand, if the primary marble on the right-hand side is black, then we have to draw another marble from box B_w. This colour will then be the result on the right-hand side. We repeat this procedure again until we are able to calculate the probabilities and the correlation function* $C(0, 3\pi/8)$ *within a sufficient accuracy.*

We can proceed in a similar way if the local parameter α *on the left-hand side is nonzero. The only thing we have to do is to fill two additional boxes on the left-hand side with an appropriate number of black and white marbles to meet the probabilities of the local interaction on this side. If* $\alpha = \pi/4$, *for example,* $\sin^2\alpha = \cos^2\alpha = 1/2$ *holds. That is, only one additional box with one white and one black marble is needed in this case on the left-hand side.*

Performing this experiment with at least 5000 single measurements for a given parameter configuration (α, β) is sufficient to approach the probabilities obtained from conventional probability theory. These probabilities are given by

$$c_{11}^2 = c_{22}^2 = \frac{1}{2} \cdot \left(\sin^2\alpha \cdot \cos^2\beta + \sin^2\beta \cdot \cos^2\alpha\right) \tag{5.114}$$

$$c_{12}^2 = c_{21}^2 = \frac{1}{2} \cdot \left(\cos^2\alpha \cdot \cos^2\beta + \sin^2\beta \cdot \sin^2\alpha\right) . \tag{5.115}$$

Let us accept these probabilities as an experimental fact.

Exercise: Development of a computer programm for the above described marble experiment. Use this program to test (5.114) and (5.115). A PYTHON code for this experiment is given in Appendix A.3.

Now we are again interested in deriving these probabilities from a Green's function in the 4-dim. event space. This can be accomplished in the same way as described in Sect. 5.1.2. We note that beside the basis $\mid \varphi_{ij}\rangle; i,j = 1,2$ defined in (5.65)–(5.71) the product vectors

$$\mid \tilde{\varphi}_{ij}^{AB}\rangle = \mid \tilde{\varphi}_{i}^{A}\rangle \mid \tilde{\varphi}_{j}^{B}\rangle \; ; \quad i,j = 1,2 \; , \tag{5.116}$$

where

$$\mid \tilde{\varphi}_{1}^{A}\rangle = (\cos\alpha, -\sin\alpha) \tag{5.117}$$

$$\mid \tilde{\varphi}_{1}^{B}\rangle = (\cos\beta, -\sin\beta) \tag{5.118}$$

$$\mid \tilde{\varphi}_{2}^{A}\rangle = (\sin\alpha, \cos\alpha) \tag{5.119}$$

$$\mid \tilde{\varphi}_{2}^{B}\rangle = (\sin\beta, \cos\beta) \; , \tag{5.120}$$

represent also a basis in the 4-dim. product space. For the sake of convenience, let us introduce the shorter notation

$$\begin{array}{lll} \mid \Xi_1\rangle := \mid \varphi_{11}\rangle & , & \mid \Xi_2\rangle := \mid \varphi_{12}\rangle \\ \mid \Xi_3\rangle := \mid \varphi_{21}\rangle & , & \mid \Xi_4\rangle := \mid \varphi_{22}\rangle \; , \end{array} \tag{5.121}$$

and

$$\begin{array}{lll} \mid \Psi_1\rangle := \mid \tilde{\varphi}_{11}^{AB}\rangle & , & \mid \Psi_2\rangle := \mid \tilde{\varphi}_{12}^{AB}\rangle \\ \mid \Psi_3\rangle := \mid \tilde{\varphi}_{21}^{AB}\rangle & , & \mid \Psi_4\rangle := \mid \tilde{\varphi}_{22}^{AB}\rangle \; , \end{array} \tag{5.122}$$

for these two systems of basis vectors. The shorter notation

$$\begin{aligned} \bar{\Lambda}_1 &= \Lambda_{11} \\ \bar{\Lambda}_2 &= \Lambda_{12} \\ \bar{\Lambda}_3 &= \Lambda_{21} \\ \bar{\Lambda}_4 &= \Lambda_{22} \; . \end{aligned} \tag{5.123}$$

is used for the corresponding products of the eigenvalues. The two expansions

$$\mathbf{D_1} = \sum_{i=1}^{4} \mid \Xi_i\rangle \, \langle \, \Xi_i \mid \tag{5.124}$$

(this is identical with (5.81)) and

$$\mathbf{D_2} = \sum_{i=1}^{4} \mid \Psi_i\rangle \langle \Psi_i \mid \tag{5.125}$$

in terms of the sum of dyadic products represent the unit operators in the respective product space before and after the interaction. And, in analogy to (5.83), the Green's function in the latter 4-dim. product space reads

$$\mathbf{G_R}(t,t') = \frac{i}{a} \sum_{n=1}^{4} \mid \Psi_n(t)\rangle\langle\Psi_n(t') \mid , \tag{5.126}$$

where

$$\mid \Psi_n(t)\rangle = e^{-\frac{i}{a}\bar{\Lambda}_n \cdot t} \cdot \mid \Psi_n\rangle , \tag{5.127}$$

and

$$\langle\Psi_n(t') \mid = e^{\frac{i}{a}\bar{\Lambda}_n \cdot t'} \cdot \mid \Psi_n\rangle . \tag{5.128}$$

Next, we introduce the T-matrix

$$\mathbf{T_{\alpha\beta}} = \begin{pmatrix} \langle \Psi_1 \mid \Xi_1\rangle & \langle \Psi_1 \mid \Xi_2\rangle & \langle \Psi_1 \mid \Xi_3\rangle & \langle \Psi_1 \mid \Xi_4\rangle \\ \langle \Psi_2 \mid \Xi_1\rangle & \langle \Psi_2 \mid \Xi_2\rangle & \langle \Psi_2 \mid \Xi_3\rangle & \langle \Psi_2 \mid \Xi_4\rangle \\ \langle \Psi_3 \mid \Xi_1\rangle & \langle \Psi_3 \mid \Xi_2\rangle & \langle \Psi_3 \mid \Xi_3\rangle & \langle \Psi_3 \mid \Xi_4\rangle \\ \langle \Psi_4 \mid \Xi_1\rangle & \langle \Psi_4 \mid \Xi_2\rangle & \langle \Psi_4 \mid \Xi_3\rangle & \langle \Psi_4 \mid \Xi_4\rangle \end{pmatrix} =$$

$$\begin{pmatrix} cos\alpha \cdot \cos\beta & -\cos\alpha \cdot \sin\beta & -\sin\alpha \cdot \cos\beta & \sin\alpha \cdot \sin\beta \\ \cos\alpha \cdot \sin\beta & \cos\alpha \cdot \cos\beta & -\sin\alpha \cdot \sin\beta & -\sin\alpha \cdot \cos\beta \\ \sin\alpha \cdot \cos\beta & -\sin\alpha \cdot \sin\beta & \cos\alpha \cdot \cos\beta & -\cos\alpha \cdot \sin\beta \\ \sin\alpha \cdot \sin\beta & \sin\alpha \cdot \cos\beta & \cos\alpha \cdot \sin\beta & \cos\alpha \cdot \cos\beta \end{pmatrix} . \tag{5.129}$$

It can be shown that the following transformation applies to these basis vectors (compare also (5.34)):

$$(\mid \Xi_1\rangle, \mid \Xi_2\rangle, \mid \Xi_3\rangle, \mid \Xi_4\rangle) = (\mid \Psi_1\rangle, \mid \Psi_2\rangle, \mid \Psi_3\rangle, \mid \Psi_4\rangle) \cdot \mathbf{T_{\alpha\beta}} . \tag{5.130}$$

Regarding $\mid \Xi_1\rangle$, for example, and if taking (5.36) into account we get

$$\mid \Xi_1\rangle = \left([T_\alpha]_{11} \cdot \mid \tilde{\varphi}_1^A\rangle + [T_\alpha]_{21} \cdot \mid \tilde{\varphi}_2^A\rangle\right) \left([T_\beta]_{11} \cdot \mid \tilde{\varphi}_1^B\rangle + [T_\beta]_{21} \cdot \mid \tilde{\varphi}_2^B\rangle\right) . \tag{5.131}$$

This can be rewritten into

$$\begin{aligned} \mid \Xi_1\rangle \;=\; [T_\alpha]_{11}\cdot[T_\beta]_{11}\cdot \mid \Psi_1\rangle \;+\; [T_\alpha]_{11}\cdot[T_\beta]_{21}\cdot \mid \Psi_2\rangle \;+ \\ [T_\alpha]_{21}\cdot[T_\beta]_{11}\cdot \mid \Psi_3\rangle \;+\; [T_\alpha]_{21}\cdot[T_\beta]_{21}\cdot \mid \Psi_4\rangle \;. \end{aligned} \tag{5.132}$$

Thus we have

$$\begin{aligned} \left[T_{\alpha\beta}\right]_{11} &= [T_\alpha]_{11}\cdot[T_\beta]_{11} \\ \left[T_{\alpha\beta}\right]_{21} &= [T_\alpha]_{11}\cdot[T_\beta]_{21} \\ \left[T_{\alpha\beta}\right]_{31} &= [T_\alpha]_{21}\cdot[T_\beta]_{11} \\ \left[T_{\alpha\beta}\right]_{41} &= [T_\alpha]_{21}\cdot[T_\beta]_{21}\;, \end{aligned} \tag{5.133}$$

and so on. The T-matrix (5.129) transforms also the amplitudes $C_n;\; n = 1,\cdots,4$ of a probability state vector given by

$$\mid \psi\rangle \;=\; C_1\cdot \mid \Xi_1\rangle \;+\; C_2\cdot \mid \Xi_2\rangle \;+\; C_3\cdot \mid \Xi_3\rangle \;+\; C_4\cdot \mid \Xi_4\rangle \tag{5.134}$$

into the new amplitudes $\tilde{C}_n;\; n = 1,\cdots,4$ of its representation

$$\mid \psi\rangle \;=\; \tilde{C}_1\cdot \mid \Psi_1\rangle \;+\; \tilde{C}_2\cdot \mid \Psi_2\rangle \;+\; \tilde{C}_3\cdot \mid \Psi_3\rangle \;+\; \tilde{C}_4\cdot \mid \Psi_4\rangle \tag{5.135}$$

in terms of the new basis. That is,

$$\begin{pmatrix} \tilde{C}_1 \\ \tilde{C}_2 \\ \tilde{C}_3 \\ \tilde{C}_4 \end{pmatrix} \;=\; \mathbf{T_{\alpha\beta}}\cdot \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{pmatrix} \tag{5.136}$$

