The Physical Role of Boundary Conditions in Quantum Mechanics

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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.

Contents

Chapter 1

Introduction

Quantum systems with boundary conditions — which term covers contact, reflection and connection (*i.e.,* two-sided boundary) conditions each — enjoy an increasing interest recently. Pointlike interactions, zero-range potentials, point defects and scatterers, junctions, reflecting boundaries, walls and egdes, and singularities of potentials find a convenient and appropriate description in terms of boundary conditions. Starting historically from the Kronig-Penney model of a crystal lattice[1] in solid state physics and the Dirac delta-like Fermi pseudopotential in nuclear physics, the subsequent improvements made by Bethe, Peierls, Thomas, and the formulation in terms of boundary condition and self-adjointness by Berezin and Faddeev gradually clarified the initially heuristic content of these considerations. More and more authors followed the pioneers, and recently it would be hard to list all the relevant and influential researchers on the field.[2] Having said that, the recognization of boundary conditions is still underdeveloped, as most physicists still believe that the boundary condition at a reflecting wall can be Dirichlet only, that the Coulomb problem is uniquely defined, *etc.*

Two obvious advantages favour for the systems related to boundary conditions. The first is their simplicity, a powerful ability to model only some essential, relevant aspects of probably highly (or, typically, too highly) complicated objects. With the aid of contact conditions, one can reduce the description to a few free parameters, the essentially characteristic ones, which makes the system comprehensible and intellectually attractive. The second advantage is solvability. Most of these systems admit exact solutions and analytical calculations, contrary to potential-based problems where perturbation theory and other approximations are required in almost all realistic cases.

Getting gradually acquainted with systems with boundary conditions, a number of further benefits have turned out. These systems exhibit a number of intriguing features, many of which have been seen before only in connection with quantum field theories. Examples include renormalization [2, 3, 4, 5, 6], Landau poles [7], anomalous symmetry breaking [6], duality [8, 9, 10], supersymmetry [10] and spectral anholonomy [10, 11, 12]. Another important aspect has become stressed on the experimental side, caused the rapid

[1] the version with a periodic sequence of Dirac delta potentials

[2] A best monograph attempting to give a thorough overview on the subject is [1].

developments of nanotechnology. Nanowires, quantum dots, nanorings and other similar objects have been manufactured and experimentally studied. Now, for most of these systems boundary conditions play a relevant role: the reflecting boundaries, the magnetic flux driven through a ring, the junctions *etc.* are all such aspects that admit a convenient formulation in terms of boundary conditions. Therefore, the interest in contact conditions comes recently not only from theoretical points of view but also because of their possible usefulness for experimental settings.

In the first decades of quantum mechanics, the difference between a symmetric and a self-adjoint Hamiltonian operator has typically been considered a mathematical aspect only, without physical relevance. Now that we understand that the difference is the possible nonuniqueness of the contact conditions that arise at boundaries, local objects and places where a potential diverges, and especially that different contact conditions lead to different, sometimes strikingly different physical consequences, this picture gradually changes. The aim of the author of the present work and of his collaborators has been to present various illustrations and possible physical applications concerning the physical role of boundary conditions.

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 spinless 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 a 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 connection conditions is char-

acterized 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 analytical 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, we give an approximate model of the deuteron and proton-neutron scattering where the nuclear interaction between the two particles is expressed not in terms of some potential but by some connection condition. The nuclear force is a short-range interaction, and our presented approach generalizes Fermi's historical delta-like pseudopotential model, containing one free parameter, to a four-parameter one. Thus even the experimentally observed weak but nonzero coupling between two angular momentum channels (which expresses 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.

Since the three discussed prototype systems are seemingly so innocent and simple, one might get the feeling that these studies are more for textbook examples than for deep scientific research. Such an opinion would be a superficial mistake.

The first highly nontrivial question is the approach to use for deriving the possible boundary conditions (cf. Sect. 2.2). One might try the method of regularizing potential sequences or the functional integral approach, or work from the eigenfunctions directly, each of which contains a number of principal and practical difficulties. For the best choice available, the boundary space value description of self-adjoint extensions, one needs to be familiar with the fine mathematical aspects at least at a level that the method can be used safely as a routine.

Even the next step, the parametrization of the found family of self-adjoint domains is to be done with care. In the literature, a number of papers use some obscure, inconvenient and sometimes even incomplete parametrizations, which make it hard for them to perceive many generally valid nice physical properties (like symmetries, dualities, *etc.*) and to present the results in simple enough form.

Then comes a relatively easy step, solving the eigenvalue problem taking into account the boundary conditions. However, the physical discussion does not stop here. On the contrary, it only starts here.

Many good physical questions are to be asked and answered to obtain a good understanding of the systems in question. There are numerous aspects that can help in the physical interpretion of the possible singular and boundary objects, or can find important practical applications. This is how we can reach connections with experiments (in solid state physics or nuclear physics) and technology (say, nanotechnology).

Answering such questions may also involve unexpectedly hard technical problems in the calculations. For example, the investigation presented in Chapter 6 requires such calculational techniques that are beyond the standard toolkit of quantum statistical physics. Finding a good approach may also simplify a calculation and decrease the amount of needed numerical work considerably, as shown in the example of Chapter 7.

At last, it is a very important general conclusion to be drawn and to be advertised that actions and interactions can be expressed in quantum mechanics in two ways, through potentials and via boundary conditions. It may depend on the physical situation that which description is more appropriate. Therefore, in every concrete situation one should be aware of both possibilities and choose the one that seems more adequate for the discussion of the given physical problem.

Except from some more-or-less elementary formulas concerning the half line, line and circle systems, all the presented calculations have been done by the author (or in a collaboration where the author played a leading or dominant role). Many of the results have been published in [13, 14, 15]. The author has participated in other collaborations

[16, 17, 18, 19] as well, where further aspects of boundary conditions have been studied, about singular potentials, the three-body Calogero problem, and a qubit suggestion based on tunable point interaction. Those works can also be viewed as applications of the ideas presented here.

Chapter 2

On self-adjoint operators

In this part, a general overview is given about the arising mathematical aspects concerning boundary conditions. After reviewing these principal and general technical questions, in the subsequent sections we will need to concentrate only on the actual concrete technical calculations for the physical systems considered in turn.

For all the necessary mathematical definitions and theorems that will arise here as directly related to self-adjointness, see Appendix A. For further prerequisites, and general, introductory, basic and/or useful material on Hilbert space operators, one may consider [20, 21, 22, 23, 24].

2.1 The domain(s)

In quantum mechanical systems that contain boundaries, pointlike defects, pointlike scatterers, Dirac delta-like pointlike singular objects, or certain potentials that diverge at infinity like $V(x) = -\text{const.}\, x^c$ $(c > 2)$ or at a finite location like the Coulomb potential, after solving the energy eigenvalue problem we can find that the found eigenfunctions are in general not pairwise orthogonal. We can also observe that the symmetricity property $(H\psi_1, \psi_2) - (\psi_1, H\psi_2) = 0$ does not hold, since, after integration by parts, the surface terms generated at these problematic locations do not generally vanish. Both phenomena indicate that, for such systems, the self-adjointness of the Hamiltonian is challenged. Consequently, we have to enter the problem how in such cases self-adjointness can be ensured.

In quantum mechanics, physical quantities are represented by self-adjoint operators. The representation happens via the spectral theorem.[1] The possible values of many physical quantities (*e.g.,* position, momentum, energy *etc.* of a point particle) run in an infinite range, thus the corresponding operator is unbounded. Now, unbounded self-

[1] In more details: physical quantities themselves can be formulated as event valued measures on the space of possible values of the given physical quantity. The event space is the Hilbert lattice, in which the events are the projection operators of the Hilbert space. Via the spectral theorem, these projection valued measures (PVM-s) are in a one-to-one correspondence with a self-adjoint operator. See [25] for a comprehensive treatment.

adjoint operators cannot be defined on the whole Hilbert space. Therefore, we have to bother with their domain of definition.[2]

Actually, in practice, it may not be easy to immediately give the self-adjoint domain for an operator. First, for differential operators, we must not confine ourselves to smooth or some finitely many times differentiable wave functions. The proper level of smoothness property is absolute continuity (in one dimensional problems, and its corresponding Sobolev space-like notion for wave functions on a higher dimensional space). Next, the bigger difficulty comes for systems with singular/problematic locations as mentioned above. The differential operator is not defined at these points, and if we simply ignore this fact then we will run into the problem that the operator is not self-adjoint on this domain of wave functions. This domain is too large and needs some restriction to obtain a self-adjoint result. The suggested method is to impose the further requirement that the wave function should vanish when approaching any of these problematic locations, to vanish such strongly that all the mentioned surface terms are guaranteed to be zero. Then we will reach a safe domain on which, however, the operator will be found only to be symmetric but not self-adjoint. The distinction between these two notions becomes important here. The reason is that when we try to extend this minimal domain back a bit to obtain a self-adjoint domain, we will find that we can do it in more than one way. The minimal operator admits multiple self-adjoint extensions, corresponding to multiple possibilities for a self-adjoint domain.[3]

To have an operator with more than one possible self-adjoint domain is not only a technical question but an essential one. That operator is "really" different on its different domains. Indeed, its spectrum and eigenfunctions will be different. A Hamiltonian may have two bound states on some of its possible domains, one on some others and none but only scattering states on the remaining possible domains. The scattering properties will also depend on the domain: an obstacle can act as a low-energy-pass filter with some domains and as a high-energy-pass filter for some other ones. An incoming wave packet may be reflected from a boundary with a considerably large time delay for some domains (so to say, for some types of boundaries), with no time delay for some others, and

[2]It is not a principal problem that the operator cannot act on all elements of the Hilbert space, so to say, on all pure states. The PVM assings a probability distribution/measure on the possible values of the physical quantity to all states, including all pure states, and this is enough for the satisfactory physical interpretation. An explanation of the situation is that not all probability distributions have a finite expectation value, or uncertainty. For example, we can think of a probability distribution on a real line with such a power-like fall at infinity that is fast enough to ensure the finite normalizability of the distribution but is slow enough that the expectation value, adding one to the power of the "tail", gives an infinite integral.

[3]One may suspect that symmetricity could be enough for the purposes of physics. Indeed, there are certain indications that the formulation of physical quantities should allow positive operator valued measures (POVM-s), not only PVM-s. (Here we are not speaking about the usage of positive operators as "fuzzy events" corresponding to imprecise measurement but about ordinary, "precise", "sharp" events.) For example, the momentum of a particle moving on a half line [26], or position in relativistic quantum mechanics [27] may force us to allow this generalization. However, the corresponding generalization of the spectral theorem [28] relates a POVM to a *maximal* symmetric operator, which is still such a symmetric operator whose domain cannot be extended to a larger symmetric domain. In addition, quantities that are the generators of some symmetry, and especially the Hamiltonian, which must provide unitary time evolution of initial states, must be self-adjoint and not only maximal symmetric.

with a considerably large time advance(!) for still other cases. The existence of multiple self-adjoint domains is not only an aspect for mathematicians. Instead, it describes the physical nonuniqueness of such a system. Exploring all the possible self-adjoint domains for a Hamiltonian means to explore all the physically possible — or, in a more careful wording: all the quantum mechanically allowed — types of boundaries, singularities and contact interactions. These entities cannot be modelled via regular potentials. (They can be given as a limit of a *sequence* of regular potentials — this approach will be discussed later.)

2.2 How to find the domains

In the pioneering and classic method by Neumann, the possible self-adjoint extensions of a symmetric operator can be found via the eigenfunctions of the adjoint operator (in our case, the Hamiltonian on the maximal domain) corresponding to a *nonreal* eigenvalue. This approach is definitely of much importance in mathematics, but for practical applications it involves the difficulty that we need to determine all these eigenfunctions and check their square integrability typically by hand.

