論文内容の要旨

論文題目：The Physical Role of Boundary Conditions in Quantum Mechanics （量子力学における境界条件の物理的意味）

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1. Abstract

The aim of the dissertation is to investigate and demonstrate the physical role of boundary conditions (contact, reflection and connection conditions) in quantum mechanics. To this end, three prototype models, a quantum particle moving on a half line with a reflecting wall, on a line under the action of a pointlike singularity, and on a circle with a pointlike singularity, respectively, are considered. Various properties are examined to present how considerably the physical properties depend on the free parameters that characterize the different possible contact conditions. Based on the results, two case studies are also provided as applications and demonstrations of the role of boundary conditions: one showing the difference in the quantum statistical behaviour for boxes with distinct boundary conditions, and another to describe the deuteron and proton-neutron scattering in terms of appropriate connection conditions. The general message of the study is that actions and interactions can be expressed in quantum mechanics in two ways, through potentials and via boundary conditions, and it may depend on the physical situation that which description is more appropriate.

2. Description

Chapter 1, the Introduction, starts with an overview of the studies of systems with boundary conditions - pointlike interactions, zero-range potentials, point defects and scatterers, junctions, reflecting boundaries, walls and egdes, and singularities of potentials. It explains the advantages of modelling appropriate systems via such contact conditions. Namely, boundary conditions can grasp the essential characteristics of singular and contact-type objects via only a few free parameters, and allow for exact and analytical calculations and investigations for many systems. Systems with boundary conditions also exhibit various interesting properties like supersymmetry, renormalization, Landau poles, quantum breaking of classical symmetries, duality and spectral anholonomy. The Introduction also stresses the importance of boundary conditions for experimental situations that have been achieved by the recent advent of nanotechnology. Nanowires, quantum dots, nanorings and similar objects are expected to require the application of boundary conditions for the theoretical description. Meanwhile, in some other fields like condensed matter physics and nuclear physics, the discussion of short-range interactions and contact effects (Dirac delta-like potentials, point defects and scatterers) in terms of boundary conditions has become a standard approach since decades. Still, the recognization of boundary conditions in their full potential and variety is a slow process in quantum physics, which explains the main motivation of the present thesis.

Chapter 2 provides the necessary mathematical background for the study of systems with boundary conditions. The existence of multiple possible boundary conditions for a quantum system is connected to that the Hamiltonian admits more than one possible self-adjoint domains within the

Hilbert space. Each self-adjoint domain is characterized by a boundary condition, and vice versa. After reviewing the physical importance of self-adjointness and the classic characterization of the family of self-adjoint domains worked out by Neumann, a more recent development, the approach of boundary value space is explained. This latter method is especially convenient for differential operators, and is used throughout the thesis. Chapter 2 also discusses the physical interpretation of the mathematically found family of boundary conditions. For some systems we can be practically sure that all the found possible boundary conditions describe physically allowed possibilities, for some others it can be shown that only some of the boundary parameters express different physics, and in a number of cases the decision is the competence of experimental investigation. Chapter 2 is assisted by Appendix A, where all the necessary mathematical definitions and theorems are collected.

In Chapter 3, the concrete investigations start, with the discussion of the systems where a nonrelativistic particle moves freely on a half line and is perfectly reflected from the wall where the half line ends. Half line systems are characterized with a free length parameter L, and are found to preserve the classically valid scale invariance only for the two cases when L is zero (Dirichlet condition) or infinity (Neumann condition). For the other cases, WKB exactness also breaks and a nonzero time delay is observed to emerge for a reflected wave packet. It is investigated whether such a time delay can be reproduced by a classical counterpart, with some reflecting potential shape. For positive L, this potential is found while, for negative L, it is proved that the time delay can not be classically reproduced, only in some weak sense. Quantum realizations are also performed, where any reflecting wall system is approached by sequences of steplike potentials.