holds. Moreover, (5.129) is again a unitary matrix, i.e.,

$$\left(\mathbf{T_{\alpha\beta}}\right)^{tp}\cdot \mathbf{T_{\alpha\beta}} \;=\; \mathbf{E}\;, \tag{5.137}$$

where $\mathbf{E}$ represents the 4×4 unit matrix. The total Green's function of the probability experiment that fits into the scheme of Fig. 5.5 can again be derived from *ansatz* (5.39) but with all quantities now defined in the product space. Replacing the additional condition (5.40) by

$$\lim_{\epsilon\to 0}\left[\sum_{i=1}^{4}\langle\, \Xi_i \mid \mathbf{G_t} \mid \Xi_i\rangle\right]_{t=t_{int}-\epsilon} \;=\; \lim_{\epsilon\to 0}\left[\sum_{i=1}^{4}\langle\, \Xi_i \mid \mathbf{G_t} \mid \Xi_i\rangle\right]_{t=t_{int}+\epsilon} \tag{5.138}$$

provides the elements

$$[W]_{nm}(\bar{t},\tilde{t}) = \frac{a}{i}\cdot e^{\frac{i}{a}\cdot\bar{\Lambda}_n\cdot\bar{t}-\frac{i}{a}\cdot\bar{\Lambda}_m\cdot\tilde{t}}\cdot[T_{\alpha\beta}]_{nm}\cdot\delta(\bar{t}-t_{int})\cdot\delta(\tilde{t}-t_{int})$$
$$n,m = 1,\cdots,4 \qquad (5.139)$$

of the corresponding interaction matrix. Thus we get finally for the Green's function

$$\mathbf{G_t}(t,t') = \frac{i}{a}\cdot H(t_{int}-t)\cdot\sum_{n,m=1}^{4}\delta_{nm}\cdot\mid\Xi_n(t)\rangle\langle\Xi_m(t')\mid +$$
$$\frac{i}{a}\cdot H(t-t_{int})\cdot\sum_{n,m=1}^{4}e^{-\frac{i}{a}\cdot(\bar{\Lambda}_m-\bar{\Lambda}_n)\cdot t_{int}}\cdot[T_{\alpha\beta}]_{nm}\cdot\mid\Psi_n(t)\rangle\langle\Xi_m(t')\mid . \qquad (5.140)$$

The first and second term on the right-hand side of (5.140) represent again the part before and after the two local interactions on both sides of the probability experiment. From (5.10), the Green's function (5.140) for observation times $t > t_{int}$, and from the two subsources (5.90) and (5.91) we get the two time dependent substates

$$\mid\psi_1(t)\rangle = \frac{1}{\sqrt{2}}\cdot\sum_{n=1}^{4}e^{-\frac{i}{a}(\bar{\Lambda}_2-\bar{\Lambda}_n)\cdot t_{int}}\cdot e^{-\frac{i}{a}\bar{\Lambda}_n\cdot t}\cdot e^{\frac{i}{a}\bar{\Lambda}_2\cdot t'_0}\cdot[T_{\alpha\beta}]_{n2}\cdot\mid\Psi_n\rangle \qquad (5.141)$$

and

$$\mid\psi_2(t)\rangle = \frac{1}{\sqrt{2}}\cdot\sum_{n=1}^{4}e^{-\frac{i}{a}(\bar{\Lambda}_3-\bar{\Lambda}_n)\cdot t_{int}}\cdot e^{-\frac{i}{a}\bar{\Lambda}_n\cdot t}\cdot e^{\frac{i}{a}\bar{\Lambda}_3\cdot t'_0}\cdot[T_{\alpha\beta}]_{n3}\cdot\mid\Psi_n\rangle . \qquad (5.142)$$

Then, from definition (5.24) it follows

$$\mid\psi_1\rangle = \sum_{n=1}^{4}\tilde{C}_n^{(1)}\cdot\mid\Psi_n\rangle = \frac{1}{\sqrt{2}}\cdot\sum_{n=1}^{4}[T_{\alpha\beta}]_{n2}\cdot\mid\Psi_n\rangle \qquad (5.143)$$

$$\mid\psi_2\rangle = \sum_{n=1}^{4}\tilde{C}_n^{(2)}\cdot\mid\Psi_n\rangle = -\frac{1}{\sqrt{2}}\cdot\sum_{n=1}^{4}[T_{\alpha\beta}]_{n3}\cdot\mid\Psi_n\rangle \qquad (5.144)$$

for the corresponding time independent expressions. $[T_{\alpha\beta}]_{n2}$ and $[T_{\alpha\beta}]_{n3}$ are given by (5.129) (i.e., the second and third column of the T-matrix). It should be mentioned that the time dependence can again be avoided by the alternative procedure described in Sect. 5.1.3 but with all quantities defined in the 4-dim. product space.

In the final step we calculate the projections according to

$$| (\psi_1)_n\rangle = | \Psi_n\rangle\langle\Psi_n | \psi_1\rangle \tag{5.145}$$

$$| (\psi_2)_n\rangle = | \Psi_n\rangle\langle\Psi_n | \psi_2\rangle \ , \quad n = 1, \cdots, 4 \ . \tag{5.146}$$

It is then straightforward to see that the probabilities (5.114) and (5.115) are the result of the sum of the scalar products

$$\tilde{C}_n^2 = \left[\tilde{C}_n^{(1)}\right]^2 + \left[\tilde{C}_n^{(1)}\right]^2 = \langle (\psi_1)_n | (\psi_1)_n\rangle + \langle (\psi_2)_n | (\psi_2)_n\rangle \ , \quad n = 1, \cdots, 4 \tag{5.147}$$

of these projections, as already discussed in conjunction with the classical probability experiment in the 2-dim. event space described in Sect. 5.1.2. Inserting these probabilities into expression (5.104) for the correlation function results in

$$C(\alpha, \beta) \ = \ - \cos 2\alpha \cdot \cos 2\beta \tag{5.148}$$

(please, note that $\tilde{C}_1^2$ corresponds with c_{11}^2, $\tilde{C}_2^2$ with c_{12}^2, $\tilde{C}_3^2$ with c_{21}^2, and $\tilde{C}_4^2$ with c_{22}^2). Since condition (5.108) holds for this correlation function we are never able to violate the CHSH-inequality (5.105) by any such classical experiment with the four different parameter configurations (α, β), (α, β'), (α', β), and (α', β'). To treat each substate of the primary impressed source separately appears moreover justified by the obvious fact that this source (the box B_p) generates only one of the two possible pairs of events in a single step of this classical probability experiment. That is, a single experimental step is related **either** to the upper **or** to the lower row of the scheme depicted in Fig. 5.5. By the way, a similar procedure is known from Helmholtz' superposition theorem of electrical circuits. It states that the response of a linear system to more than one independent sources is given by the sum of the responses caused by each independent source acting alone.

The check of condition (5.96) reveals that the two substates (5.143) and (5.144) are nonentangled. But on the other hand and according to our definition, these two substates are now nondisjoint since having all the basis vectors $| \Psi_n\rangle$ in common. We may therefore expect that the superposition of these two substates to the total state

$$| \psi\rangle \ = | \psi_1\rangle + | \psi_2\rangle \ = \ \frac{1}{\sqrt{2}} \cdot \sum_{n=1}^{4} \left([T_{\alpha\beta}]_{n2} \ - \ [T_{\alpha\beta}]_{n3} \right) \cdot | \Psi_n\rangle \tag{5.149}$$

and the calculation of the probabilities

$$\tilde{C}_n^2 \ = \ \langle \psi_n | \psi_n\rangle \ , \quad n = 1, \cdots, 4 \tag{5.150}$$

from the projections

$$| \psi_n\rangle \ = | \Psi_n\rangle\langle\Psi_n | \psi\rangle \ , \quad n = 1, \cdots, 4 \tag{5.151}$$

result in probabilities which differ from these one given in (5.114) and (5.115). And indeed, in so doing we end up with

$$c_{11}^2 \;=\; c_{22}^2 \;=\; \frac{1}{2}\cdot \sin^2(\alpha-\beta) \tag{5.152}$$

$$c_{12}^2 \;=\; c_{21}^2 \;=\; \frac{1}{2}\cdot \cos^2(\alpha-\beta)\;. \tag{5.153}$$

But these probabilities are not in agreement with our experience from the marble experiment or any other experiment with classical objects that fits into the scheme of Fig. 5.5! The corresponding correlation function reads

$$C(\alpha,\beta) \;=\; -\cos 2(\alpha-\beta)\;. \tag{5.154}$$

Now there are parameter configurations (α,β) for which the necessary condition (5.113) of the violation of the CHSH-inequality (5.105) holds! For example, a maximum violation of the CHSH-inequality can be observed if the four different parameter configurations

$$(\alpha,\beta) = \left(0,\frac{\pi}{8}\right) \tag{5.155}$$

$$(\alpha,\beta\,') = \left(0,\frac{3\pi}{8}\right) \tag{5.156}$$

$$(\alpha',\beta) = \left(\frac{\pi}{4},\frac{\pi}{8}\right) \tag{5.157}$$

$$(\alpha',\beta\,') = \left(\frac{\pi}{4},\frac{3\pi}{8}\right)\;, \tag{5.158}$$

are used. This provokes again the question we already ask at the end of Sect. 5.1.2: Is there any experiment that would end up with these probabilities? And the answer is "yes", if using quantum objects like spin-entangled electrons, polarization-entangled photons, etc.. These are the quantum mechanical Bell's experiments. But, unfortunately, performing a quantum mechanical Bell's experiment is not as simple as the classical counterpart experiment since it requires a much more sophisticated equipment than boxes filled with certain numbers of differently coloured marbles. The first real experiment with polarization-entangled photons was performed by A. Aspect and co-workers in 1980, as mentioned in Sect. 1.3 of the Prologue. A. Aspect and co-workers used a primary impressed source that emits pairs of polarization-entangled photons produced by a calcium cascade source. Today, sources that are based on parametric down-conversion are more common (see Zhu et al. (2012), for example). The scheme of such an experiment is as follows: We tacitly assume that there exists a source that emits two polarization-entangled photons (let us say horizontally (h)- and vertically (v)-polarized with respect to a fixed but arbitrary plane) into opposite directions in a single event. But we do not know the state of