To circumvent this problem, another method has been developed, which is especially convenient for differential operators.[4] In this approach, the concept of boundary value space is introduced and utilized. For our purposes of differential operators, it practically means that if we are able to express our problematic surface terms in a given standard form (A.5) then the method provides for us all the possible self-adjoint domains, in terms of a boundary (surface/contact/reflecting/connection) condition (A.7) that contains an arbitrary unitary operator (or matrix). Each self-adjoint domain is in a one-to-one correspondence with one such unitary operator. For reflecting walls, and pointlike singular objects and potentials, the required standard form will contain simply the limiting values of the wave function and its derivative when approaching such a location. For singular potentials, the wave functions will diverge but there is a systematic method how the diverging behaviour of the wave functions can be characterized with some finite limit numbers, and then these finite numbers can be used for the boundary value space approach. For this, we will need to know only the approximate behaviour of the eigenfunctions near the singular locations, and only for an arbitrary real eigenvalue (*e.g.,* for the zero eigenvalue).

Throughout the dissertation, we will call the unitary operator that characterizes a given self-adjoint domain the *characteristic operator* (actually, in all cases discussed hereafter, it will be a matrix, the *characteristic matrix*).

While Appendix A contains all the mathematical details, one thing to mention here is that, in physics, the space coordinate is not a real number but a quantity with the dimension of length. Since the two maps Γ_1, Γ_2 needed in the boundary value space approach must be of the same dimension by construction, and because the limit numbers combine the wave function ψ and its space derivative ψ', ψ and ψ' must be brought into

[4]Nevertheless, it works at the completely general level as well.

the same dimension, with the aid of an auxiliary nonzero constant length L_0. This L_0 does not play any deeper principal role than this, and a change of it can be compensated by an appropriate change of the characteristic operator U so that the same self-adjoint domain is assigned.[5] From conditions that do not mix the wave function with its derivative, like the Dirichlet or the Neumann boundary condition (vanishing of the wave function, resp. its derivative), L_0 drops out, indicating the possibility of scale invariance for the given self-adjoint system. For the other cases, scale invariance is broken, even if it was present at the classical level. We will see examples for this scale anomaly in the subsequent chapters.

A common multiplier of Γ_1 and Γ_2 can be dropped since (A.7) is linear in them. Therefore, we don't have to bother with the dimension of the Hamiltonian, as its effect on the Γs can be changed by such an appropriate overall factor in (A.7).

Experience shows that the boundary value space approach is a very convenient and generally applicable method to determine the possible self-adjoint domains. Nevertheless, it is worth commenting some alternative ways how this task can be completed.

First, we may, by hand, form complete orthogonal systems from the eigenfunctions, and each determined complete orthogonal system will correspond to one self-adjoint domain. (See [30] for such a treatment.) The technical difficulty here is that we will need to solve the eigenvalue problem for all eigenvalues, and then to calculate the scalar product of any pair of eigenfunctions, and to prove that any orthogonal system that we can form is really complete (probably involving infinite sums and integrals that must lead to Kronecker or Dirac delta). Another disadvantage is that we may reach the result in a parametrization in which some general features (*e.g.,* symmetries) are hard to perceive.

Another possibility is to give the possible self-adjoint Hamiltonians as a limit of a sequence of Hamiltonians where the singularities and sharp objects a regularized via some everywhere regular potentials. We will also provide such a scheme (Sect. 3.2). However, we will do this already knowing what the possible boundary conditions are, and this will make our work much easier. If one does not know in advance what the general form of the possible boundary conditions will be then it is hard to ensure that all the possibilities have been produced. One may also choose too general forms of potentials that are hard to work with, or too restricted ones with which it is not possible to reach all possibilities. It is especially easy to miss many of the possible self-adjoint cases since a general practical observation is that most boundary conditions require a fine tuning. It is not the leading form but some fine-tuned subleading behaviour of the potential sequences that will provide the required boundary condition.

In principle, it is also possible to find the possible self-adjoint domains via the path integral representation. There, the different boundary conditions may be achieved by a nontrivial action contribution applied when the path bounces on a reflecting or singular point. The failure of complete WKB exactness discussed later in this dissertation suggests that it may be hard to find the appropriate bounce action contributions with which all the

[5] Apart from L_0, we will not need to deal with that mathematics usually restricts itself to dimensionless quantities while most quantities used in physics are dimensionful. Nevertheless, it is worth mentioning that in [25] quantum mechanics is treated in a mathematical form that fully gives account of the physical dimensions of operators and all other quantities involved. For a "reader-friendly" introduction to the mathematical description of physical dimensions, see [29].

boundary conditions can be reproduced — especially if those are not known in advance.

2.3 How to solve the eigenproblem for such a domain

While some authors make a talented use of functional analysis — such as Krein's formula for resolvents — for solving the eigenproblem of a differential Hamiltonian operator, for our purposes the simple approach of solving the differential equation plus the boundary conditions will be enough. In addition, for cases when one needs confirmation of that the given self-adjoint operator does not admit a continuous singular spectrum, or about where the continuous spectrum lies, or about some similar other information, many criterions are available in the mathematical literature. See Appendix A for more details.

There is another question that may arise concerning the eigenfunctions: the physicist's intuitive expectation is that scattering states also have to fulfil the boundary conditions that characterize a given self-adjoint domain. However, scattering states are not normalizable and are not in the domain so it is a question whether they really should share the same conditions as the normalizable eigenfunctions. Fortunately, the mathematical literature provides an affirmative answer, at least for the one dimensional systems we will encounter.[6] Therefore, in the subsequent paragraphs we won't need to worry about this question.

2.4 The physical interpretation of multiple self-adjoint domains

We may be able to determine the mathematically possible self-adjoint domains for a given Hamiltonian differential operator, and this operator has different eigenvalues and eigenfunctions for different domains, but do these different cases really express a variety of physically allowed possibilities or are just a technical artifact, a situation which probably needs to be cured by some additional principle for quantum mechanics in general or for each such concrete system done case by case? The answer is: it depends.

The first thing to tell is that there has not been wide enough experimental work done for investigating this question. The free parameter of the three dimensional Dirac delta-like "potential", the so-called Fermi potential is a widely accepted physical parameter for experimental fits in nuclear physics and condensed matter physics. The Aharonov-Bohm flux driven through a ring and felt by the quantum particles propagating in the ring is an experimentally verified effect [32, 33, 34]. There is much less knowledge about the free parameters that parametrize the family of possible self-adjoint domains for other systems like reflecting walls, point-sized singularities (Dirac delta, delta-prime = epsilon, *etc.*) in one dimension, or the singular centre of a Coulomb or $1/x^2$ potential. Even when a

[6] It is also probable that a completely general proof can be given, along the lines of the generalized eigenstate expansion in the rigged Hilbert space approach by Gelfand (for a first consultation and further literature, see [31]).

measurement happens (*e.g.,* [35] on a reflecting wall), it is evaluated assuming some model potentials. For walls of boxes and boundaries of space regions, the textbook paradigm of Dirichlet condition, the vanishing of the wave function itself, is the only case that is widely believed to be possible quantum mechanically, hence the only case considered. It is interesting that many physicists do not get suspicious that, if the physical properties of a boundary or edge of a material are different — say, its small-length-scale surface roughness, a very thin oxide layer that covers it from the outside, or some inhomogeneity as approaching the outmost atomic layer —, then for quantum particles in states with much larger length scale these differences should effectively manifest themselves as differences in a reflecting parameter of the boundary. This should rather be an experimental question to test than a belief in the textbook standard condition. The theoretical aspects seem to restrict the physical thinking of many physicists. Even the Neumann condition, vanishing of the derivative of the wave function, which is a well-known other type of boundary condition from classical electrodynamics, is mostly neglected to be a possible alternative.

The fact that such singular, contact objects (effectively, the various self-adjoint domains) can be expressed as a limit of a diverging sequence of finite potentials (see Sect. 3.2, as well as [3, 4, 5, 6]) may help in physically accepting the existence of the other possibilities. These sequence-of-potentials realization can also serve as a guide how an approximate experimental setup can be designed for such cases. It can also be fruitful to think of the arising open parameters as some analogue of other well-known nontrivial degrees of freedom of pointlike objects: mass, charge and especially spin of a point particle, or the multipole moments that can be attributed to (effectively) pointlike electrodynamical or gravitational objects.

For the Coulomb problem (both the nonrelativistic and the special relativistic one), careful enough treatments observe the nonuniqueness of self-adjoint domain, at least in some form. There the typical attitude is to (do handwaving, or) work out some argument why the usual choice, the least singular (Dirichlet) one should only be accepted. Dirac, at the time when neither the mathematical aspects nor the quantum mechanical role of distributions were clear, imposed the condition that the eigenfunctions must be eigenfunctions in the distribution derivative sense. The same opinion is shared, later, in [22]. The problem with this is that, according to our present knowledge, it is not necesary to impose this requirement. Neither does mathematics restrict us to do so, nor can we tell what is present physically at the centre of an otherwise Coulomb potential. Maybe some short-range nontrivial richness exists there, which cannot effectively be observed outside locally but manifests itself when the particle is near enough to it. For example, when we use the Coulomb problem as a model for the hydrogen atom, the short-sized charge distribution of the proton may appear from the outside as a deviation from the historically used self-adjoint domain for the electron. In case of two oppositely charged, and strongly also interacting particles, such a scenario is even more plausible. It may cause a rather big error to neglect that short-range but strong interaction from the quantum mechanical description. And if it is not neglected then it is fairly logical to try to describe it first as a pointlike effect, via a non-Dirichlet boundary condition for the relative wave function at the centre. (Repeating the idea how the Fermi potential was introduced.)

Furthermore, the distributional argument may be carried out for a relatively mild

singularity (like $1/r$ in three dimensions) but not for stronger ones (stronger power, fewer dimensions). Namely, a stronger singularity may not be a locally integrable function and then the multiplication of it with a wave function (the term $V\psi$ in a Schrödinger equation $i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\triangle\psi + V\psi$) may be ill-defined in the distribution sense, especially since the energy eigenfunctions and, actually, all functions in the maximal domain will also be singular where the potential is singular. Thus the method for such cases should include a regularization or other manipulation, but with such mathematics we may get more and more distant from the physical situation.

Two more arguments are also usually applied for excluding the historically nonstandard cases in the Coulomb problem. For example, both are used in [36]. One of them is that the domain of the total energy operator should be a domain for the kinetic and the potential energy terms separately as well. This condition sounds nice but, as far as our present physical knowledge is concerned, this is not a physical requirement. On similar ground, we could impose that momentum, and/or position should also admit the same self-adjoint domain as kinetic energy but we know that both unavoidably have some different domains. As mentioned above, the domains themselves mean no problem for the physical interpretation of a self-adjoint operator as a physical quantity. Hence, this requirement does not seem physically satisfactory.

The other argument shows that, if the singular centre is regularized and a limiting procedure is performed then the limit leads to the standard self-adjoint operator. This really can be an acceptable argument for charges that are known to be smeared out to some extent.[7] Nevertheless, it may not be a universally acceptable principle – let us think again of the two oppositely charged particles that interact strongly as well.

To summarize, principal considerations may not be enough to choose a self-adjoint domain for a given system: this question is to be investigated by experiments. Potentials are determined and/or checked experimentally; similarly, the boundary type properties of a system are also to be explored and fixed by experiments.