Chapter 4 considers the systems where a free particle moves on a line that hosts a pointlike singular object. Here the family of all possible fitting conditions is characterized by distinct $U(2)$ matrices. From the corresponding four free parameters, two prove to be two independent length scales, a third one measures the mixing between the two sides of the point singularity, and the fourth - the phase jump at the place of the singularity - is found to be an unphysical gauge freedom. Similarly to the half line systems, which admit one bound state in the cases of positive L, line systems can have maximally two bound states, when both length scales are positive. The family of possible point singularities possesses various subfamilies distinguished by certain symmetry properties (scale invariance, parity invariance, time reversal invariance, etc.) and a continuous generalization of duality-type relationships connecting different line systems. An extensive treatment of these generalized symmetries, via boundary transformations, is provided in Appendix C.

In Chapter 5, the linelike configuration space is changed to a circular one. It is shown how the entering additional length scale, the circumference, reduces the symmetry and generalized symmetry properties, and how the closed topology makes the phase jump parameter physical, gaining interpretation as the magnetic flux driven through the circle. The finite configuration space also makes the energy spectrum discrete; all possible spectra are determined. The family of circle systems still possesses subfamilies admitting certain symmetries. Two supersymmetric cases are also identified, where supersymmetry is shown to be present in the strict sense where the supersymmetry algebra is valid not only in the sense of differential operators but also in the sense of operator domains. WKB exactness is investigated as well.

In Chapters 6 and 7, two case studies are presented, as applications of the previous results and for illustrating the role of boundary conditions. In Chapter 6, a box with Dirichlet outer walls is considered, into which a thin separating wall is placed with Dirichlet boundary condition on one of its sides and with Neumann condition at the other. The two half boxes are of the same length, and are considered to contain the same number of identical noninteracting particles, kept at the same temperature. The difference of the quantum statistically emerging pressure (or force) on the two sides is calculated. The net force acting on the separating wall is found nonzero at zero temperature, to gradually decrease for increasing temperature but, after reaching a nonzero minimum, to increase again and to diverge as temperature tends to infinity. This qualitative behaviour is valid both for bosonic and fermionic particles but with quantitative differences. Since the arising infinite sums are not exactly summable, the force is determined both numerically and via analytic approximations performed in the various temperature domains (low, medium, high).

Chapter 7 reports about a work that exhibits the power of description by boundary conditions. Here, an approximate model of the deuteron and proton-neutron scattering is given where the nuclear interaction between the two particles is expressed not in terms of some potential but by some fitting condition. The nuclear force is a short-range interaction, and the present approach generalizes Fermi's historical delta-like pseudopotential model, with one free parameter, to a four-parameter one. Thus even the experimentally observed weak but nonzero coupling between two angular momentum channels (the spin dependence of the nuclear force) may be effectively characterized. The bound state and the scattering states are calculated in this framework. Some of the free parameters are adjusted via certain experimentally known quantities of the deuteron, and the remaining ones are to be fitted using the scattering data. The comparison of the prediction of the model with the experimental results shows a good agreement.

3. Discussion

Concerning the significance of the results presented in the thesis, let us first consider the discussed systems in turn. The importance of the wall/half-line systems lies in that they appear in many practically relevant models, such as the nontrivial radial part of two and three dimensional delta-type singularities, or the reflecting boundaries of boxes. In parallel, they also serve as a prototype for many features of quantum systems with boundary conditions, including the quantum breaking of classical scale invariance, the time delay and it classical (non)reproducability, and the aspects how they can be produced as a sequence of regularizing potentials. The latter gains practical importance, e.g., when one wishes to experimentally realize the various reflecting walls.

The point singularities on a line are models for any possible short-range interaction, impurity, etc., in an (effectively) one dimensional configuration space. Many of the properties of one such pointlike singular object will appear repeatedly for a sequence of more than one point singularities, leading to models of a crystal lattice, or, if distributed randomly, of defects in a crystal lattice yielding electric resistance, for example. In addition, the one singularity case has proved to be important in the suggestion of spacelike (`abacus') qubit realization, which might become a real alternative compared to the recent spin-based realizations. Two coupled angular momentum channels - like the ones in the chapter about the proton-neutron system - also appear as application.