polarization of the photon emitted in a certain direction. That is, we do not know if we have the combination (h,v) or (v,h) with respect to the polarization of both photons in a single event. We only know that each pair is emitted with the probability of $1/2$! Let us further assume that a detector is mounted on each side that produces a click if a h-polarized photon is detected. There will be no click otherwise. Without any additional interactions on both sides we measure the probabilities (5.95). This probability experiment can be described in exactly the same way used above for the classical experiment if $t < t_{int}$. But the situation changes if we place additional polarizing filters on both sides the photons are interacting with. The orientation of the polarizing filters with respect to a fixed plane (i.e., the angles α and β on the left- and right-hand side) can be continuously varied between $[0, \pi]$. The local interactions become in this way functions of the local parameters α and β. Finally, the detectors are replaced by new detectors which act in such a way that a click is produced if a photon is detected, independent of its state of polarization. There will be no click otherwise. This experiment fits into the scheme of Fig. 5.5 and provides the probabilities (5.152) and (5.153). In the last years there have been performed several other experiments which confirm these probabilities although there are some discussions about possibly existing loopholes in the experimental design. However, the violation of the CHSH-inequality with corresponding quantum mechanical experiments is accepted among most of the physicists in our days. To conclude this discussion I want to emphasize again that the different probabilities obtained in our experiment with the black and white marbles and the quantum mechanical Bell's experiment may be considered as a consequence of a necessary superposition of the nonentangled but nondisjoint substates in the latter experiments and the separate treatment of each substate in the former experiment. That is, the different probabilities are traced back to a reason we encountered already in conjunction with the double-slit experiment (see also the last section in the Prologue).

Let us now discuss another but not less interesting point of view on the probability experiments considered in this chapter that provides us with another explanation of the different probabilities. Introducing the normalized probability states

$$| \tilde{\Phi}_1\rangle := \sum_{n=1}^{4} [T_{\alpha\beta}]_{n2} \cdot | \Psi_n\rangle \tag{5.159}$$

$$| \tilde{\Phi}_2\rangle := -\sum_{n=1}^{4} [T_{\alpha\beta}]_{n3} \cdot | \Psi_n\rangle \tag{5.160}$$

$$| \tilde{\Phi}_3\rangle := \frac{1}{\sqrt{2}} \cdot [| \Psi_2\rangle + | \Psi_3\rangle] \tag{5.161}$$

$$| \tilde{\Phi}_4\rangle := \frac{1}{\sqrt{2}} \cdot [| \Psi_1\rangle + | \Psi_4\rangle] \tag{5.162}$$

will allow us to relate the following "statistical operator" to these experiment:

$$\mathbf{S} := \sum_{i=1}^{2/4} p_i \cdot \mid \tilde{\Phi}_i \rangle \langle \tilde{\Phi}_i \mid \tag{5.163}$$

with weights p_i given by

$$p_1 = p_2 = \frac{1}{2} \tag{5.164}$$

$$p_3 = -p_4 = 2 \cdot w(\alpha, \beta) \ , \tag{5.165}$$

and

$$w(\alpha, \beta) = \sin\alpha \cdot \sin\beta \cdot \cos\alpha \cdot \cos\beta \ . \tag{5.166}$$

The upper summation index $i = 2$ belongs to the classical marble experiment, and $i = 4$ is the upper summation index for the quantum mechanical Bell's experiment. $\mid \tilde{\Phi}_1 \rangle$ and $\mid \tilde{\Phi}_2 \rangle$ (these two states are identical with (5.143) and (5.144) but for the prefactors $1/\sqrt{2}$) as well as $\mid \tilde{\Phi}_3 \rangle$ and $\mid \tilde{\Phi}_4 \rangle$ are again orthogonal among each other. Moreover,

$$\sum_{i=1}^{2/4} p_i = 1 \tag{5.167}$$

holds for the weights. Please, note the negative weight (negative quasi-probability) p_4! The measured probabilities (5.152) and (5.153) for any parameter configuration (α, β) are then the result of

$$c_{11}^2 = \langle \Psi_1 \mid \mathbf{S} \mid \Psi_1 \rangle \tag{5.168}$$

$$c_{12}^2 = \langle \Psi_2 \mid \mathbf{S} \mid \Psi_2 \rangle \tag{5.169}$$

$$c_{21}^2 = \langle \Psi_3 \mid \mathbf{S} \mid \Psi_3 \rangle \tag{5.170}$$

$$c_{22}^2 = \langle \Psi_4 \mid \mathbf{S} \mid \Psi_4 \rangle \ , \tag{5.171}$$

Operator (5.163) may be called the "basic statistical operator" since it is related to an experiment with a fixed parameter configuration α and β. On the other hand, if we have a mixture of N such experiments (i.e., if different parameter configurations (α_k, β_k) with $k = 1, \cdots, N$ are considered) with weights r_k, $\sum_{k=1}^{N} r_k = 1$, then we can relate the following statistical operator to the mixture:

$$\mathbf{S}^{\text{mix}} = \sum_{k=1}^{N} r_k \cdot \mathbf{S_k} = \sum_{k=1}^{N} \sum_{i=1}^{2/4} r_k \cdot p_i^{(k)} \cdot \mid \tilde{\Phi}_i^{(k)} \rangle \langle \tilde{\Phi}_i^{(k)} \mid \ . \tag{5.172}$$

Regarding the statistical operator (5.163) the question of the linear independence of the normalized probability states $\mid \tilde{\Phi}_i\rangle$ is of some importance. If this happens, then we are able to represent any probability state of our 4-dim. event space by a linear combination of these vectors. To prove the linear independence we have to consider Grams' matrix

$$\mathbf{Gr} \;=\; \langle\, \tilde{\Phi}_i \mid \tilde{\Phi}_j \rangle \;; \quad i,j \;=\; 1, \cdots, 4 \;. \tag{5.173}$$

Because of (5.159)–(5.162) this matrix is a symmetric one,

$$\mathbf{Gr} \;=\; \begin{pmatrix} 1 & 0 & g_1 & g_2 \\ 0 & 1 & -g_1 & g_2 \\ g_1 & -g_1 & 1 & 0 \\ g_2 & g_2 & 0 & 1 \end{pmatrix} \tag{5.174}$$

with elements g_1 and g_2 given by

$$g_1 \;=\; \frac{1}{\sqrt{2}} \cdot \cos(\alpha \;+\; \beta) \tag{5.175}$$

$$g_2 \;=\; \frac{1}{\sqrt{2}} \cdot \sin(\alpha \;-\; \beta) \;. \tag{5.176}$$

Its determinant reads

$$\det\,(\mathbf{Gr}) \;=\; \frac{8}{\sqrt{2}} \cdot w(\alpha, \beta) \tag{5.177}$$

with $w(\alpha, \beta)$ according to (5.166). Thus we have to meet the condition

$$w(\alpha, \beta) \;\neq\; 0 \tag{5.178}$$

to ensure the linear independence of the vectors (5.159)–(5.162). On the other hand, if

$$w(\alpha, \beta) \;=\; 0 \tag{5.179}$$

holds (this happens if we have ($\alpha \;=\; 0$ or $\pi/2, \beta \;\neq\; 0$) or ($\alpha \;\neq\; 0, \beta \;=\; 0$ or $\pi/2$)), both weights p_3 and p_4 are identical zero. If calculating the probabilities only from the two states $\mid \tilde{\Phi}_1\rangle$ and $\mid \tilde{\Phi}_2\rangle$ (i.e., if restricting the summation in (5.163) to $\sum_{i=1}^{2}$!) we get the probabilities (5.114) and (5.115) of the marble experiment. The two states $\mid \tilde{\Phi}_3\rangle$ and $\mid \tilde{\Phi}_4\rangle$ can therefore be considered to represent the interference contribution that results from the superposition of the two substates (5.143) and (5.144). From (5.163) we can see moreover that $\mid \tilde{\Phi}_3\rangle$ acts as a "source state". That is it adds a certain amount to the probabilities c_{12}^2 and c_{21}^2

calculated from the states $|\ \tilde{\Phi}_1\rangle$ and $|\ \tilde{\Phi}_2\rangle$. Contrary, $|\ \tilde{\Phi}_4\rangle$ acts as a "sink state" since it removes the same amount from the probabilities c_{11}^2 and c_{22}^2 calculated from the states $|\ \tilde{\Phi}_1\rangle$ and $|\ \tilde{\Phi}_2\rangle$. A similar behaviour was already discussed in Chap. 4 in conjunction with the interaction of a linearly polarized plane wave with a polarizing filter (see the discussion subsequent to Eq. (4.80)).

Chapter 6
Outlook or Something Like an End

The best end is an end that provokes a new beginning

Congratulation! We (i.e., the readers who followed me up to this point and the author himself) have reached the last chapter of this book. Based on the results of the second and third chapter this final chapter is aimed at providing a short and fragmented look at relations between some of the classical Green's functions derived so far, and some of the Green's functions used in Quantum Mechanics. We start with a relation between the Green's function of a free point mass derived in the second chapter, the Green's function of the diffusion- or heat transfer equation derived in the third chapter, and the free particle Green's function of the Schrödinger equation. To this end, we will employ again the Fourier transform method described in Sect. 3.4. We want to discuss further the issue of the transfer of this relation to other problems. This will lead us to a relation between the Fokker-Planck- and Schrödinger equation. A relation between the Green's function of the Klein-Gordon- and Dirac equation is discussed finally. All these considerations are restricted to the 1-dim. case. They provide only a first aid kit for those readers who want to get deeper into the Green's function formalism used in Quantum Mechanics, Quantum Statistics, or in Quantum Field Theory. However, a more thoroughly treatment of these nonclassical fields by use of Green's functions is outside the scope of this book and would be a project of its own.

6.1 Classical Free Point Mass and Green's Function of the Diffusion Equation

To spare the reader the burden of going back and forth in this book let us write down the relevant equations from the foregoing chapters.

$$G_{tt}^{(PM)}(t,t') \;=\; \frac{1}{m}\cdot\delta(t-t') \tag{6.1}$$

was the equation of motion for the Green's function of a free point mass (please, note again the shorter notation used for the twofold derivative with respect to time).