As an independent physical aspect of multiple self-adjoint domains, it is interesting to remark that, according to Koshmanenko [37], in interacting and self-interacting quantum field theories, the Hamiltonian (after an infrared cutoff imposed) admits multiple self-adjoint extensions (with infinite deficiency indices). The challenge there is thus to choose a possibly distinguished one and to give the domain and the operator on it explicitly. He actually presents such a choice, which is similar to the procedure when a quantum mechanical pointlike or contact object is given as a limit of diverging regular potentials. Those diverging quantities may be interpeted as the ultraviolet divergences of field theory. Therefore, it is a nice pedagogical possibility to explain the ultraviolet divergences via the much simpler, finite degree-of-freedom example of, say, a delta "potential" (renormalized Dirac delta, see [1]) in three dimensions, or the even simpler case of a one dimensional half line system with a reflecting wall (Sec. 3).

[7]However, the result might depend on the way of regularization, like in Sect. 3.2. It may happen that, similarly as $L = 0$ walls are realized most easily and with least "tricky" sequences, the Dirichlet case is similarly distinguished in the Coulomb problem. Even then, that property should be proved.

Chapter 3

Reflecting walls: the half line systems

In this chapter, a free particle is considered moving on a half line $x \geq 0$, along the lines of [13] but also adding some new components. This model is a simple prototype of the systems with contact condition. It also appears as a special case of various more complicated settings, and as the radial part of any higher dimensional system of a delta-type point interaction [1]. The family of quantum mechanically allowed impenetrable reflecting walls at $x = 0$ is parametrized by an arbitrary real length parameter L. After discussing the basic properties of these systems — including the spectrum and eigenfunctions, scale (non)invariance and the time delay of a reflected wave packet —, realizations are provided for all these walls as limits of sequences of regular, steplike, potentials. Then we then study the classical analogues of the quantum walls, by seeking a classical counterpart which admits the same time delay in scattering from the quantum wall, and the semiclassical aspects by examining the WKB-exactness of the transition kernel, incorporating the found potential realizations as well.

3.1 Basic properties of the wall systems

For our present Hamiltonian, $H = -\hbar^2/(2m)\,\mathrm{d}^2/\mathrm{d}x^2$, the infinity is limit-point, and thus the lhs difference in (A.5) evaluates, by partial integration, to

$$(\psi_1^*\psi_2' - \psi_1^{*\prime}\psi_2)(0) = W[\psi_1^*, \psi_2](0)\,, \tag{3.1}$$

up to a constant that is irrelevant for our present purposes (see Sect. 2.2). As has also been mentioned in Sect. 2.2, with such a regular potential all wave functions of any self-adjoint domain are also regular at $x = 0$. Hence, the identification of Γ_1, Γ_2 is very simple here: we can choose

$$\Gamma_1\psi = \psi(0)\,, \qquad \Gamma_2\psi = L_0\psi'(0) \tag{3.2}$$

(see Sect. 2.2 concerning L_0). Then, using (A.5), the possible self-adjoint domains are given by the condition

$$(e^{i\vartheta}-1)\psi(0)+i(e^{i\vartheta}+1)L_0\psi'(0)=0\,, \tag{3.3}$$

where the characteristic matrix U is now simply the $U(1)$ complex phase factor $e^{i\vartheta}$, with $\vartheta\in[0,2\pi)$. We can rearrange this condition in a simpler form,

$$\psi(0)+L\,\psi'(0)=0\,, \tag{3.4}$$

where, consequently,

$$L=L_0\cot\frac{\vartheta}{2}\in(-\infty,\infty)\cup\{\infty\} \tag{3.5}$$

is an arbitrary real length parameter. $L=0$ gives the most well-known case, the Dirichlet boundary condition while "$L=\infty$" ($\vartheta=0$) represents the Neumann boundary condition.[1]

Under the boundary condition (3.4) the positive energy eigenfunctions are

$$\varphi_k(x)=\frac{1}{\sqrt{2\pi}}\left(e^{-ikx}-\frac{1-ikL}{1+ikL}\,e^{ikx}\right)\,, \tag{3.6}$$

or, in a form that displays the scattering phase,

$$\varphi_k(x)=\tfrac{1}{\sqrt{2\pi}}\left(e^{-ikx}+e^{i\delta_k}e^{ikx}\right) \tag{3.7}$$

with $\delta_k=2\mathrm{arccot}\,kL$. In addition, for $L>0$, we also have one negative energy state,

$$\varphi_{\mathrm{bound}}(x)=\sqrt{\tfrac{2}{L}}\;e^{-\frac{x}{L}}\qquad\qquad(L>0)\,, \tag{3.8}$$

which is a bound state localized at the wall with its characteristic size L. The existence of this bound state is indicated also by the pole of the reflection coefficient $-\frac{1-ikL}{1+ikL}$ on the complex k-plane, $k_{\mathrm{pole}}=i\frac{1}{L}$, which lies on the positive half of the imaginary axis for $L\in(0,\infty)$, predicting a bound state of energy $\frac{\hbar^2}{2m}k_{\mathrm{pole}}^2=-\frac{\hbar^2}{2mL^2}$. From (3.8) we can see that this bound state is localized at the wall, at the edge of the system. Its characteristic size is just the parameter L itself.

One may find it strange that, although apparently there is no negative potential present in the system, the energy is allowed to be negative for the $L\in(0,\infty)$ systems. This suspicion is based on that, for any usual system on the whole line with Hamiltonian $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)$, the minimal value of the potential $V(x)$ provides a lower bound for the energy,[2]

$$(\psi,H\psi)\geq V_{\min}\,. \tag{3.9}$$

[1] Why self-adjointness excludes a condition like $\psi(0)=c\neq 0$ is easy to understand based on that a domain must be a linear subspace in the Hilbert space *i.e.,* to satisfy the superposition principle. Why a nonreal L is not allowed in (3.4) can also be understood in a simple way, since the wall does not allow a probability flux through $x=0$, and rearranging the vanishing of the probability current $j(0)=\frac{\hbar}{2im}(\psi^*\psi'-\psi\psi^{*\prime})(0)=0$ gives $\psi(0)/\psi'(0)=[\psi(0)/\psi'(0)]^*$. For more complicated systems, it gets less apparent which boundary conditions are admitted by self-adjointness so in general it is better to apply the general result (A.5).

[2] This statement is valid in higher space dimensions, too. For our purposes we quote it in its one dimensional form.

However, if we apply the argument that yields this inequality for our system on the half line, now the boundary condition produces an additional term on the rhs of (3.9). More closely, we find

$$(\psi, H\psi) = \int_0^\infty \mathrm{d}x\, \psi^*\Big(-\frac{\hbar^2}{2m}\psi''\Big) = \frac{\hbar^2}{2m}\int_0^\infty \mathrm{d}x\, |\psi'|^2 \, - \frac{\hbar^2}{2m}\frac{1}{L}|\psi(0)|^2 \;\geq\; -\frac{\hbar^2}{2m}\frac{1}{L}|\psi(0)|^2 \qquad (3.10)$$

by partial integration and using the boundary condition (3.4) (and supposing that ψ and its derivative tend to zero for $x \to \infty$), which lower bound is negative for $L \in (0, \infty)$. Further, observing that the expectation value of the Hamiltonian can be expressed as

$$(\psi, H\psi) = \frac{\hbar^2}{2m}\frac{1}{L^2}\int_0^\infty \mathrm{d}x\, |\psi(x) + L\psi'(x)|^2 - \frac{\hbar^2}{2m}\frac{1}{L^2} \qquad (3.11)$$

for a state normalized to one, we obtain that the lower bound of the energy is $-\frac{\hbar^2}{2m}\frac{1}{L^2}$ if the system admits a state that possesses the property $\psi(x) + L\psi'(x) = 0 \quad (\forall x)$. Now, this property is fulfilled by the function $\psi(x) = \text{const.} \cdot e^{-x/L}$, which is normalizable iff $L \in (0, \infty)$. This way we actually recovered the bound state (3.8).

For the other Ls, this property cannot hold for any normalizable state, and actually, the extra term on the rhs of (3.10) is non-negative, showing that for these systems the lower bound of the energy is zero.

The phenomenon that the energy can be negative in a half line system can be further understood through the physical picture provided by the realizations of the reflecting wall by potential sequences with thin potentials located at $x = 0$, as discussed in Sect. 3.2.

The appearance of a length parameter in the physical properties of the quantum wall systems shows that scale invariance, which is present at the classical level, is broken quantum mechanically. Indeed, the wave function and its derivative are transformed in a different way under scale transformation. Hence, their ratio, and thus L, does not remain invariant. This scale anomaly is a nice and simple example for the phenomenon of quantum breaking of a continuous classical symmetry, which was historically observed first in quantum field theory. Scale invariance remains present only in the two cases $L = 0$ and $L = \infty$, the Dirichlet and Neumann cases.

Another apparent role of the parameter L in the physical behaviour of half line systems is played in the time delay that occurs when an incoming particle is reflected from the wall. The time delay in quantum scattering processes has been studied extensively (see, *e.g.,* [31, 38] and references therein), but is not solely a quantum phenomenon but a generic wave property: the time shift between the instant when the peak of an incoming wave packet arrives at the scattering object and the instant when the peak of the scattered wave packet leaves it. This quantity provides an interesting characterization of the scattering process. Its definition and calculation are given for our simple system as follows.[3] Let us consider a wave packet formed out of the positive energy states (3.7),

$$\begin{aligned}\psi(x,t) &= \int_0^\infty \mathrm{d}k\, f(k)\, e^{ikx_0} e^{-\frac{i\hbar k^2}{2m}t}\varphi_k(x) \\ &= \tfrac{1}{\sqrt{2\pi}}\int_0^\infty \mathrm{d}k\, f(k)\, e^{ikx_0} e^{-\frac{i\hbar k^2}{2m}t} e^{-ikx} + \tfrac{1}{\sqrt{2\pi}}\int_0^\infty \mathrm{d}k\, f(k)\, e^{ikx_0} e^{i\delta_k} e^{-\frac{i\hbar k^2}{2m}t} e^{ikx} \qquad (3.12)\end{aligned}$$

[3]Compare this with the classical mechanical definition of time delay, presented in Sect. 3.3.

where $f(k)$ is a real function peaked at $k_0 > 0$. The first term describes the incident packet whose maximum starts from x_0 at $t = 0$ and moves to the left with velocity magnitude $v_0 = \hbar k_0/m$, as can be seen from a stationary phase argument,

$$\mathrm{d}/\mathrm{d}k \left(-\hbar k^2/(2m)\, t + kx_0 - kx\right)\Big|_{k=k_0} = 0 \qquad \Rightarrow \qquad x^{(1)}_{\max}(t) = x_0 - (\hbar k_0/m)\, t\,. \tag{3.13}$$

Similarly, the reflected packet given by the second term moves as

$$x^{(2)}_{\max}(t) = -x_0 + (\hbar k_0/m)\, t + 2L/[1 + (k_0 L)^2]\,. \tag{3.14}$$

As t increases, the first packet moves towards the wall at $x = 0$, and its maximum reaches it at $t_1 = x_0/v_0$. Meanwhile, the second packet comes from the left (if we allow $x < 0$ as well) moving to the right and arrives at the wall at $t_2 = (x_0 - \frac{2L}{1+(k_0L)^2})/v_0$. The difference between the two instants gives the time delay,

$$\tau = t_2 - t_1 = -\frac{2mL}{\hbar k_0[1 + (k_0 L)^2]}\,. \tag{3.15}$$

For $L = 0$ and $L = \infty$, this time delay is zero, as one would expect on the ground that for such cases there is no parameter in the system possessing the dimension of time. Note that for negative L the time delay is positive, whereas for positive L it is negative.