A pointlike object on a circle is again a prototype, and is the first necessary step towards a circle with two or more singularities. On the theoretical side, the presented supersymmetry results have motivated other authors to study supersymmetry on a circle with more than one singularities. On the other side, it has opened the possibility to provide an explanation of a recent experiment about how the magnetic flux influences the energy levels in a nanoring. The two junctions where the electric current enters and leaves the ring, respectively, may admit a good effective characterization as pointlike singularities. That work is presently in progress by the author and his collaborators.

The investigation of the quantum pressure difference caused by distinct boundary conditions has originally intended to provide an illustrative example of the physical consequences of different boundary conditions. The found apparently nonzero (and even diverging) net force really serves this aim. Although such a force on a separating wall may be experimentally hard to observe, we plan to repeat the treatment for a similar setting, in which the chemical potential difference drives an electric current between two boxes. That effect may well be verified experimentally with the recent nanotechnology and measurement methods. In parallel, the work also required to invent a number of alternative calculational techniques to treat quantum statistical systems when the standard approximation recipes do not provide enough preciseness. Therefore, the methodology is also expected to be of value for quantum statistical physics.

The application for the proton-neutron system is also originally an illustration, but as well a test whether the idea can work quantitatively for nuclear force. Since this attempt seems successful, the idea can be applied for other, theoretically less understood, cases as well (like certain experimental results for hadrons with strangeness).

Considering the dissertation as a whole, the aim has always been to fill the gap between two typical approaches existing on the field of boundary conditions. One typical class of papers is where proper and high-quality mathematical methods are applied but the analysis stops at solving the energy eigenvalue problem, not studying further physical consequences. Such works do not penetrate into physics well enough both because of the language and because they may not discuss questions which physicists are interested in. On the other side, another class of papers aims at answering a physicist's question, but the approach may use improper mathematics, and be incomplete both in the considered family of boundary conditions and in the derived conclusion. The author's motivation has been to appear in between: to be mathematically simple still complete, and to answer questions raised by a physicist's way of thinking.

The other aim has been to advertise boundary conditions for physicists, showing how appropriate and relevant they can be in various quantum physical settings. Boundary conditions are definitely a valuable aspect to be aware of whenever one works with quantum systems.

Throughout the chapters we could see many various faces and aspects of boundary conditions. Although being local in their formulation, they can influence the systems considerably. It may be said that effects and interactions in quantum physics can be modelled in two ways, via a potential and in terms of some boundary condition. Quantum mechanics can formulate physical effects in these two possible forms. Some phenomena may be better described by a potential and others by some contact-type condition. Boundary conditions provide a technically simple description which can be an advantage for a number of physical situations, while in others they may be too restrictive. Potentials and contact conditions can also act together, expressing such richness that could remain unexplored in a potential-only theoretical attitude. Therefore, boundary conditions should be recognized as a relevant part of quantum mechanics.

The third message of this material is hopefully that, right because of their richness, boundary conditions may apply various practical applications in physics. Tunable quantum devices: qubits, quantum switches, filters and other objects may be designed and manufactured making use of them. This aspect adds to the virtues and relevance of contact conditions. If the present work and the related literature inspires experimentalists to carry out measurements and realize practical applications related to boundary conditions then physics and technology may benefit from these studies.

At last, we have been happy to find that many properties historically observed related to quantum field theoretical models appear in quantum physical systems with boundary conditions. Therefore, renormalization, quantum breaking of a classical symmetry, duality, Landau poles, plus other seminal quantum properties like supersymmetry and the Berry-like anholonomy in energy, can be demonstrated on these technically simple systems, and by analytical tools. Quantum mechanical systems with boundary conditions are thus also of much pedagogical and illustrative value.