T. Rother, *Green's Functions in Classical Physics*, Lecture Notes in Physics 938, DOI 10.1007/978-3-319-52437-5_6

Its solution was given by

$$G^{(PM)}(t,t') \;=\; F(t,t')\cdot H(t-t')\;, \tag{6.2}$$

where

$$F(t,t') \;=\; \frac{(t-t')}{m} \tag{6.3}$$

was representing a special solution of the corresponding homogeneous equation

$$F_{tt}(t,t') \;=\; 0\;. \tag{6.4}$$

$H(t-t')$ is the Heaviside function.

$$a^2\cdot G_t^{(D)}(x,t;x',t') \;-\; G_{xx}^{(D)}(x,t;x',t') \;=\; -\delta(x-x')\cdot\delta(t-t')\;. \tag{6.5}$$

was the 1-dim. diffusion equation. Its solution was given by

$$G^{(D)}(x,t;x',t') \;=\; F^{(D)}(x,t;x',t')\cdot H(t-t')\;. \tag{6.6}$$

Starting from the 1-dim. equation of telegraphy, it was derived from the limiting situation of an assumed infinitely large velocity of light.

$$F^{(D)}(x,t;x',t') \;=\; \frac{1}{\sqrt{4\,\pi\,a^2\,(t-t')}}\cdot e^{\;-\dfrac{a^2}{4}\,\cdot\,\dfrac{(x-x')^2}{(t-t')}} \tag{6.7}$$

was again a special solution of the corresponding homogeneous equation

$$a^2\cdot F_t^{(D)}(x,t;x',t') \;-\; F_{xx}^{(D)}(x,t;x',t') \;=\; 0\;. \tag{6.8}$$

Is there any relation between these two Green's functions? To answer this question we have to go back to the action defined in (2.2). From the Lagrangian of the free particle we thus get

$$W(x,t;x',t') \;=\; \frac{(x-x')^2}{2\,F(t,t')} \tag{6.9}$$

with $F(t,t')$ according to (6.3). This allows as to write instead of (6.6)

$$G^{(D)}(x,t;x',t') \;=\; \frac{1}{\sqrt{4\,\pi\;\,m\,a^2\,F(t,t')}}\cdot e^{\;-\dfrac{a^2}{2\,m}\,\cdot\,W(x,t;x',t')}\cdot H(t-t')\;. \tag{6.10}$$

$F(t,t')$ in the square root of the denominator and in the function (6.9) of the action establishes a link between the Green's function of the 1-dim. diffusion equation and the special solution (6.3) of the Green's function of the free point mass.

Now we want to apply the Fourier transform method to derive the Green's function of the diffusion equation once again. Using *ansatz* (3.216) for the Green's function and (3.215) for Dirac's time dependent delta function it follows from Eq. (6.5)

$$-\,i\,\omega\,a^2\cdot G^{(D)}(x,x';\omega)\;-\;G^{(D)}_{xx}(x,x';\omega)\;=\;-\,\delta(x-x')\;. \tag{6.11}$$

Assuming that we know the continuous or discrete number of eigenvalues k_n and the related eigenfunctions $\varphi_n(x)$ of the eigenvalue problem

$$-\,[\varphi_n(x)]_{xx}\;-\;k_n\cdot\varphi_n(x)\;=\;0 \tag{6.12}$$

we can approximate the unknown quantity $G^{(D)}(x,x';\omega)$ by the series expansion

$$G^{(D)}(x,x';\omega)\;=\;\sum\!\!\!\!\!\!\int_n\;G_n(x',\omega)\cdot\varphi_n(x)\;dk\;. \tag{6.13}$$

On the right-hand side of (6.11) we use the completeness relation

$$\delta(x-x')\;=\;\sum\!\!\!\!\!\!\int_n\;\varphi_n^*(x')\cdot\varphi_n(x)\;dk \tag{6.14}$$

of Dirac's delta function $\delta(x-x')$. This results in

$$G_n(x',\omega)\;=\;\frac{1}{ia^2}\cdot\frac{\varphi_n^*(x')}{\omega+i\,\dfrac{k_n}{a^2}} \tag{6.15}$$

for the unknown expansion coefficients in (6.13). The poles are located on the negative imaginary axis of the complex ω-plane. Inserting (6.13) with (6.15) into (3.216) and taking into account that we have to close the path of integration in the lower complex ω-plane at infinity (see the discussion in Sect. 2.5.3 in conjunction with the Kramers-Kronig relation) gives

$$G^{(D)}(x,t;x',t')\;=\;\frac{1}{a^2}\sum\!\!\!\!\!\!\int_n\;e^{-\dfrac{k_n}{a^2}\cdot(t-t')}\cdot\varphi_n^*(x')\cdot\varphi_n(x)\;dk\;. \tag{6.16}$$

Fortunately, regarding the problem at hand we know the continuous eigenvalues and the corresponding eigenfunctions of (6.12). The eigenvalues are $k_n=k^2$, and

$$\varphi_n(x)\;=\;\frac{1}{\sqrt{2\pi}}\cdot e^{\,ikx} \tag{6.17}$$

are the related eigenfunctions. Equation (6.16) reads therefore

$$G^{(D)}(x,t;x',t') \;=\; \frac{1}{2\pi a^2}\;\int_{-\infty}^{\infty} e^{\;-\dfrac{k^2}{a^2}\cdot(t-t')\;+\;ik(x-x')}\;dk\;. \tag{6.18}$$

By means of completing the square this expression can be reformulated as follows:

$$G^{(D)}(x,t;x',t') \;=\; \frac{1}{2\pi a^2}\;\cdot\; e^{\;-\dfrac{a^2}{4}\cdot\dfrac{(x-x')^2}{(t-t')}}\;\cdot$$
$$\int_{-\infty}^{\infty} e^{\;-\,i\,\dfrac{(t-t')}{ia^2}\cdot\left[k\,-\,\dfrac{ia^2}{2}\cdot\dfrac{(x-x')}{(t-t')}\right]^2}\;dk\;. \tag{6.19}$$

Substituting

$$\tilde{\lambda} \;=\; k-\frac{ia^2}{2}\cdot\frac{(x-x')}{(t-t')} \tag{6.20}$$

and taking the Gaussian integral

$$\int_{-\infty}^{\infty} e^{\,-\,i\,\kappa\,\tilde{\lambda}^2}\,d\tilde{\lambda} \;=\; \left(\frac{\pi}{i\kappa}\right)^{1/2} \tag{6.21}$$

into account results finally in expression (6.7) of the Green's function of the 1-dim. diffusion equation.

Now, let us once again derive our pivotal relation for solving the equation

$$a^2\cdot\psi_t^{(D)}(x,t)\;-\;\psi_{xx}^{(D)}(x,t)\;=\;-\,\rho(x,t) \tag{6.22}$$

which is of our actual interest. Its derivation can be accomplished in close analogy to the way described in Sect. 3.2.3 in conjunction with the general solution of the 1-dim. wave equation. But, now, only a single derivative with respect to time must be considered. As a consequence and due to Reciprocity with respect to time the adjoint equation with a negative sign in front of the term with the time derivative must be used, as frequently practiced in the second chapter in the presence of friction. We start therefore from the equations

$$a^2\cdot\psi_{t'}^{(D)}(x',t')\;-\;\psi_{x'x'}^{(D)}(x',t')\;=\;-\,\rho(x',t') \tag{6.23}$$

and

$$-\;a^2\cdot G_{t'}^{(D)}(x,t;x',t')\;-\;G_{x'x'}^{(D)}(x,t;x',t')\;=\;-\,\delta(x-x')\cdot\delta(t-t')\;. \tag{6.24}$$

In the next step we consider the integral expression

$$\int dx'\, dt' \, \Big\{ \psi^{(D)}(x',t') \cdot \Big[-a^2 \cdot G^{(D)}_{t'}(x,t;x',t') \, - \, G^{(D)}_{x'x'}(x,t;x',t') \Big] \\ - \, G^{(D)}(x,t;x',t') \cdot \Big[a^2 \cdot \psi^{(D)}_{t'}(x',t') \, - \, \psi^{(D)}_{x'x'}(x',t') \Big] \Big\} \, . \tag{6.25}$$

This gives

$$\int dx'\, dt' \, \{ \cdots \} \, = \, - \psi^{(D)}(x,t) \, + \, \int dx'\, dt'\, G^{(D)}(x,t;x',t') \cdot \rho(x',t') \tag{6.26}$$

(note that its left-hand side is identical with (6.25)). On the other hand, if applying Green's theorem to (6.25), and from the requirements of homogeneous boundary conditions with respect to the spatial boundaries and Causality with respect to time we get

$$\psi^{(D)}(x,t) \, = \, \int dx'\, dt'\, G^{(D)}(x,t;x',t') \cdot \rho(x',t') \\ + \, a^2 \cdot \int dx'\, G^{(D)}(x,t;x',t') \cdot \psi^{(D)}(x',t') \, . \tag{6.27}$$

Inhomogeneous spatial boundary conditions would result in additional contributions on the right-hand side which can alternatively be expressed by corresponding sources, as already demonstrated in conjunction with the general solution of the wave equation. This holds also for the second term on the right-hand side of (6.27). It may be considered to be the result of the source

$$\rho(x',t') \, = \, a^2 \cdot \psi^{(D)}(x') \cdot \delta(t') \tag{6.28}$$

acting at the initial time $t' \, = \, 0$. With this understanding we arrived at our pivotal relation (3.1). Relation (3.1) together with the source (6.28) and the general condition

$$G(x,t;x',t') \, = \, 0 \, ; \quad t < t' \tag{6.29}$$

for the Green's function provide a causal relation between the initial state $\psi(x', t' = 0)$ and the state $\psi(x,t)$ at a later time $t > 0$. It is exactly this structure that allows us to establish a link to Quantum Mechanics. Let us therefore consider the Green's function related to the Schrödinger equation of a free quantum particle.