3.2 Wall realizations by potential sequences

Now let's study how the possible walls can be realized as a limit of finite (regularizing) potentials. The potentials we consider are step-like and may be manufactured using, *e.g.,* thin layers of different types of semiconductors in the future. Naturally, such an experimental realization would provide only one such potential and not the limiting case but it may provide a very good approximation to the theoretical model. We shall show that it is indeed possible to realize any wall out of the step-like potentials if we fine-tune the limiting procedure. Our regularization method will be analogous to those used earlier for point singularities [1, 5].

We extend the space to the entire line $-\infty < x < \infty$ and seek a potential $V(x)$ with finite support such that, in the limit of vanishing support, the boundary condition (3.4) at $x = 0$ can be realized. Obviously, since no probability flow is admitted through the wall at $x = 0$, such a regularized potential has to become infinitely high for $x < 0$ in the limit. A simple choice for the potential fulfilling the demand is

$$V(x) = \begin{cases} V_1\,, & x < -d & \text{(domain I)} \\ V_2\,, & -d < x < 0 & \text{(domain II)} \\ 0\,, & x > 0 & \text{(domain III)} \end{cases} \tag{3.16}$$

with constants $V_1 > 0$ and $V_2 < 0$. Here, the scale of the support is given by the regularization parameter d, and V_1 and V_2 are assumed to be functions of d such that V_1, $|V_2| \to \infty$ as $d \to 0$.

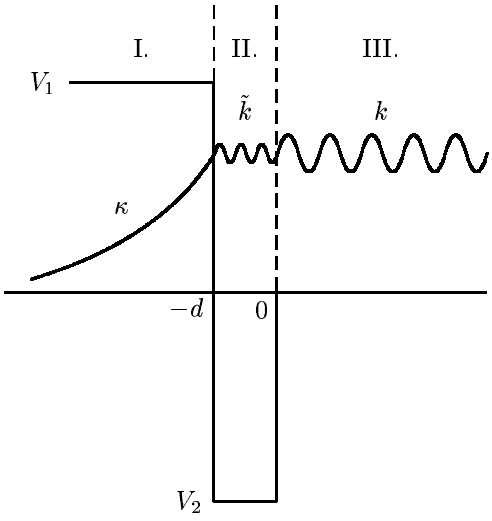

Figure 3.1: The regularized potential (3.16) and the eigenfunction (3.17).

To find the appropriate dependence of $V_1(d)$ and $V_2(d)$, let us consider an energy eigenstate φ in the potential (3.16) with energy $E < V_1$ (see Fig. 3.1):

$$\varphi(x) = \begin{cases} \varphi_{\rm I}(x) = Ne^{\kappa x}, & x < -d\ , & \kappa = \sqrt{\frac{2m}{\hbar^2}(V_1 - E)}\ , \\ \varphi_{\rm II}(x) = Ae^{i\tilde{k}x} + Be^{-i\tilde{k}x}, & -d < x < 0\ , & \tilde{k} = \sqrt{\frac{2m}{\hbar^2}(|V_2| + E)}\ , \\ \varphi_{\rm III}(x) = Ce^{ikx} + De^{-ikx}, & x > 0\ , & k = \sqrt{\frac{2mE}{\hbar^2}} \end{cases} \tag{3.17}$$

(for $E < 0\,,\ \varphi_{\rm III}(x) = Me^{-\sqrt{\frac{2m|E|}{\hbar^2}}x}$). Under such finite potentials (*i.e.*, without infinity or singularity), the wave function and its derivative are required to be continuous. The condition which is dynamically important is provided by the continuity of the ratio φ'/φ which is free from the ambiguity of overall normalization. From this continuity condition, we obtain

$$\kappa = \frac{i\tilde{k}(Ae^{-i\tilde{k}d} - Be^{i\tilde{k}d})}{Ae^{-i\tilde{k}d} + Be^{i\tilde{k}d}}\,, \qquad \frac{\varphi'_{\rm III}}{\varphi_{\rm III}}(0) = \frac{i\tilde{k}(A-B)}{A+B} \tag{3.18}$$

at $x = -d$ and $x = 0$. Note that both $\tilde{k}$ and κ are d-dependent $\tilde{k} = \tilde{k}(d)$, $\kappa = \kappa(d)$ through $V_1(d)$ and $V_2(d)$ and so are the two ratios in (3.18). If we introduce

$$R(d) = \frac{\varphi'_{\rm III}}{\varphi_{\rm III}}(0)\ , \qquad \alpha = \arctan\frac{\kappa}{\tilde{k}}\ , \qquad \beta = \tilde{k}d\ , \tag{3.19}$$

then from (3.18) we find

$$R(d) = \tilde{k}\,\frac{(Ae^{-i\beta} - Be^{i\beta})\cos\beta - i(Ae^{-i\beta} + Be^{i\beta})\sin\beta}{(Ae^{-i\beta} + Be^{i\beta})\cos\beta - i(Ae^{-i\beta} - Be^{i\beta})\sin\beta} = \tilde{k}\tan(\alpha - \beta)\,. \tag{3.20}$$

The boundary condition (3.4) is realized if

$$R(d) \to -\tfrac{1}{L} \qquad \text{as} \quad d \to 0\ , \tag{3.21}$$

independently of the energy E. In what follows we present a set of regularized potentials fulfilling this requirement.

To this end, we first define

$$\alpha_0 = \lim_{d\to 0}\alpha\ , \qquad \beta_0 = \lim_{d\to 0}\beta\ , \tag{3.22}$$

and note that, since $V_1(d) \to \infty$ as $d \to 0$, we always have $\kappa \to \infty$, whereas since $0 < \alpha < \pi/2$ by definition, we have $0 \le \alpha_0 \le \pi/2$. Note also that, if $V_2(d)$ used in our regularization is such that $\beta \to \infty$, then $\tan(\alpha - \beta)$ will oscillate between $-\infty$ and ∞ so $R(d)$ will not have a limit. We therefore confine ourselves to cases in which β has a finite (zero or nonzero) limit β_0. Now, let us suppose $\beta_0 \neq \alpha_0 \,(\mathrm{mod}\ \pi)$, that is, $\tan(\alpha - \beta) \to \tan(\alpha_0 - \beta_0) \neq 0$. Then, if $|V_2| \to \infty$ we have $\tilde{k} \to \infty$ and, consequently, $R(d) \to \pm\infty$. If $|V_2|$ remains finite, on the other hand, then we find $\alpha_0 = \pi/2$ and $\beta_0 = 0$ and hence $R(d) \to \infty$. We thus see that these regularizations yield necessarily the standard wall $L = 0$.

The foregoing argument shows that nonstandard walls with $L \neq 0$ can be realized only by such realizations in which V_1 and V_2 are fine-tuned as

$$\beta_0 = \alpha_0 \,(\mathrm{mod}\ \pi)\,. \tag{3.23}$$

We shall suppose (3.23) from now on, and consider the limit of $R(d)$ for the cases $\alpha_0 = 0$, $0 < \alpha_0 < \pi/2$ and $\alpha_0 = \pi/2$, separately.

(i) case $\alpha_0 = 0$:

We then have, as $d \to 0$, $\alpha \approx \tan\alpha = \kappa/\tilde{k} \to 0$ and $\beta - \beta_0 \to 0$ and hence $\tan(\alpha - \beta) = \tan(\alpha - \beta + \beta_0) \approx \kappa/\tilde{k} - \beta + \beta_0$. Thus the ratio is approximated as

$$R(d) \approx \kappa - \tilde{k}(\beta - \beta_0)\,. \tag{3.24}$$

Now, if $\beta_0 = 0$ then the rhs reads $\kappa - \tilde{k}^2 d$. Hence, to get a finite $R(d)$, $\tilde{k}^2 d$ has to compensate the divergence of κ. This can be done if κ and $\tilde{k}$ behave as

$$\kappa \sim c\, d^{\nu} - \tfrac{1}{L}\,, \qquad \tilde{k} \sim c^{\frac{1}{2}}\, d^{\frac{\nu-1}{2}} \qquad (-1 < \nu < 0)\,, \tag{3.25}$$

which is realized if, for instance, we put

$$V_1(d) = \tfrac{\hbar^2}{2m}\left(c^2 d^{2\nu} - \tfrac{2c}{L} d^{\nu}\right)\,, \qquad V_2(d) = -\tfrac{\hbar^2}{2m}\, c\, d^{\nu-1}\,, \tag{3.26}$$

with a constant $c > 0$. It is then readily confirmed that this regularized potential (3.26) does lead to $R(d)$ fulfilling (3.21) for all $E > 0$. If $\beta_0 > 0$, on the other hand, then $\beta_0 d^{-1}(\beta - \beta_0)$ on the rhs of (3.24) has to cancel the divergence of κ. This means $\tilde{k} \sim \beta_0 d^{-1} + (1/\beta_0)\kappa$. The needed finite term $-\frac{1}{L}$ can be provided again by κ if $\kappa \sim c_1 d^{\nu} - \frac{1}{L}$. This is achieved, for example, by

$$V_1(d) = \tfrac{\hbar^2}{2m}\left(c^2 d^{2\nu} - \tfrac{2c}{L}\, d^{\nu}\right)\,, \qquad V_2(d) = -\tfrac{\hbar^2}{2m}\left(\beta_0^2\, d^{-2} + 2c\, d^{\nu-1}\right)\,. \tag{3.27}$$

It is again easy to confirm that (3.27) yields $R(d)$ fulfilling (3.21) for $\nu > -1/2$.

(ii) case $0 < \alpha_0 < \pi/2$:

In this case, we have $\tilde{k} \sim \beta_0 d^{-1}$ and $\kappa \sim (\beta_0 \tan\beta_0)\, d^{-1}$. Using the Taylor expansion,

$$\alpha = \arctan(\kappa/\tilde{k}) \approx \alpha_0 + \cos^2\alpha_0 \left(\kappa/\tilde{k} - \tan\alpha_0\right), \tag{3.28}$$

we find

$$R(d) \approx \tilde{k}\, \tan\left[\alpha_0 - \beta_0 + \cos^2\alpha_0\, (\kappa/\tilde{k} - \tan\alpha_0)\right] \approx \cos^2\alpha_0\, (\kappa - \tilde{k}\tan\alpha_0\,). \tag{3.29}$$

Hence the choice,

$$\kappa \sim (\beta_0 \tan\beta_0)\, d^{-1} - (1/\cos^2\beta_0)\, \tfrac{1}{L} \tag{3.30}$$

may lead to (3.21). A possible regularized potential realizing (3.30) is

$$V_1(d) = \tfrac{\hbar^2}{2m}\left[(\beta_0^2 \tan^2\beta_0)\, d^{-2} - \tfrac{2}{L}\,(\beta_0 \tan\beta_0/\cos^2\beta_0)\, d^{-1}\right], \quad V_2(d) = -\tfrac{\hbar^2}{2m}\,\beta_0^2\, d^{-2}\,, \tag{3.31}$$

which can be shown to give $R(d)$ satisfying (3.21).

(iii) case $\alpha_0 = \pi/2$:

We still have $\tilde{k} \sim \beta_0 d^{-1}$ but now $\kappa/\tilde{k} \to \infty$ so $\alpha \approx \pi/2 - \tilde{k}/\kappa$, and therefore

$$R(d) \approx \tilde{k} \tan\left[\frac{\pi}{2} - \frac{\tilde{k}}{\kappa} - (\beta - \beta_0) - \beta_0\right] \approx \tilde{k}\left[-\frac{\tilde{k}}{\kappa} - (\beta - \beta_0)\right]. \tag{3.32}$$

The realization (3.21) will be attained if, for example, we have $\kappa/\tilde{k}^2 \to \infty$ and provide $-\frac{1}{L}$ through $\tilde{k}$ by assuming $\tilde{k} \sim \beta_0 d^{-1} + \frac{1}{L}\frac{1}{\beta_0}$. This is the case with the regularization,

$$V_1(d) = \tfrac{\hbar^2}{2m}\, c_1^2\, d^{2\nu} \quad (\nu < -2)\,, \qquad V_2(d) = -\tfrac{\hbar^2}{2m}\left(\beta_0^2 d^{-2} + \tfrac{2}{L}\, d^{-1}\right). \tag{3.33}$$

To summarize, the regularization by means of the step-like potential (3.16) leads generically to the standard wall $L = 0$. It can also lead to nonstandard walls $L \neq 0$ but only as exceptional cases under the fine-tuning (3.23). It is worth emphasizing that the crucial factor in determining the limit of $R(d)$, *i.e.*, the boundary condition at $x = 0$, is not the leading asymptotic behaviour of V_1 and V_2 in $d \to 0$ but always a subleading term. A similar phenomenon has been observed for the regularization of the Dirac delta point interactions in higher space dimensions [1].

The regularizations we used are based on a step-like potential. Needless to say, other types of potentials can also be used for realizing the walls. It is possible, for instance, to use a sequence of steeper and steeper slopes. Since such a sequence itself leads again necessarily to the Dirichlet wall[4] similarly to when we have only one higher and higher steplike potential, again one would need some additional well-like structure to provide the other cases. One can also look for a potential which leads to the realization for any L without involving the mass parameter m. Such a regularization may be more desirable than that we constructed — where the potentials turned out to be m-dependent — for the reason that potentials should be independent of the particle. Nonetheless, our simple

[4]The details of this result are not included here.

regularization can well exhibit universal features of the realization of the (standard and nonstandard) walls, as we can see, for example, the bound state being accommodated in the negative middle part of the step-like potential we used.

It also deserves discussion that, while we can choose rather arbitrary regularizing potential shapes governed by many free parameters, surprisingly, the limit of any such sequence will be dependent on only one parameter, L. Apparently, what happens is that any sequence falls into one universality class, the classes indexed by the limiting property L. Similarly, potential sequences that realize a pointlike singularity on a line will fall into university classes indexed by finitely many — four — parameters. It seems a general rule that the possible richness becomes restricted as we reach the limit of an exactly pointlike contact interaction. It is physically not obvious why this should be the case: for example, the infinitely many multipole moments of an electric charge distribution all survive the pointlike limit. The situation seems more similar to another (unrelated) analogue: classical [25] as well as quantum mechanics allows only finitely many parameters for a free pointlike particle: the mass and the spin.

Some closer simple understanding of this restrictedness of contact interactions can be achieved for one dimensional cases as follows. Any self-adjoint domain / physically consistent system is fully determined by the solution of the energy eigenvalue problem. The energy eigenvalue equation is a second order linear differential equation so the connection or boundary conditions at the place of a contact interaction can only contain the wave function and its first derivative (at both sides of the contact interaction, if applies) and only in some linear combination. Therefore, the linear coefficients are clearly only finitely many in number.[5]

In higher dimensions, a pointlike singularity is even more "lost" (less freedom) than in one dimension. However, a linelike singularity in a plane, for example, has infinitely many free parameters. Intuitively, it has finitely many at each point of the line, but because of some regularity properties of the wave function along the direction of the line, only a discretely infinite freedom results.[6]

3.3 Classical counterparts of quantum walls

We then turn to the question whether the quantum walls admit classical analouges, at least from some specific points of view. This will be examined by looking at the time delay of the particle in scattering, which is the time difference between the moments of incidence and reflection at the wall. It will be shown that quantum walls with $L < 0$, which are characterized by positive time delay, have no classical counterpart possessing the same time delay. Such classical equivalents are possible only in some weaker sense.

What we ask is whether there is a classical system with some appropriate potential $V(x)$ which can account for the same amounts of time delay as those observed under

[5]In fact, self-adjointness imposes some further restriction on even this limited freedom.

[6]Square integrable functions form a separable Hilbert space so the deficiency index can also be only countably infinite.

the walls. Note that systems with the regularized potentials discussed above are not applicable for this purpose, because in those systems the time a classical particle spends in a potential (3.16) tends necessarily to zero as $d \to 0$ (since, as $V_2 \to -\infty$, the distance run by the particle becomes zero while its velocity becomes infinity).

To find a potential for the classical particle that reproduces the quantum time delay, we shall first consider the walls with $L > 0$. In this case the time delay (3.15) is negative, and if the classical picture is available, the incident particle with velocity magnitude $v = \frac{\hbar k}{m}$ must return earlier by

$$|\tau| = \frac{2L}{v}\,\frac{1}{1+\left(\frac{mL}{\hbar}\,v\right)^2} \tag{3.34}$$

than we would expect when it collided with the wall at $x = 0$. Observe that, for small v the time advance $|\tau|$ approaches $\frac{2L}{v}$. This suggests that a slow particle sees the wall at (around) $x = L$, not $x = 0$. Consequently, the reflecting potential $V(x)$ is expected to begin to grow at $x = L$. For definiteness, let us search for the potential in the qualitative form as shown in Fig. 3.2. (This fixes an arbitrariness in the choice of the potential. As we will see, demanding a positive, monotonically decreasing potential determines the potential uniquely.) Now, let us introduce

$$\tilde{\tau} = \frac{2L}{v} + \tau = \sqrt{2mL^2E}\Big/\Big(\tfrac{\hbar^2}{2mL^2} + E\Big)\,, \tag{3.35}$$

(where $E = \frac{1}{2}mv^2$ is the incoming energy) which is the time spent by the particle in the region left to the point $x = L$. Our problem is then an inverse problem: Determine a potential $V(x)$ from a given $\tilde{\tau}(E)$ as a function of E. This can be answered if we follow the well-known argument of Landau and Lifshitz [39] used for the problem of determining a well-shaped potential from the period time with which a particle moves.

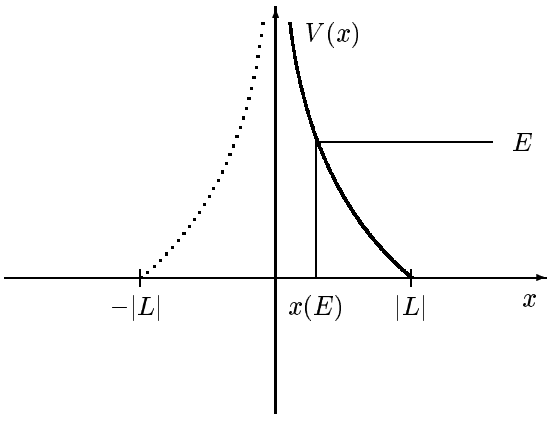

Figure 3.2: The realizing potential (3.39) is shown by the solid line for $L > 0$. For $L < 0$ the obtained potential becomes the dotted line and is unphysical.

We start by writing the relationship between the potential and $\tilde{\tau}$ as

$$\tilde{\tau}(E) = \sqrt{2m}\int_{x(E)}^{L} \frac{\mathrm{d}x}{\sqrt{E-V(x)}} = \sqrt{2m}\int_{0}^{E}\left(-\frac{\mathrm{d}x(V)}{\mathrm{d}V}\right)\frac{\mathrm{d}V}{\sqrt{E-V}}\,. \tag{3.36}$$

Dividing by $\sqrt{W-E}$ with W being an auxiliary parameter, and integrating with respect to E from 0 to W leads to

$$\int_0^W \frac{\tilde{\tau}(E)\,\mathrm{d}E}{\sqrt{W-E}} = \sqrt{2m}\int_0^W \mathrm{d}V\left(-\frac{\mathrm{d}x}{\mathrm{d}V}\right)\int_V^W \frac{\mathrm{d}E}{\sqrt{(W-E)(E-V)}}\,. \tag{3.37}$$

The inner integral (the one with respect to E) gives π, while on the lhs we can evaluate the integral explicitly [cf. (3.35)]. From the result,

$$\pi\sqrt{2m}\,L\left(1-1\Big/\sqrt{1+\tfrac{2mL^2}{\hbar^2}\,W}\right) = \pi\sqrt{2m}\,\left[L-x(W)\right]\,, \tag{3.38}$$

we obtain $x(W) = L[1+\frac{2mL^2}{\hbar^2}W]^{-\frac{1}{2}}$, inverting which yields[7]

$$V(x) = \tfrac{\hbar^2}{2mL^2}\left(\tfrac{L^2}{x^2}-1\right). \tag{3.39}$$

We can see that this wall-realizing potential sits on the positive half line. This is unavoidable: Indeed, if a potential is identically zero on the whole positive half line and is nonzero only on the negative half line then the time delay is necessarily non-negative. The most we can reach is that the penetration of the wall-realizing potential to the positive half line is finite. (3.39) presents such a solution. We will see that, for $L<0$, we have to pay more.

For $L<0$, the time delay is positive, *i.e.,* the quantum wave packet returns later than expected:

$$\tau = \frac{2|L|}{v}\,\frac{1}{1+(\frac{m|L|}{\hbar}\,v)^2} = \sqrt{2m}|L|\,\frac{1}{\sqrt{E}\left(1+\frac{2mL^2}{\hbar^2}E\right)}\,. \tag{3.40}$$

This is the time delay we try to reproduce with the corresponding classical particle as its classical time delay

$$\tau_{\mathrm{cl},\,x_0}(E) = \sqrt{2m}\int_{x(E)}^{x_0}\frac{\mathrm{d}x}{\sqrt{E-V(x)}} - \frac{2x_0}{\sqrt{2E/m}}\,, \tag{3.41}$$

where x_0 is the initial position of the particle. For small v, (3.40) becomes $\frac{2|L|}{v}$, which suggests that a slow particle enters the $x<0$ region and sees the wall near $x=-|L|$. For this, the realizing potential $V(x)$ is expected to start to increase at $x=-|L|$, and to keep increasing for smaller x. However, if one repeats the same argument used for the $L>0$ case, one ends up with (3.39) again, with now the left branch of this function (see Fig. 3.2).

[7]We remark that, while this potential reproduces the time delay classically, it does not reproduce the boundary condition (3.4) and hence cannot serve as a potential to realize the walls quantum mechanically.

The obvious problem with this branch, *i.e.*, it increases for x to the right of $-|L|$ and is unphysical, can be understood intuitively as follows. For high energies E, the particle is expected to move approximately freely, and since the particle travels at least until $x = -|L|$, the $E \to \infty$ asymptotics of the time delay would be at least $\frac{2|L|}{v}$. However, the time delay we have to reproduce has only a v^{-3} asymptotic behaviour. This means that the coefficient of the v^{-1} term must vanish for $E \to \infty$, imlplying that in the limit the particle reaches only until $x = 0$.

The situation cannot be helped with any additional potential in $-|L| < x < 0$ or in $0 < x$, nor by any other modification. Actually, it can be proven that no classically acceptable reflecting potential can fulfil the requirement that the time delay (3.40) be reproduced exactly for all $x_0 > x_{\text{thresh}}$, that is, for all initial positions of the incoming particle above a finite, possibly positive threshold position x_{thresh}. To see this, let us consider an arbitrary piecewise differentiable potential, even possibly diverging at the discontinuity points. Then the classical force $-V'(x)$ exists everywhere except for finitely many points, while at a discontinuity point an incoming classical trajectory can be continued with the outgoing trajectory that has the same energy E as the incoming one. The potential is further required to act as a completely reflecting wall, that is, for every positive energy E, there has to be a turning point $x(E)$ (like in Fig. 3.2). Note that then the function $x(E)$ is necessarily nonincreasing, and its inverse is $V(x)$ locally, *i.e.*, it reproduces at least parts of the function $V(x)$.