6.2 Schrödinger Equation of the Free Particle and Green's Function

The Green's function of the Schrödinger equation in Quantum Mechanics—also referred to as a "propagator"— is often introduced via the relation

$$\psi(x,t) \;=\; \int_{-\infty}^{\infty} dx'\, G^{(S)}(x,t;x',t') \cdot \psi(x',t') \tag{6.30}$$

between the quantum state $\psi(x',t')$ at a certain initial time t' and the quantum state $\psi(x,t)$ at a later time $t > t'$ (see Müller-Kirsten (2006), Chap. 21 therein, for example). But we have just seen that this causal relation can be understood as the result of the underlying equation with only a single derivative with respect to time and an appropriate source. This will now be demonstrated for the Schrödinger equation of a **N**onrelativistic, **F**orceless, **S**pinless, and **M**ass-carrying quantum particle (a "NFSM-quantum particle") given by

$$-\, i\hbar \cdot \psi_t(x,t) \;-\; \frac{\hbar^2}{2m} \cdot \psi_{xx}(x,t) \;=\; -\,\rho(x,t)\;. \tag{6.31}$$

In contrast to the conventional formulation one can find in textbooks, a source is already introduced on the right-hand side of this equation. It is to be understood as an impressed source that generates the initial state. The corresponding equation of the Green's function reads

$$-\, i\hbar \cdot G_t^{(S)}(x,t;x',t') \;-\; \frac{\hbar^2}{2m} \cdot G_{xx}^{(S)}(x,t;x',t') \;=\; -\,\delta(x-x') \cdot \delta(t-t')\,. \tag{6.32}$$

There is an obvious analogy to the diffusion equation. The same method as described in the foregoing Sect. can be applied to solve this equation. But due to the different prefactors, instead of expression (6.16) it now follows

$$G^{(S)}(x,t;x',t') \;=\; -\,\frac{1}{i\hbar} \sum\!\!\!\!\!\!\int_n e^{\,-\frac{i}{\hbar}\,k_n\,(t-t')} \cdot \varphi_n^*(x') \cdot \varphi_n(x)\; dk\;, \tag{6.33}$$

from *ansatz* (6.13). The eigenvalues are given by

$$k_n \;=\; \frac{\hbar^2\,k^2}{2m}\;. \tag{6.34}$$

In the course of deriving (6.33) we have to take moreover into account that the poles of the corresponding expression (6.15) are now real-valued. It is therefore helpful to add a "$-i\epsilon$" to shift these poles into the direction of the negative imaginary axis. This will allow us to close the path of integration of the inverse transformation at

infinity in the lower complex ω-plane (please, remember that a similar trick was already applied in Sect. 2.1.4 to derive the Green's function of the simple harmonic oscillator). Equation (6.33) is then obtained from the residual theorem, and if ϵ is finally set to zero. From (6.34) and the eigenfunctions (6.17) we thus get

$$G^{(S)}(x,t;x',t') \;=\; \frac{1}{2\pi(-i\hbar)} \int_{-\infty}^{\infty} e^{\,-ik^2\frac{\hbar}{2m}\cdot(t-t') \;+\; ik\,(x-x')}\, dk\;. \tag{6.35}$$

The integral can again be solved by completing the square. But we can also benefit from the analogy to the diffusion equation. Comparing (6.18) and (6.35) we find that

$$G^{(S)}(x,t;x',t') \;=\; \frac{a^2}{(-i\hbar)} \cdot G^{(D)}(x,t;x',t') \tag{6.36}$$

holds if

$$a^2 \;=\; \frac{2m}{i\hbar} \tag{6.37}$$

is used. And with (6.36) and (6.37) we can moreover transform the equation (6.32) of the Green's function of the Schrödinger equation into the equation (6.5) of the Green's function of the diffusion equation. Looking at (6.10) the Green's function of the NFSM-quantum particle reads therefore

$$G^{(S)}(x,t;x',t') \;=\; \frac{1}{(-i\hbar)} \cdot \frac{1}{\sqrt{2\,\pi\, i\,\hbar\, F(t,t')}} \cdot e^{\,\frac{i}{\hbar}\cdot W(x,t;x',t')} \cdot H(t-t')\;, \tag{6.38}$$

where $F(t,t')$ and $W(x,t;x',t')$ are again given by the classical expressions (6.3) and (6.9)! Except for the prefactor $1/(-i\hbar)$, expression (6.38) agrees with that one known from the literature. But this prefactor vanishes if we ask for the solution of equation (6.31) which is of our actual interest. Application of Green's theorem in exactly the same way as described in the foregoing section provides

$$\begin{aligned}\psi(x,t) \;=\; &\int dx'\; dt'\; G^{(S)}(x,t;x',t') \;\cdot \rho(x',t') \\ &-\, i\hbar \int dx'\; G^{(S)}(x,t;x',t') \cdot \psi(x',t')\end{aligned} \tag{6.39}$$

with $G^{(S)}(x,t;x',t')$ given by (6.38). The second term on the right-hand side can be considered as a result of the impressed source

$$\rho(x',t') \;=\; -i\hbar \cdot \psi(x') \cdot \delta(t') \tag{6.40}$$

if the initial time is set to $t' = 0$. The resulting solution agrees with the definition (6.30) of a Green's function without the prefactor $1/(-i\hbar)$. The restriction of (6.39) to the first term on the right-hand side together with the impressed source (6.40) is precisely what I called the "source picture" of Quantum Mechanics in the Prologue (see the end of Sect. 1.3). According to the point of view on physics formulated in the Prologue, the Green's function (6.38) provides a complete characterization of the abstract object "NFSM-quantum particle" and avoids the recourse to the uncertainty relation between momentum and position.

To summarize the procedure we can use to determine the Green's function of the Schrödinger equation (6.32): We multiply the special solution (6.7) of the classical diffusion equation by $a^2/(-i\hbar)$, and replace a^2 afterwards by $2m/i\hbar$. Multiplication by the Heaviside function $H(t-t')$ provides the Green's function. This raises the question if this simple procedure can also be applied to other problems in Quantum Mechanics?

6.3 Classical Fokker-Planck Equation and Schrödinger Equation

To answer this question let us go back to Eq. (6.10). We want to find out the condition for

$$F^{(FP)}(x,t;x',t') = \frac{1}{\sqrt{4\pi\, m a^2 F(t,t')}} \cdot e^{-\frac{a^2}{2m} \cdot W(x,t;x',t')} \tag{6.41}$$

with the more general expression

$$W(x,t;x',t') = \frac{1}{2F(t,t')} \cdot \left[(x^2 + x'^2) \cdot m \cdot F_t(t,t') - 2xx'\right] \tag{6.42}$$

of the action being the solution of the homogeneous Fokker-Planck equation

$$a^2 \cdot F_t^{(FP)}(x,t;x',t') - F_{xx}^{(FP)}(x,t;x',t') - \frac{a^4}{2m} \cdot V(x) \cdot F^{(FP)}(x,t;x',t') = 0 \tag{6.43}$$

for time independent potentials $V(x)$. This special Fokker-Planck equation is of our interest here since it can be transformed into the Schrödinger equation

$$(-i\hbar) \cdot F_t^{(S)}(x,t;x',t') - \frac{\hbar^2}{2m} \cdot F_{xx}^{(S)}(x,t;x',t') + V(x) \cdot F^{(S)}(x,t;x',t') = 0 \tag{6.44}$$

for time independent potentials $V(x)$ by assuming the relation

$$F^{(S)}(x,t;x',t') \;=\; \frac{a^2}{(-i\hbar)} \cdot F^{(FP)}(x,t;x',t') \tag{6.45}$$

between the solutions of these two equations. Please, note that this relation agrees with the former relation (6.36). The Fokker-Planck equation becomes identical with the diffusion equation if $V(x) = 0$. Insertion of (6.41) into (6.43) results in

$$\begin{aligned} 0 \;=\; -\frac{1}{2\sqrt{4\,\pi\; m\, a^2\, F(t,t')}} \cdot e^{-\frac{a^2}{2\,m}\cdot W(x,t;x',t')} \cdot \Bigg\{ & \frac{F_t(t,t')}{F(t,t')} \\ & + \frac{a^2}{m} \cdot W_t(x,t;x',t') \;-\; \frac{1}{m} \cdot W_{xx}(x,t;x',t') \\ & + \frac{a^2}{m} \cdot \left[\frac{W_x^2(x,t;x',t')}{2m} \;+\; V(x) \right] \Bigg\} \;. \end{aligned} \tag{6.46}$$

Because of (6.42) we have the identity

$$\frac{F_t(t,t')}{F(t,t')} \;-\; \frac{1}{m} \cdot W_{xx}(x,t;x',t') \;=\; 0\;. \tag{6.47}$$

Equation (6.46) then becomes

$$\begin{aligned} 0 \;=\; -\frac{a^2}{2m} \cdot \frac{1}{\sqrt{4\,\pi\; m\, a^2\, F(t,t')}} \cdot e^{-\frac{a^2}{2\,m}\cdot W(x,t;x',t')} \cdot \\ \left[W_t(x,t;x',t') + \frac{W_x^2(x,t;x',t')}{2m} \;+\; V(x) \right] \;. \end{aligned} \tag{6.48}$$

The expression in the square brackets is nothing but the well-known Hamilton-Jacobi partial differential equation of the action. It is identical zero in the presence of conservative potentials. Equation (6.41) is therefore a solution of (6.43) for the corresponding potentials $V(x)$. We will now use this knowledge to determine the Green's function of the object "quantum mechanical harmonic oscillator".

We start from the classical expressions of the simple harmonic oscillator derived already in the second chapter.

$$G_{tt}^{(O)}(t,t') \;+\; \omega^2 \cdot G^{(O)}(t,t') \;=\; \frac{1}{m} \cdot \delta(t-t') \tag{6.49}$$

was the equation of motion of the related Green's function. Its solution was given by

$$G^{(O)}(t,t') \;=\; F^{(O)}(t,t') \cdot H(t-t') \;, \tag{6.50}$$

where

$$F^{(O)}(t,t') \;=\; \frac{\sin\omega(t-t')}{m\,\omega} \;. \tag{6.51}$$

was again a special solution of the corresponding homogeneous equation

$$F^{(O)}_{tt}(t,t') \;+\; \omega^2 \cdot F^{(O)}(t,t') \;=\; 0 \;. \tag{6.52}$$

From (6.42) we get the following expression for the action of the simple harmonic oscillator:

$$W^{(O)}(x,t;x',t') \;=\; \frac{m\,\omega}{2\,\sin\omega(t-t')} \cdot \left[(x^2+x'^2)\cdot\cos\omega(t-t') \;-2\,x\,x'\right] \;. \tag{6.53}$$

Applying the procedure described at the end of the foregoing section we thus get the Green's function

$$\begin{aligned} G^{(S)}(x,t;x',t') \;=\; & \frac{1}{(-i\hbar)} \cdot \frac{1}{\sqrt{2\,\pi\,i\,\hbar\,F^{(O)}(t,t')}} \\ & \cdot e^{\dfrac{i}{\hbar}\cdot W^{(O)}(x,t;x',t')} \cdot H(t-t') \end{aligned} \tag{6.54}$$

of the quantum mechanical harmonic oscillator in a straightforward way. Except for the prefactor $1/(-i\hbar)$, expression (6.54) is well-known from the literature. The Green's function (6.38) of the NFSM-quantum particle results from $\omega = 0$. In Parker and Petrosian (1995), for example, one can find the Green's function of the Fokker-Planck equation for a large number of other conservative potentials. However, the knowledge of the solution $F(t,t')$ of the corresponding homogeneous equations is a necessary precondition to benefit from the above procedure.