First let us discuss the case when V is differentiable (and hence continuous) everywhere. The x_0-independence of the time delay $\tau_{\text{cl},\,x_0}(E)$ [cf. (3.41)] implies

$$\frac{\mathrm{d}}{\mathrm{d}x_0}\,\tau_{\text{cl},\,x_0}(E) = \sqrt{2m}\left[\frac{1}{\sqrt{E - V(x_0)}} - \frac{1}{\sqrt{E}}\right] = 0 \tag{3.42}$$

and thus that $V = 0$ above x_{thresh}. Let x_{pos} denote the lowest x above which the potential is nonpositive. Naturally, one has $x_{\text{pos}} \le x_{\text{thresh}}$ and can write $x_{\text{pos}} = \sup\{x \,|\, V(x) > 0\}$, from which one finds $x_{\text{pos}} = \lim_{E \searrow 0} x(E)$, that is, x_{pos} is the "turning point for zero energy".

If there exists an energy E_* with a turning point on the negative half line, $x(E_*) < 0$, then for larger energies E the time delay is at least

$$\sqrt{2m}\int_{x(E_*)}^{x_0} \frac{\mathrm{d}x}{\sqrt{E - V}} - \sqrt{2m}\,\frac{x_0}{\sqrt{E}} \tag{3.43}$$

which is obtained by omitting the time of travelling through the interval $[x(E),\, x(E_*)]$. Since V is continuous on the interval $[x(E_*),\, x_0]$, it is bounded and hence the high-energy asymptotics of (3.43) is

$$\sqrt{2m}\,\frac{x_0 - x(E_*)}{\sqrt{E}} - \sqrt{2m}\,\frac{x_0}{\sqrt{E}} = \sqrt{2m}\,\frac{|x(E_*)|}{\sqrt{E}} \sim \frac{1}{\sqrt{E}}\,. \tag{3.44}$$

This is in contradiction with the asymptotics $E^{-3/2}$ of the demanded time delay (3.40). Consequently, all turning points have to be on the non-negative half line,

$$x(E) \ge \lim_{E' \to \infty} x(E') =: x_\infty \ge 0\,. \tag{3.45}$$

Next we prove that in $(x_\infty,\, x_{\rm pos}]$ the potential V decreases strictly. Namely, if we assume the contrary then there will be at least one point x_1 in this interval that is not a turning point [see Fig. 3.3(a)]. Within $[x_1,\, x_{\rm pos}]$, let x_2 denote the turning point with the highest energy E_2. Then, in the function $\tau_{{\rm cl},\,x_0}(E)$ there will be a discontinuity at $E = E_2$:

$$\frac{1}{\sqrt{2m}}\left[\lim_{E\searrow E_2}\tau_{{\rm cl},\,x_0}(E) - \lim_{E\nearrow E_2}\tau_{{\rm cl},\,x_0}(E)\right] = \lim_{E\searrow E_2}\int_{x(E)}^{x_0}\frac{{\rm d}x}{\sqrt{E-V}} - \lim_{E\nearrow E_2}\int_{x(E)}^{x_0}\frac{{\rm d}x}{\sqrt{E-V}} \tag{3.46}$$

$$= \lim_{E\searrow E_2}\left[\int_{x(E)}^{x_2}\frac{{\rm d}x}{\sqrt{E-V}} + \int_{x_2}^{x_0}\frac{{\rm d}x}{\sqrt{E-V}}\right] - \lim_{E\nearrow E_2}\int_{x(E)}^{x_0}\frac{{\rm d}x}{\sqrt{E-V}} \tag{3.47}$$

$$= \lim_{E\searrow E_2}\int_{x(E)}^{x_2}\frac{{\rm d}x}{\sqrt{E-V}} > \lim_{E\searrow E_2}\int_{x_1}^{x_2}\frac{{\rm d}x}{\sqrt{E-V}} = \int_{x_1}^{x_2}\frac{{\rm d}x}{\sqrt{E_2-V}} > 0\,. \tag{3.48}$$

However, the required quantum time delay, (3.40), is a continuous function everywhere. This result tells us that on the region $(x_\infty,\, x_{\rm pos}]$ $x(E)$ is the inverse of $V(x)$ and is differentiable. We have also obtained the qualitative behaviour of the candidate potential function [see Fig. 3.3(b)]: Coming from the right, it is zero above $x_{\rm thresh}$, nonpositive in $x_{\rm pos} < x < x_{\rm thresh}$, and is positive and increasing in $x_\infty < x \le x_{\rm pos}$, diverging to $+\infty$ at x_∞.

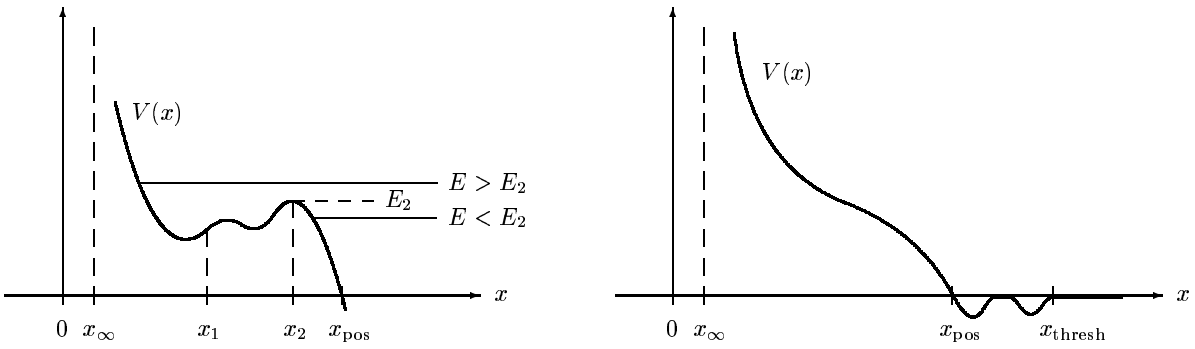

Figure 3.3: Left: A nondecreasing part in the potential in $(x_\infty,\, x_{\rm pos}]$ causes a discontinuity in the time delay. Right: The obtained qualitative shape of the potential.

Now we are ready to investigate the requirement $\frac{1}{\sqrt{2m}}\,\tau(E) = \frac{1}{\sqrt{2m}}\,\tau_{{\rm cl},\,x_0}(E)$:

$$\frac{|L|}{\sqrt{E}\left(1+\frac{2mL^2}{\hbar^2}E\right)} = \int_{x(E)}^{x_{\rm pos}}\frac{{\rm d}x}{\sqrt{E-V}} + \int_{x_{\rm pos}}^{x_0}\frac{{\rm d}x}{\sqrt{E-V}} - \frac{x_0}{\sqrt{E}}\,. \tag{3.49}$$

Observe that the second integral is bounded from above by $\frac{x_0 - x_{\rm pos}}{\sqrt{E}}$, since the potential is nonpositive on that interval. Employing again the 'Landau trick' to the first integral (*i.e.,* changing the variable from x to V, dividing by $\sqrt{W-E}$, and integrating between 0 and W), we find

$$\pi|L|\Big/\sqrt{1+\tfrac{2mL^2}{\hbar^2}W} \le -\pi\,x(W)\,, \tag{3.50}$$

or

$$x(W) \le -|L| \Big/ \sqrt{1 + \tfrac{2mL^2}{\hbar^2} W} < 0\,. \tag{3.51}$$

This, however, contradicts our previous result that all turning points have to be on the non-negative half line, showing that the requirement (3.49) cannot be fulfilled.

We can show that the preceding argument remains valid even if we allow discontinuity points in the potential — only slight modifications are necessary. The x_0-independence of the time delay implies $V = 0$ at all continuity points, and hence everywhere, above x_{thresh}. x_{pos} is introduced in the same way and with the same properties as before. (3.45) also remains valid: When assuming $x(E_*) < 0$, the possible discontinuity points falling between $x(E_*)$ and x_0 can be covered by intervals of a total length less than, say, $\frac{1}{2}|x(E_*)|$. We omit even these covering intervals from the time delay, and on the remaining intervals the potential is continuous and has overall upper and lower bounds. Consequently, the high-energy asymptotics of the time delay is still at least $\sim 1/\sqrt{E}$.

The proof of the strict decreasing of V in $(x_\infty,\, x_{\mathrm{pos}}]$ holds, too. This also rules out discontinuity points x_{disc} in $(x_\infty,\, x_{\mathrm{pos}}]$ with $V(x_{\mathrm{disc}} - 0) < V(x_{\mathrm{disc}} + 0)$. Others are allowed but do not cause any trouble in the behaviour of $x(E)$ because, for energies $E \in [V(x_{\mathrm{disc}} + 0),\, V(x_{\mathrm{disc}} - 0)]$, we then have $x(E) = x_{\mathrm{disc}} = \mathrm{const.}$ and $\frac{\mathrm{d}}{\mathrm{d}E}\, x(E) = 0$. The transformation of the integration variable in the first integral in (3.49) remains applicable, while the second integral can also be estimated as before, in spite of any discontinuity points in $(x_{\mathrm{pos}},\, x_{\mathrm{thresh}}]$. Therefore, we reach the same contradictory result (3.50) again.

Hence, interestingly enough, the walls with negative L do not admit a classical counterpart, so to say, they are genuinely quantum. We can help the situation only partially: if we demand only that the quantum time delay be reproduced in the $x_0 \to \infty$ limit of $\tau_{\mathrm{cl},\, x_0}(E)$, then the required realization can be achieved. See Appendix B for how this can be done.

3.4 Semiclassical aspects

From the eigenfunctions (3.7) and (3.8) the Feynman kernel describing the transition of the particle from $x = a$ at $t = 0$ to $x = b$ at $t = T$ can be calculated (see [40, 41, 42]). The result is

$$K(b, T; a, 0) = \sqrt{\tfrac{m}{2\pi i\hbar T}} \left[e^{\frac{im}{2\hbar T}(b-a)^2} \mp e^{\frac{im}{2\hbar T}(b+a)^2} \right]\,, \tag{3.52}$$

for $L = 0$ ("$-$"-sign) and $L = \infty$ ("$+$"-sign). For $L < 0$ the kernel is given by

$$\sqrt{\tfrac{m}{2\pi i\hbar T}} \left[e^{\frac{im}{2\hbar T}(b-a)^2} + e^{\frac{im}{2\hbar T}(b+a)^2} - \tfrac{2}{|L|} \int_0^\infty \mathrm{d}z\, e^{-z/|L|}\, e^{\frac{im}{2\hbar T}(b+a+z)^2} \right]\,, \tag{3.53}$$

and for $L > 0$ by

$$\sqrt{\tfrac{m}{2\pi i\hbar T}} \left[e^{\frac{im}{2\hbar T}(b-a)^2} + e^{\frac{im}{2\hbar T}(b+a)^2} - \tfrac{2}{L} \int_0^\infty \mathrm{d}z\, e^{-z/L}\, e^{\frac{im}{2\hbar T}(b+a-z)^2} \right] + \tfrac{2}{L} e^{\frac{i\hbar T}{2mL^2}} e^{-\frac{b+a}{L}}\,. \tag{3.54}$$

The salient feature of the result is that, for $L = 0$ and $L = \infty$, the kernel (3.52) almost coincides with that obtained by WKB semiclassical approximation, because the two terms

in (3.52) correspond to the free kernels for the direct path from $(a,0)$ to (b,T) and for the bounce path which hits the wall once during the transition, respectively. The only problem for the complete WKB-exactness is the appearance of the $\mp$ sign factor attached to the contribution from the bounce path. We shall show here that this sign factor can be attributed to the classical action $\Delta S_{\rm bounce}=\hbar\pi$ gained by the bounce effect at the wall so that $e^{\frac{i}{\hbar}\Delta S_{\rm bounce}}=\mp 1$. On the other hand, it will be proved here that, for other Ls, the WKB-exactness cannot hold.

What we wish to see is whether the sum of amplitudes along the classical two paths, the direct world line from $(x,t)=(a,0)$ to (b,T) and the bouncing path which hits the wall $x=0$ before arriving at (b,T), give the exact result (see Fig. 3.4). The question, therefore, is if the kernels (3.52), (3.53) and (3.54) can be rewritten in the form of a sum of the corresponding two terms as

$$K(b,T;a,0)=\sqrt{\frac{m}{2\pi i\hbar T}}\,e^{\frac{im}{2\hbar T}(b-a)^2}+\sqrt{\frac{1}{2\pi i\hbar}\frac{\partial^2 S_{\rm bounce}}{\partial a\,\partial b}}\,e^{\frac{i}{\hbar}S_{\rm bounce}(b,T;a,0)}\,, \tag{3.55}$$

where $S_{\rm bounce}(b,T;a,0)$ is the classical action for the bounce path, and the factor before the second exponential term comprises the van Vleck determinant and the Maslov phase factor corresponding to the turning point (see [43] for the details). In the spirit of the preceding sections, here again the wall is considered not necessarily to be simply the infinitely high vertical potential wall at the origin but to be realized by some sequence of more general reflecting potentials. What we require is that the potential sequence must converge uniformly to zero for all $x\geq x_{\rm wall}$ with some $x_{\rm wall}$ which may be positive, and that, for any $a,b>x_{\rm wall}$, the bounce path tends to the standard bounce world line depicted on Fig. 3.4, at least on the spacetime region $x>x_{\rm wall}$. Otherwise we let the reflecting potential sequence be arbitrary to the left of $x_{\rm wall}$ and, therefore, at the limit of the sequence, the resultant action $S_{\rm bounce}$ can differ from the action $S^{(0)}_{\rm bounce}=\frac{m(a+b)^2}{2T}$ that corresponds to the simplest case of the infinitely high vertical potential wall with no extra action contribution caused by the wall.

Even these very mild assumptions allow us to observe some important, generally valid, properties. The first one is that, although the direct path is also influenced by a non-vanishing potential, its WKB contribution $\sqrt{\frac{i}{2\pi\hbar}\frac{\partial^2 S_{\rm direct}}{\partial a\,\partial b}}\,e^{\frac{i}{\hbar}S_{\rm direct}}$ will still reduce to the first term of (3.55). Indeed, since in the limit we have $V\to 0$ and hence the velocity of the particle tends uniformly to $\frac{b-a}{T}$, we trivially find $E\to E^{(0)}_{\rm direct}=\frac{m}{2}\frac{(b-a)^2}{T^2}$ and $S_{\rm direct}\to S^{(0)}_{\rm direct}=\frac{m}{2}\frac{(b-a)^2}{T}$. The nontrivial question that remains to be shown concerns with the property of the derivative, $\frac{\partial^2 S_{\rm direct}}{\partial a\,\partial b}\to\frac{\partial^2 S^{(0)}_{\rm direct}}{\partial a\,\partial b}$, but this can be seen by writing the action as

$$S_{\rm direct}=\int_0^T {\rm d}t\,(E-2V)=-TE+2\int_0^T {\rm d}t\,(E-V)=-TE+\sqrt{2m}\int_a^b {\rm d}x\sqrt{E-V} \tag{3.56}$$

which is valid for $a,b>x_{\rm wall}$, and evaluating

$$\frac{\partial^2 S_{\rm direct}}{\partial a\,\partial b}=-\frac{\sqrt{m/2}}{\sqrt{E-V(a)}}\frac{\partial E}{\partial b}=-\sqrt{2m}\left[\sqrt{E-V(a)}\sqrt{E-V(b)}\int_a^b\frac{{\rm d}x}{\sqrt{E-V}^3}\right]^{-1}. \tag{3.57}$$

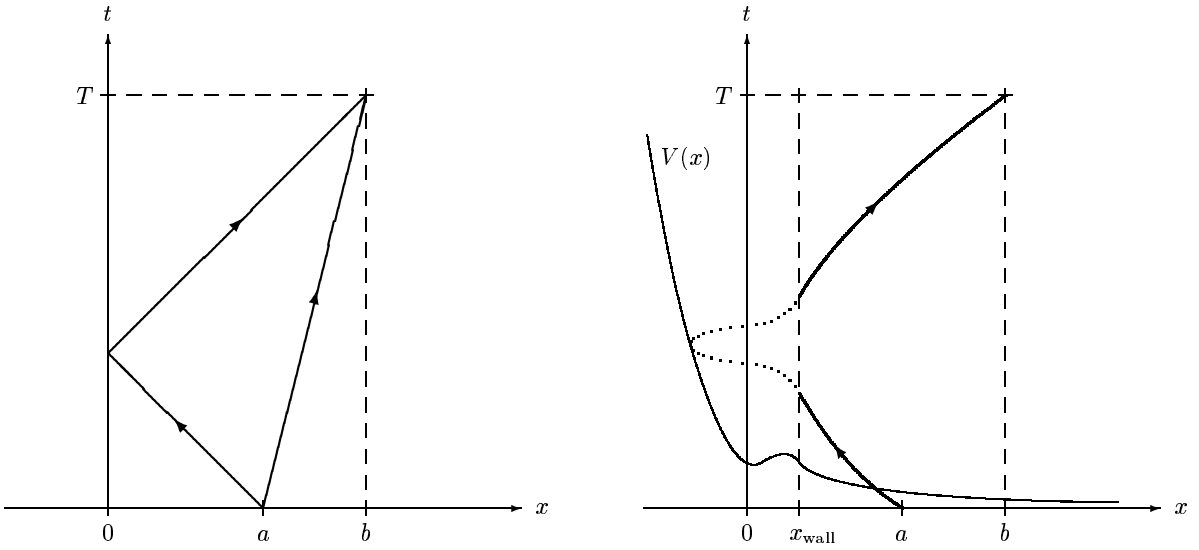

Figure 3.4: Left: The direct and the bounce paths. Right: The bounce path under a wall-realizing potential.

Here, the energy E of the direct path is determined by the condition

$$\sqrt{\tfrac{m}{2}} \int_a^b \frac{\mathrm{d}x}{\sqrt{E-V}} = T \tag{3.58}$$

which is used to evaluate $\frac{\partial^2 S_{\text{direct}}}{\partial a\, \partial b}$ in (3.57). Plugging the limiting values for the energies and the potential in (3.57), we find the required property.

Second, we make the observation that the energy of the bounce path converges to $E^{(0)}_{\text{bounce}} = \frac{m}{2}\frac{(a+b)^2}{T^2}$. This follows from our requirement that the bounce path must tend to the standard bounce world line outside x_{wall} because then the velocity of the particle tends uniformly to $\frac{a+b}{T}$ under the vanishing potential. In addition, we find that, although $\Delta S_{\text{bounce}} = S_{\text{bounce}} - S^{(0)}_{\text{bounce}}$ does not necessarily tend to zero, in the limit it becomes independent of a and b. This can be seen as follows:

$$S_{\text{bounce}} = -TE + \sqrt{2m}\int_{x(E)}^{a} \mathrm{d}x\sqrt{E-V} + \sqrt{2m}\int_{x(E)}^{b} \mathrm{d}x\sqrt{E-V} \tag{3.59}$$

and

$$\partial S_{\text{bounce}}/\partial a = \sqrt{2m}\sqrt{E-V(a)}\,, \tag{3.60}$$

where now the energy of the bounce path is determined by

$$\sqrt{\tfrac{m}{2}} \int_{x(E)}^{a} \frac{\mathrm{d}x}{\sqrt{E-V}} + \sqrt{\tfrac{m}{2}} \int_{x(E)}^{b} \frac{\mathrm{d}x}{\sqrt{E-V}} = T \tag{3.61}$$

[again, (3.61) is used also for the result (3.60)]. Since now $E \to E^{(0)}_{\text{bounce}}$, it follows that

$$\partial S_{\text{bounce}}/\partial a \;\to\; m(a+b)/T = \partial S^{(0)}_{\text{bounce}}/\partial a \tag{3.62}$$

so $\partial\Delta S_{\rm bounce}/\partial a \to 0$. The b-independence of $\Delta S_{\rm bounce}$ is proven analogously.

Third, if we restrict ourselves to the potential sequences of the type (3.16) then (3.59) and (3.61) read

$$S_{\rm bounce} = -TE + \sqrt{2m}\,(a+b)\sqrt{E} + 2\sqrt{2m}\,d\sqrt{E+|V_2|} \tag{3.63}$$

and

$$\sqrt{m/2}\;\frac{a+b}{\sqrt{E}} + \sqrt{m/2}\;\frac{d}{\sqrt{E+|V_2|}} = T\,. \tag{3.64}$$

From (3.63) we have that

$$\lim_{d\to 0}\Delta S_{\rm bounce} = \lim_{d\to 0}\left(2\sqrt{2m}\,d\sqrt{|V_2|}\right)\,. \tag{3.65}$$

In parallel, $\partial^2 S_{\rm bounce}/(\partial a\,\partial b)$ can be computed by differentiating (3.60), and using $\partial E/\partial b$, the latter obtained by expressing $b = b(E)$ from (3.64) and applying $\partial E/\partial b = 1/[\partial b/\partial E]$. Taking the limit of the result gives m/T so we find that, in the limit, the square root factors in the two terms of (3.55) equal each other for these step-like potential sequences.

By virtue of these properties, we are able to discuss the question of complete WKB-exactness. In the cases $L = 0$ and $L = \infty$, it is possible to reproduce the required action contribution $\Delta S_{\rm bounce} = \pi\hbar$ and $\Delta S_{\rm bounce} = 0$, respectively, for example with the step-like potential sequences (3.16). In fact, choosing for $L = 0$

$$V_1(d) = \text{const.}\,d^{-1}\,, \qquad V_2(d) = -\tfrac{\hbar^2}{2m}\left(\tfrac{\pi}{2}\right)^2 d^{-2} \tag{3.66}$$

(a potential sequence with $\alpha_0 = 0$ and $\beta_0 = \pi/2$), and for $L = \infty$

$$V_1(d) = \tfrac{\hbar^2}{2m}\,c^2\,d^{-1}\,, \qquad V_2(d) = -\tfrac{\hbar^2}{2m}\,c\,d^{-\frac{3}{2}}\,, \tag{3.67}$$

which is the case $\nu = -1/2$ of (3.26), provides just these needed action contributions [cf. (3.65)]. Note that these potential sequences are, at the same time, correct realizations of the quantum boundary condition with $L = 0$, respectively $L = \infty$, as well. Nevertheless, they are not unique even among the step-like realizations with these properties, and presumably other potential shapes can also serve as examples for even both the complete WKB-exactness and realizing the quantum boundary condition.