In certain cases, if the particle in a box model with impenetrable barriers at either end is considered, for example, expression (6.33) becomes

$$G^{(S)}(x,t;x',t') \;=\; -\frac{1}{i\hbar}\sum_n e^{-\dfrac{i}{\hbar}E_n\,(t-t')} \cdot \varphi_n^*(x') \cdot \varphi_n(x) \;. \tag{6.55}$$

The infinitely-countable number of energy values E_n and the related eigenfunctions $\varphi_n(x)$ are again the solutions of the corresponding eigenvalue problem we have to solve in conjunction with the Fourier transform method. Such a representation is

also known for the Green's function (6.54) of the quantum mechanical harmonic oscillator. The characteristic eigenvalues and normalized eigenfunctions are in this case given by

$$E_n \;=\; \hbar\,\omega\left(n \;+\; \frac{1}{2}\right) \;; \quad n = 0, 1, \cdots \tag{6.56}$$

and

$$\varphi_n(x) \;=\; \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot \frac{1}{\sqrt{2^n n!}} \cdot \Phi_n(\xi) \cdot e^{-\xi^2/2} \,. \tag{6.57}$$

$\Phi_n(\xi)$ are the Hermitian polynomials with

$$\xi \;=\; \sqrt{\frac{m\omega}{\hbar}} \cdot x \,. \tag{6.58}$$

It is interesting to note that this representation can be derived from (6.54) if the trigonometric relations

$$\sin\omega(t-t') \;=\; \frac{1}{2i}\, e^{\,i\omega(t-t')}\left(1 \;-\; e^{\,-2i\omega(t-t')}\right) \tag{6.59}$$

$$\cos\omega(t-t') \;=\; \frac{1}{2i}\, e^{\,i\omega(t-t')}\left(1 \;+\; e^{\,-2i\omega(t-t')}\right) \tag{6.60}$$

are used, and if an appropriate series expansion is applied to the exponential functions afterwards. This was demonstrated by Feynman and Hibbs in (Feynman and Hibbs 1965) in the context of the path integral formulation of Quantum Mechanics. Unfortunately, this is impossible for the Green's function of the classical Fokker-Planck equation (6.43) that considers the same potential.

Taking the square of (6.54),

$$\left|(i\hbar)\cdot G^{(S)}(x,t;x',t')\right|^2 \;=\; \frac{m\omega}{2\pi\hbar\,\sin[\omega(t-t')]} \,, \tag{6.61}$$

provides the "transition probability" of detecting the quantum object at time t in position dx around x if its initial position at time $t' < t$ is given by dx' around x'. The corresponding transition probability for the NFSM-quantum particle considered before results from (6.61) if $\omega = 0$. But the more common interpretation that is associated with conventional Quantum Mechanics results from the representation (6.55)–(6.57). According to the point of view formulated in the Prologue, this representation provides also a complete physical characterization of the object "quantum mechanical harmonic oscillator". Inserting (6.55) and the source (6.40)

into the first term on the right-hand side of (6.39) gives

$$\psi(x,t) \;=\; \sum_n a_n \cdot e^{-\frac{i}{\hbar} E_n t} \cdot \varphi_n(x) \;. \tag{6.62}$$

$$a_n \;=\; \int \psi(x') \cdot \varphi_n^*(x')\; dx' \tag{6.63}$$

are the complex-valued expansion coefficients, in general. The state (6.62) is normalized to unity,

$$\int \psi^*(x,t) \cdot \psi(x,t)\; dx \;=\; 1 \;, \tag{6.64}$$

so that

$$\sum_n a_n^2 \;=\; 1 \tag{6.65}$$

holds. The resulting a_n^2 are then the probabilities to measure the energy value E_n in a corresponding experiment if the quantum mechanical harmonic oscillator was prepared before to be in state $\psi(x,t)$. The time dependence that appears in (6.62) is washed out by taking its square. This is the same interpretation we mentioned already in the foregoing chapter to calculate the probabilities from the probability states in classical event spaces, in the absence of additional stochastic interactions. Using again the conventional "bra-ket"- formulation, and with the definitions

$$\mid \phi_n(x,t)\rangle \;:=\; e^{-\frac{i}{\hbar} E_n t} \cdot \varphi_n(x) \tag{6.66}$$

and

$$\langle f(x,t) \mid g(x,t)\rangle \;:=\; \int f^*(x,t) \cdot g(x,t)\; dx \tag{6.67}$$

the corresponding "source picture" reads

$$\mid \psi(x,t)\rangle \;=\; \hat{G}^{(S)}(x,t;x',t') \;\mid \rho(x',t')\rangle \tag{6.68}$$

with the source $\mid \rho(x',t')\rangle$ and the Green's function given by (6.40) and

$$\hat{G}^{(S)}(x,t;x',t') \;=\; -\frac{1}{i\hbar} \sum\!\!\!\!\!\!\int_n |\phi_n(x,t) >< \phi_n(x',t')|\; dk \;. \tag{6.69}$$

There exists another function—the so-called "spectral function"—which is of some importance in Quantum Statistics, and which is strongly related to the Green's function. Let us have a very short and incomplete look at this function. In this context it should be first mentioned that, if $x = x'$ is used in (6.55), and if integration with respect to x is performed, the introduction of the complex time difference

$$(t - t') \;=\; -\,i\,\hbar\,\beta \tag{6.70}$$

with

$$\beta \;=\; \frac{1}{k_B\,T} \tag{6.71}$$

allows one to establish a link to the partition function

$$Z \;=\; \sum_n e^{\,-\dfrac{E_n}{k_B\,T}}\;, \tag{6.72}$$

and, therefore, to equilibrium problems in Quantum Statistics. k_B represents the Boltzmann constant, and T denotes the temperature. This complex time technique results in the so-called "Matsubara representation" of the Green's functions. The equation of motion of the Fourier transform of these Green's functions are governed by the Dyson equation. This approach is similar to what was discussed in Sect. 2.5.2, and in conjunction with the Fourier transform method in the third chapter. Let us therefore ask for the structure of the spectral function $A(\omega)$, introduced by

$$G^{(S)}(x,t;x',t') \;=\; \int_{-\infty}^{\infty} \frac{d\omega}{2\,\pi}\,A(\omega)\cdot e^{\,-\,i\,\omega\,(t\,-\,t')}\;, \tag{6.73}$$

that results in the representation (6.55). Applying the Fourier transform method to the Green's function of the Schrödinger equation of the quantum mechanical harmonic oscillator gives at first

$$-\hbar\,\omega\,G(x,x';\omega) - \frac{\hbar^2}{2m}\,G_{xx}(x,x',\omega) + \frac{m\,\omega^2}{2}\,x^2\,G(x,x',\omega) \;=\; -\,\delta(x{-}x') \tag{6.74}$$

in the Fourier transform domain with respect to the time. Solving the corresponding eigenvalue problem

$$-\;\frac{\hbar^2}{2m}\;[\varphi_n(x)]_{xx} \;+\; \frac{m\,\omega^2}{2}\,x^2\,\varphi_n(x) \;=\; E_n\,\varphi_n(x) \tag{6.75}$$

results in the series expansion

$$G(x,x';\omega) \;=\; \frac{1}{\hbar}\sum_n \frac{\varphi_n^*(x')\cdot\varphi_n(x)}{\omega - E_n/\hbar}\;. \tag{6.76}$$

E_n are the eigenvalues (6.56), and $\varphi_n(x)$ are the related eigenfunctions (6.57). If the spectral function is now defined by

$$A(\omega) \;:=\; -\lim_{\epsilon\to 0}\left[G(x,x';\omega+i\epsilon) \;-\; G(x,x';\omega-i\epsilon)\right]\;, \tag{6.77}$$

we get from (6.76) and Dirac's identity

$$\lim_{\epsilon\to 0}\frac{1}{\omega \pm i\epsilon} \;=\; \mathrm{pv}\left(\frac{1}{\omega}\right) \mp i\,\pi\,\delta(\omega) \tag{6.78}$$

(please, note that "pv" denotes the principal value) the expression

$$A(\omega) \;=\; \frac{2\,\pi\,i}{\hbar}\sum_n \delta(\omega - E_n/\hbar)\cdot\varphi_n^*(x')\cdot\varphi_n(x)\;. \tag{6.79}$$

Inserting this spectral function into (6.73) results actually in representation (6.55). It should be mentioned that definition (6.77) of the spectral function differs in the prefactor "$-i$" from its usual definition

$$A(\omega) \;:=\; i\lim_{\epsilon\to 0}\left[G(x,x';\omega+i\epsilon) \;-\; G(x,x';\omega-i\epsilon)\right] \tag{6.80}$$

in Quantum Statistics. This is a consequence of the additional prefactor "$i/\hbar$" in the Green's function (6.55) that disappears only in combination with the source (6.40). Both the Green's function (6.55) as well as the spectral function (6.79) provide a complete characterization of the idealized object "quantum mechanical harmonic oscillator". In Quantum Statistics the spectral function results from the so-called "causal Green's function". It is closely related to the correlation- and thermodynamic functions and provides a complete characterization of the idealized object "quantum mechanical ensemble" (canonical, grand-canonical, etc.) in the case of Hermitian Hamilton operators. For example, the spectral function that is calculated from the causal Green's function of a grand-canonical ensemble of interaction-free Fermion particles results in the Fermi distribution function for the average number of particles in a certain energy state. The equation of motion of the causal one-particle Green's function is the so-called Dyson-Schwinger equation that relates the one-particle Green's function to the two-particles Green's function, and so on. It allows the incorporation of interaction processes to describe the influence of the environment on the eigenvalues and the decay of probabilities of single states, for example. But, unfortunately, in most of these cases the Hermitian character of the Hamiltonian, and, as a consequence, the simple structure (6.79) of the spectral

function get lost. But let us stop the discussion at this point. The interested reader can find a very good and detailed treatment of these methods in Kadanoff and Baym (1962), and an application of this method to different problems in the physics of charged particle systems in Kraeft et al. (1986), for example.

6.4 A Relation Between the Green's Functions of the Klein-Gordon- and Dirac Equation

It was demonstrated in Sect. 2.5.1 how to decompose the equation of motion for the Green's function of the simple harmonic oscillator—a second-order equation in its time derivative—into two differential equations of first order, and how to combine the solutions of these two equations to the Green's function of the simple harmonic oscillator. Moreover, relation (2.208) between the Green's function of one of the first-order equations and the Green's function of the second-order equation was formally derived. Such a decomposition of a second-order equation was an essential idea of Dirac in the course of deriving a relativistic equation of massive spin-1/2 particles like electrons—the Dirac equation, as it is called today. In the early efforts undertaken in Quantum Mechanics to find a relativistic alternative to Schrödinger's wave equation the Klein-Gordon equation was considered as a potential candidate. This happened because time and position are treated equally in this equation. The derivatives are both of second order. But due to the second-order time derivative of this equation a problem arises with the formulation of an equation of continuity for the probability $\psi^* \psi$. In contrast, this can be accomplished without any problems by use of Schrödinger's equation with only a first-order time derivative. It was a bright idea of Dirac to decompose the Klein-Gordon equation into two first-order equations with respect to the time and space. In so doing, Dirac was also able to solve the problem of the spin-orbit interaction in the hydrogen atom. The original paper (Dirac 1928) is highly recommended for those readers who may be interested in a detailed discussion of the problems which forces Dirac to seek for a better quantum mechanical treatment of the hydrogen atom.

The decomposition of the Klein-Gordon equation into two first-order equations as well as the derivation of a relation between the Green's function of the Dirac- and Klein-Gordon equation similar to that one given by (2.208) will be demonstrated in what follows. For the sake of simplicity and to give only a very first impression of the idea behind Dirac's equation these derivations are restricted to the 1-dim. case. Any quantum mechanical considerations are moreover avoided. As I mentioned at the beginning: A more thoroughly treatment of the aspects touched in this chapter would be a book of its own. To start with, let us write down the Klein-Gordon equation (3.62) once again but in a somewhat different form:

$$\left(\frac{1}{c^2}\cdot\partial_t^2 \;-\; \partial_x^2 \;+\; \frac{a^2}{c^2}\right) G^{(KG)}(x,t;x',t') \;=\; \delta(x-x')\cdot\delta(t-t')\;. \tag{6.81}$$

The differential operator of second order in the brackets on the left-hand side shall now be decomposed into two operators each of which contains only first-order derivatives with respect to time and space. This can be accomplished by choosing the following *ansatz* for these operators:

$$\hat{L}_1 = \frac{1}{c}\,\partial_t - \alpha \cdot \partial_x - i\,\frac{a}{c} \cdot \beta \tag{6.82}$$

and

$$\hat{L}_2 = \frac{1}{c}\,\partial_t + \alpha \cdot \partial_x + i\,\frac{a}{c} \cdot \beta\ . \tag{6.83}$$

α and β are so far unknown quantities. They will be derived from the requirement that

$$\hat{L}_2\,\hat{L}_1 = \frac{1}{c^2} \cdot \partial_t^2 - \partial_x^2 + \frac{a^2}{c^2} \tag{6.84}$$

must hold. Because of

$$\hat{L}_2\,\hat{L}_1 = \frac{1}{c^2}\,\partial_t^2 - \alpha^2 \cdot \partial_x^2 + \frac{a^2}{c^2} \cdot \beta^2 - i\,\frac{a}{c} \cdot [\beta\,\alpha + \alpha\,\beta] \tag{6.85}$$

the relations

$$\begin{aligned} \alpha^2 &= 1 \\ \beta^2 &= 1 \\ \beta\,\alpha + \alpha\,\beta &= 0 \end{aligned} \tag{6.86}$$

must hold for these quantities. The fulfilment of these relations is obviously impossible in the realm of complex numbers. But, interestingly, this is possible if α and β are allowed to represent the two matrices $\mathbf{A}$ and $\mathbf{B}$ given by

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{6.87}$$

$$\mathbf{B} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\ . \tag{6.88}$$

These matrices are nothing but two of Pauli's spin matrices. With $\mathbf{E}$ representing the 2×2 unit matrix we thus get

$$\hat{L}_1 = \frac{1}{c}\,\mathbf{E} \cdot \partial_t - \mathbf{A} \cdot \partial_x - i\,\frac{a}{c}\,\mathbf{B} \tag{6.89}$$

and

$$\hat{L}_2 \;=\; \frac{1}{c}\,\mathbf{E}\cdot\partial_t \;+\; \mathbf{A}\cdot\partial_x \;+\; i\,\frac{a}{c}\,\mathbf{B} \tag{6.90}$$

for the two first-order operators. If the equation for the Green's function $\mathbf{G}^{(\mathbf{D})}$ of the "1-dim. Dirac equation" is defined by

$$\hat{L}_2\,\mathbf{G}^{(\mathbf{D})}(x,t;x',t') \;=\; \mathbf{E}\cdot\delta(x-x')\,\delta(t-t') \tag{6.91}$$

we are able to calculate this Green's function from the Green's function (3.68) of the 1-dim. Klein-Gordon equation according to

$$\begin{aligned}\mathbf{G}^{(\mathbf{D})} \;&=\; \hat{L}_1\,G^{(KG)}(x,t;x',t') \;=\\ &\left(\frac{1}{c}\,\mathbf{E}\cdot\partial_t \;-\; \mathbf{A}\cdot\partial_x \;-\; i\,\frac{a}{c}\,\mathbf{B}\right) G^{(KG)}(x,t;x',t')\;,\end{aligned} \tag{6.92}$$

as already demonstrated for the Green's function of the simple harmonic oscillator in Sect. 2.5.1. Is there any classical experiment that can be described by this equation? To find an answer to this question is liberally left to the reader!

Appendix

This Appendix provides 3 simple routines which can be used as starting points for solving the numerical exercises formulated in Chaps. 4 and 5. The following software packages have been used:

- Python Release 3.4.4
- NumPy Release 1.11.0
- SciPy Release 0.18.0
- Matplotlib Release 1.5.1

All these packages are Open Source (see http://www.opensource.org for more details) and available for different operating systems. One can simply copy these files into an appropriate editor (Spyder for Python 3.4, for example) to run the programs. Or one can get the original Python files from the author on request (please, mail to: tom.rother@dlr.de).

A.1: Program "ssl_vs_dsl_e.py" and Module "slbasics_e.py"

These two programs refer to the exercise at the end of Sect. 4.2.1. To run the main program "ssl_vs_dsl_e.py", module "slbasics_e.py" must be imported and copied to the working directory. This module can simply be extended beyond the triple-slit to solve the last part of the exercise.

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```
#      ssl_vs_dsl_e.py

# Intensity distribution in the far field of a single- and double slit
# (note, that double-slits with identical slit width are considered!)

print()
print()
print("     Intensity distribution of a single- and double-slit!")
print()
print()

import numpy as np
import slbasics_e as slb
import matplotlib.pyplot as plt


# Input slit width "s1", slit distance "d", and size parameter "ks1":

s1 = float(input('slit width s1: '))
s2 = s1
d = float(input('slit distance d: '))
ks1 = float(input('size parameter ks1: '))


# Calculation of the intensity distribution:

alpha = np.linspace(-50.0, 50.0, 1000)
y1 = slb.ssl(s1, ks1, alpha)
y2 = slb.dsl(s1, s2, d, ks1, alpha)


# Plotting the results as a function of \alpha
# (forward direction: alpha = 0):

plt.plot(alpha,y1,linewidth=2.0, label="ssl")
plt.plot(alpha,y2,linewidth=2.0, label="dsl")
plt.legend()
plt.xlabel("alpha [deg]")
plt.ylabel("intensity")
plt.show()

############### End of the main program ################


#          slbasics_e.py

# Python module with routines to calculate the intensity distribution
# in the far field of a single-, double-, and tiple -slit! Must be imported
# in the main program!

import numpy as np
from scipy import sin, exp, pi


# Function to calculate the intensity distribution of a single slit.
# Parameter: slit width "s1"; size parameter "ks1", and angle "\alpha".
# Slit "s1" is located symmetrically with respect to the x-axis.

def ssl(s1, ks1, alpha):
    k = ks1 / s1
```

```
    Gam_s1 = k * s1 / 2 * sin(alpha * pi / 180)
    z1 = 0 + 1.0j
    ss1 = z1 * (k * s1 / 2 / pi) * sin(Gam_s1) / Gam_s1
    intensity = ss1 * np.conj(ss1)
    intensity = np.real(intensity)
    return intensity

# Function to calculate the intensity distribution of a double-slit.
# Parameter: slit width "s1", "s2"; slit distance "d"; size parameter
# "ks1", and angle "\alpha".

def dsl(s1, s2, d, ks1, alpha):
    k = ks1 / s1
    Gam_s1 = k * s1 / 2 * sin(alpha * pi / 180)
    Gam_s2 = k * s2 / 2 * sin(alpha * pi / 180)
    Gam_d = k * d / 2 * sin(alpha * pi / 180)
    z1 = 0 + 1.0j
    z2 = z1 * (Gam_d + Gam_s1)
    z3 = z1 * (Gam_d + Gam_s2)
    ss1 = z1 * (k * s1 / 2 / pi) * sin(Gam_s1) / Gam_s1 * exp(-z2)
    ss2 = z1 * (k * s2 / 2 / pi) * sin(Gam_s2) / Gam_s2 * exp(z3)
    ss = ss1 + ss2
    intensity = ss * np.conj(ss)
    intensity = np.real(intensity)
    return intensity


# Function to calculate the intensity distribution of a triple-slit.
# Parameter: slit width "s1", "s2", "s3"; slit distances "d1", "d2";
# size parameter "ks1", and angle "\alpha".

def tsl(s1, s2, s3, d1, d2, ks1, alpha):
    k = ks1 / s2
    z1 = 0 + 1.0j
    pref = z1 * k / 2 / pi

    ul1 = s1 / 2
    ul2 = ul1 + d1 + s2
    ul3 = - (s1 /2 + d2)

    ll1 = - ul1
    ll2 = ul2 - s2
    ll3 = ul3 - s3

    eu1 = z1 * k * ul1 * sin(alpha * pi / 180)
    eu2 = z1 * k * ul2 * sin(alpha * pi / 180)
    eu3 = z1 * k * ul3 * sin(alpha * pi / 180)

    el1 = z1 * k * ll1 * sin(alpha * pi / 180)
    el2 = z1 * k * ll2 * sin(alpha * pi / 180)
    el3 = z1 * k * ll3 * sin(alpha * pi / 180)
    ss1 = z1 / k /sin(alpha * pi / 180) * pref * (exp(- eu1) - exp(- el1))
    ss2 = z1 / k /sin(alpha * pi / 180) * pref * (exp(- eu2) - exp(- el2))
    ss3 = z1 / k /sin(alpha * pi / 180) * pref * (exp(- eu3) - exp(- el3))
    ss = ss1 + ss2 + ss3
    intensity = ss * np.conj(ss)
    intensity = np.real(intensity)
    return intensity
```

A.2: Program “sphere_hDP.py”

This program refers to the exercise at the end of Chap. 4. It calculates the differential and total scattering cross-sections of an acoustically soft sphere. A small modification and the usage of special SciPy routines will allow you to handle also the acoustically hard sphere. In so doing, the homogeneous Dirichlet condition must be replaced by the homogeneous von Neumann condition that contains the derivatives of the eigensolutions at the spherical surface.

```
#              sphere_hDP.py

# Scattering on an acoustically soft sphere (homogeneous Dirichlet problem).
# The differential and total scattering cross-sections are calculated in steps
# of 0.5 degrees in [0,\pi]!

print()
print()
print("Scattering on an acoustically soft sphere")
print()
print()

import numpy as np
import scipy as scp
import scipy.special as scs
import matplotlib.pyplot as plt


# Input: radius "a" of the sphere and size parameter "beta = ka":

a = float(input('radius a [mm]: '))
beta = float(input('size parameter beta: '))
N_cut = int(beta + 5.)  # truncation parameter of series expansion!
k = beta / a

# Calculation of the differential scattering cross-section at "theta" in [0,\pi]:

theta = np.linspace(0.0, 180.0, 361)
ctheta = np.cos(theta * scp.pi / 180.)
zi = 0. + 1.0j
pref = zi / k
dscross = []
psi_s = []
for i in range(0, 361):
    psi = 0.0
    y = scs.lpn(N_cut,ctheta[i])
    y1 = y[0]
    for n in range(0, N_cut +1):
        u = scs.spherical_jn(n,beta)
        v0 = scs.spherical_yn(n,beta)
        v = u + zi * v0
        d_n = (2 * n + 1)
        sum_n = d_n * y1[n] * u / v
        psi = psi + sum_n
    psi = pref * psi
    psi_s = psi_s + [psi]
    dscross = dscross + [psi * np.conj(psi)]
dscross = np.real(dscross)


# Calculation of the total scattering cross-section and efficiency by use of
# the optical thorem:

w = np.imag(psi_s[0])
sca_tot = 4 * scp.pi * w / k
sca_eff = ext_tot/ scp.pi / a**2
print()
print("total scattering cross-sect.: sca_tot = ", sca_tot)
print("extinction efficiency: sca_eff = ", sca_eff)
input()

# Plotting the differential scattering cross-section:

plt.yscale('log')
plt.plot(theta, dscross, linewidth=2.0)
plt.xlabel("scat angle [deg]")
plt.ylabel("diff. scat. cross-sect.")
plt.show()
```

A.3: Program “c_bell.py”

This program refers to the exercise formulated in Sect. 5.2.3. It is only one possible way to accomplish the described marble experiment related to the classical Bell’s experiment, and to check the validity of the CHSH-inequality with such a classical experiment. If this program is modified to handle more than one input file, you can run the four different experimental configurations required to check the CHSH inequality at once.

```
#       c_bell.py

# Classical Bell's experiment with differently coloured marbles
# as described in Sect. 5.2.3

# Note that the additional 2 boxes on each side are complementary
# filled with black and white marbles! It is therefore sufficient
# to specify only 1 box on each side!

import numpy as np

# Read the input parameter from file "bell_input_data_e.txt":
# Note, that

# "RBw_Nw" represents the number of white marbles in box Bw on the right-hand side
# "RBw_Ns" represents the number of black marbles in box Bb on the right-hand side
# "LBw_Nw" represents the number of white marbles in box Bw on the left-hand side
# "LBw_Ns" represents the number of black marbles in box Bb on the left-hand side
# "Nexp" represents the total number of runs for a given configuration

fobj = open("bell_input_data_e.txt", "r")  # this file must exist in the
#                                          working directory

z = []
for line in fobj:
    arr = line.split('=')
    wert = int(arr[1])
    z = z + [wert]
fobj.close()

RBw_Nw = z[0]
RBw_Ns = z[1]

LBw_Nw = z[2]
LBw_Ns = z[3]

Nexp = z[4]

# Boxes on the right-hand side:

RBw_Ng = RBw_Nw + RBw_Ns
RBw_L = int(RBw_Ns * 100 / RBw_Ng) - 1
RBs_Nw = RBw_Ns
RBs_Ns = RBw_Nw
RBs_Ng = RBs_Nw + RBs_Ns
RBs_L = int(RBs_Nw * 100 / RBs_Ng) - 1

# Boxes on the left-hand side:

LBw_Ng = LBw_Nw + LBw_Ns
LBw_L = int(LBw_Ns * 100 / LBw_Ng) - 1
LBs_Nw = LBw_Ns
LBs_Ns = LBw_Nw

LBs_Ng = LBs_Nw + LBs_Ns
LBs_L = int(LBs_Nw * 100 / LBs_Ng) - 1

# Definition of the possible events!

ev_ws = ['white', 'black']
ev_sw = ['black', 'white']
ev_ww = ['white', 'white']
ev_ss = ['black', 'black']
```

```
# Generating the random numbers related to the primary box Bp:

za_Bp = np.random.randint(2, size = Nexp)


# Generating the random numbers related to the additional boxes
# on the left- and right-hand sie:

za_RBws = np.random.randint(100, size = Nexp)
za_LBws = np.random.randint(100, size = Nexp)

# Generating the single events for a given experimental configuration:

res = []
for i in range(0, Nexp):
   zr_Bp = za_Bp[i]
   zr_RBs = za_RBws[i]
   zr_RBw = zr_RBs
   zl_LBs = za_LBws[i]
   zl_LBw = zl_LBs

   if zr_Bp == 0:

      if zr_RBs > RBs_L and zl_LBw > LBw_L:
         zr = ["black"]
         zl = ["white"]
      elif zr_RBs <= RBs_L and zl_LBw > LBw_L:
         zr = ["white"]
         zl = ["white"]
      elif zr_RBs > RBs_L and zl_LBw <= LBw_L:
         zr = ["black"]
         zl = ["black"]
      elif zr_RBs <= RBs_L and zl_LBw <= LBw_L:
         zr = ["white"]
         zl = ["black"]

   elif zr_Bp == 1:

      if zr_RBw > RBw_L and zl_LBs > LBs_L:
         zr = ["white"]
         zl = ["black"]
      elif zr_RBw <= RBw_L and zl_LBs > LBs_L:
         zr = ["black"]
         zl = ["black"]
      elif zr_RBw > RBw_L and zl_LBs <= LBs_L:

         zr = ["white"]
         zl = ["white"]
       elif zr_RBw <= RBw_L and zl_LBs <= LBs_L:
         zr = ["black"]
         zl = ["white"]
```

```
    a = zl + zr
    res = res + [a]

anz_ev_ws = 0
anz_ev_sw = 0
anz_ev_ww = 0
anz_ev_ss = 0

for i in range(0, Nexp):
    if res[i] == ev_ws:
        anz_ev_ws = anz_ev_ws + 1
    elif res[i] == ev_sw:
        anz_ev_sw = anz_ev_sw + 1
    elif res[i] == ev_ww:
        anz_ev_ww = anz_ev_ww + 1
    elif res[i] == ev_ss:
        anz_ev_ss = anz_ev_ss + 1

whs_ev_ws = anz_ev_ws / Nexp
whs_ev_sw = anz_ev_sw / Nexp
whs_ev_ww = anz_ev_ww / Nexp
whs_ev_ss = anz_ev_ss / Nexp

summe = whs_ev_ww + whs_ev_ss + whs_ev_ws + whs_ev_sw
corr = whs_ev_ww + whs_ev_ss - whs_ev_ws - whs_ev_sw

# Experimental numbers and probabilities of each event:

print()
print('Experimental numbers and probabilities:')
print()
print('number of event ', ev_ws, ':   ', anz_ev_ws, ' ;', '  whs_ws: ', whs_ev_ws)
print('number of event ', ev_sw, ':   ', anz_ev_sw, ' ;', '  whs_sw: ', whs_ev_sw)
print('number of event ', ev_ww, ':     ', anz_ev_ww, ' ;', '  whs_ww: ', whs_ev_ww)
print('number of event ', ev_ss, ': ', anz_ev_ss, ' ;', '  whs_ss: ', whs_ev_ss)
# input()

print('sum of probabilities: ', summe)
print()
print('correlation C = whs_ww + whs_ss - whs_ws - whs_sw: ', corr)

# Calculation of the theoretical probabilities:

c2beta = RBw_Nw / RBw_Ng
s2beta = RBw_Ns / RBw_Ng
c2alpha = LBw_Nw / LBw_Ng
s2alpha = LBw_Ns / LBw_Ng

th_whs_ev_ws = (c2beta * c2alpha + s2beta * s2alpha)/ 2.
th_whs_ev_sw = th_whs_ev_ws

th_whs_ev_ww = (s2beta * c2alpha + c2beta * s2alpha) / 2.
th_whs_ev_ss = th_whs_ev_ww
```

```
print()
print('theoretical probabilities:')
print()
print('probability of event ', ev_ws, ':   ', '  Whs: ', th_whs_ev_ws)
print('probability of event ', ev_sw, ':   ', '  Whs: ', th_whs_ev_sw)
print('probability of event ', ev_ww, ':     ', '  Whs: ', th_whs_ev_ww)
print('probability of event ', ev_ss, ': ', '  Whs: ', th_whs_ev_ss)
input()

############ End of main program ######################


# Example of the file "bell_input_data_e.txt". Start with the first line!

RBw_Nw = 17
RBw_Ns = 3
LBw_Nw = 1
LBw_Ns = 1
Nexp = 5000
```

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