On the other side, for the other walls $L \neq 0, \infty$, one can prove that no potential sequence can account for the kernels (3.53) and (3.54) irrespective of whether the potential sequence reproduces the correct quantum boundary condition or not. To see this, let us write these kernels in the form

$$\sqrt{\tfrac{m}{2\pi i\hbar T}}\left[e^{\frac{im}{2\hbar T}(b-a)^2} + A_L(a,b,T)\,e^{\frac{i}{\hbar}S^{(0)}_{\rm bounce}}\right]\,. \tag{3.68}$$

If the complete WKB-exactness holds then $\arg A_L(a,b,T)$ should correspond to the limit of $\Delta S_{\rm bounce}/\hbar$, which we know is unavoidably independent of a and b. However, actually

$\arg A_L(a,b,T)$ does depend on a and b, as can be checked simply for example, on the large-T asymptotics of $A_L(a,b,T)$,

$$A_L(a,b,T) \approx \begin{cases} -\sqrt{\frac{m}{2\pi i\hbar T}}\ e^{-\frac{2imL}{\hbar T}(a+b-L)}\,, & L<0\,, \\ \frac{2}{L}\ e^{-\frac{a+b}{L}}\ e^{-\frac{im}{2\hbar T}\left[(a+b)^2-\left(\frac{\hbar T}{mL}\right)^2\right]}\,, & L>0\,, \end{cases} \tag{3.69}$$

as one finds from (3.53) and (3.54).

We thus learn that the quantum walls with $L=0$ and $L=\infty$, which correspond to the Dirichlet and the Neumann boundary condition, respectively, are distinguished in the $U(1)$ family of walls with respect to the WKB-exactness. We can observe that these two cases are the ones distinguished by their scale invariance, too. The relationship between the two, the WKB-exactness and scale invariance, is however unclear yet.

Chapter 4

Free motion on a line with a point interaction (defect, scatterer)

Next, we consider the basic properties of systems where a free particle moves on a full line, with a point interaction / pointlike disturbance at $x = 0$. Basically, this short chapter reviews results [9, 10, 12] which are included here because they will be utilized and referred at various places in the subsequent chapters. Furthermore, this discussion also serves to put the *new* results, a fuller treatment of generalized symmetries (Appendix C), into context.

For earlier results on 'point interaction on a line' systems, see, *e.g.,* [7, 44, 45, 46, 47].

4.1 Characterization of the line systems

With the two infinities being limit-point-type, the surface term regarding (A.5) is now

$$W[\psi_1^*, \psi_2](+0) - W[\psi_1^*, \psi_2](-0) \tag{4.1}$$

(again up to an irrelevant overall factor). We can identify Γ_1, Γ_2 as

$$\Gamma_1\psi := \Psi \equiv \begin{pmatrix} \psi(+0) \\ \psi(-0) \end{pmatrix}, \qquad \Gamma_2\psi := L_0\Psi' \equiv L_0 \begin{pmatrix} \psi'(+0) \\ -\psi'(-0) \end{pmatrix}. \tag{4.2}$$

Note the minus sign in the second component of Ψ', which is actually connected to the fact that, on the negative half line, the coordinate x runs with inward orientation. If an outward-oriented coordinate $x_- = -x \in [0, \infty)$ is introduced there then the symmetric arrangement can be achieved. It is worth mentioning that it is this latter symmetric form how it is practical to generalize these formulas for an arbitrary star graph system, where a general n number of half-line "legs" are running out from a common junction, with outward-oriented coordinates $x_i \in [0, \infty)\,,\ \ i = 1, \ldots n\,.$

The condition determining the self-adjoint domains for our present line systems is

$$(U - I)\Psi + i(U + I)L_0\Psi' = 0\,, \tag{4.3}$$

with the characteristic operator U being an arbitrary $U(2)$ matrix. We note that, similarly to the half line systems, the presence of the length L_0 again indicates an inherent scale dependence, broken scale invariance for generic self-adjoint domains. It is only a lower dimensional subfamily of $U(2)$ where L_0 actually drops out from the connection condition and which, consequently, are scale invariant.

A practical parametrization for U is given by

$$U = e^{i\xi} \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix} = e^{i\xi} \begin{pmatrix} \alpha_R + i\alpha_I & \beta_R + i\beta_I \\ -\beta_R + i\beta_I & \alpha_R - i\alpha_I \end{pmatrix}, \tag{4.4}$$

where $\xi \in [0, \pi)$ and α, β are complex parameters satisfying

$$|\alpha|^2 + |\beta|^2 = \alpha_R^2 + \alpha_I^2 + \beta_R^2 + \beta_I^2 = 1 \ . \tag{4.5}$$

The diagonalized form of $U = V^{-1}DV$ and the eigenvalues $e^{i\theta_+}$, $e^{i\theta_-}$ ($\theta_\pm \in [0, 2\pi)$) play an important role for the spectral and other physical aspects. Hence, we also introduce the parameters[1]

$$\{(L_+, L_-, \mu, \nu) \,|\, L_\pm \in (-\infty, \infty) \cup \{\infty\}, \, \mu \in [0, \pi], \, \nu \in [0, 2\pi)\} \ , \tag{4.6}$$

where the two length scales appear as

$$D = \begin{pmatrix} e^{i\theta_+} & 0 \\ 0 & e^{i\theta_-} \end{pmatrix} \ , \qquad L_\pm := L_0 \cot \frac{\theta_\pm}{2} \tag{4.7}$$

and the two angle parameters as the Euler angles of V

$$V = e^{i\chi\sigma_3} e^{i\frac{\mu}{2}\sigma_2} e^{i\frac{\nu}{2}\sigma_3} \ , \qquad \mu \in [0, \pi], \quad \nu \in [0, 2\pi) \, , \tag{4.8}$$

(the first factor $e^{i\chi\sigma_3}$ being irrelevant since it is cancelled in the product $U = V^{-1}DV$). As we will see, these parameters carry more direct physical meaning for the point interaction systems.

In the case of the so-called separating connection conditions ($\beta = 0$), when the point interaction is not transparent and the two half line configuration subspaces decouple, $L_\pm$ become the parameters of the resulting two half line systems. For the other, nonseparating, cases the connection conditions can be written in another useful form,

$$\Lambda \begin{pmatrix} \psi(-0) \\ \psi'(-0) \end{pmatrix} = \begin{pmatrix} \psi(+0) \\ \psi'(+0) \end{pmatrix} \tag{4.9}$$

where the *transit matrix* Λ takes the form

$$\Lambda = e^{i\zeta} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \ , \qquad \zeta \in [0, \pi), \quad a, L_0^{-1}b, L_0 c, d \in \mathbb{R}, \quad ad - bc = 1 \, . \tag{4.10}$$

This shows that the family of nonseparating systems is topologically $U(1) \times SL(2, \mathbb{R})$. The phase jump ζ is essentially equivalent to ν as well as with $\arg \beta$. Further relationship with the generally valid parametrization (4.4) is provided by

$$\Lambda = \frac{i}{\beta_R - i\beta_I} \begin{pmatrix} \sin\xi - \alpha_I & -L_0(\cos\xi + \alpha_R) \\ L_0^{-1}(\cos\xi - \alpha_R) & \sin\xi + \alpha_I \end{pmatrix} \ . \tag{4.11}$$

[1] which, with these intervals running in, cover $U(2)$ actually twice [12] so some care is needed when using them

4.2 Energy eigenvalues and eigenfunctions

Concerning the eigenvalue problem, the bound states allowed for a given H_U are of the form

$$\varphi_\kappa(x) = \begin{cases} A^-_\kappa e^{\kappa x}, & x < 0 \\ B^+_\kappa e^{-\kappa x}, & x > 0 \end{cases} \tag{4.12}$$

where κ determines the bound state energy $E_{\text{bound}} = -\hbar^2\kappa^2/(2m)$, and the constants A^-_κ and B^+_κ are subject to the normalization condition $|A^-_\kappa|^2 + |B^+_\kappa|^2 = 2\kappa$. The connection conditions require $\begin{pmatrix} B^+_\kappa \\ A^-_\kappa \end{pmatrix}$ to be an eigenvector of U and κ to fulfil

$$\kappa = \frac{1}{L_+} \qquad \text{or} \qquad \kappa = \frac{1}{L_-} \ , \tag{4.13}$$

which shows that there exist two bound states if $L_+ > 0$ and $L_- > 0$, one if $L_+L_- < 0$, and none if $L_+ < 0$ and $L_- < 0$. In terms of (4.8) the coefficients are found to be

$$\begin{pmatrix} B^+_\kappa \\ A^-_\kappa \end{pmatrix} = \sqrt{\frac{2}{L_+}} \begin{pmatrix} e^{-i\nu}\cos\frac{\mu}{2} \\ \sin\frac{\mu}{2} \end{pmatrix} \ , \qquad \begin{pmatrix} B^+_\kappa \\ A^-_\kappa \end{pmatrix} = \sqrt{\frac{2}{L_-}} \begin{pmatrix} -e^{-i\nu}\sin\frac{\mu}{2} \\ \cos\frac{\mu}{2} \end{pmatrix} \ , \tag{4.14}$$

for $\kappa = 1/L_+$ and $1/L_-$, respectively. Naturally, having seen the half line system,[2] we are not surprised that a naively 'almost' free system may possess bound states. Roughly saying, we just expect maximally two since the point defect acts as a wall from both sides, and one wall is known to allow (maximally) one bound state. Now this 'point-wide' wall is, generically, partially transmitting, and this explains that a bound state on one half line is partially copied to the other side.

We might nevertheless be surprised that a pointlikely "wide" potential well admits only maximally two bound states while potential wells in general can admit arbitrarily many. A simple explanation of this may be provided by observing that, on the two semi-infinite free sides, a bound state must be an expontentially decreasing wave function (and with the same characteristic length on both sides). Therefore, it is only the ratio of the weights of this exponential on the two sides in which we can have some freedom. Now, different bound states must be mutually orthogonal to each other and this is what limits our freedom to have only two bound states as the maximum.

The scattering states for the particle (with velocity $v = \hbar k/m$) incident from the negative side are

$$\varphi^{(-)}_k(x) = \frac{1}{\sqrt{2\pi}} \begin{cases} e^{ikx} + r^{(-)}_k e^{-ikx}, & x < 0, \\ t^{(-)}_k e^{ikx}, & x > 0 \end{cases} \ , \tag{4.15}$$

with the reflection and the transmission amplitudes determined by the connection conditions as

$$r^{(-)}_k = \frac{\alpha\, q + \alpha^* q^{-1} - (\eta + \eta^*)}{\eta\, q + \eta^* q^{-1} - (\alpha + \alpha^*)} \ , \qquad t^{(-)}_k = \frac{-\beta(q - q^{-1})}{\eta\, q + \eta^* q^{-1} - (\alpha + \alpha^*)} \ , \tag{4.16}$$

[2] as well as bearing in mind that "potential wells" like a Dirac delta potential is also among the possible point intreactions

where we have used

$$\eta = e^{i\xi} \ , \qquad q = \frac{1 - kL_0}{1 + kL_0} \ . \tag{4.17}$$

Similarly, the right-incoming plane wave is

$$\varphi_k^{(+)}(x) = \frac{1}{\sqrt{2\pi}} \begin{cases} t^{(+)} e^{-ikx}, & x < 0, \\ e^{-ikx} + r^{(+)} e^{ikx}, & x > 0, \end{cases} \tag{4.18}$$

with

$$r^{(+)} = \frac{\alpha^* q + \alpha\, q^{-1} - (\eta + \eta^*)}{\eta\, q + \eta^* q^{-1} - (\alpha + \alpha^*)} \ , \qquad t^{(+)} = \frac{\beta^* (q - q^{-1})}{\eta\, q + \eta^* q^{-1} - (\alpha + \alpha^*)} \ . \tag{4.19}$$

These scattering states are "orthonormalized" to $\delta(k - k')$. In terms of the parameters (4.6), the amplitudes read

$$\begin{pmatrix} r_k^{(\pm)} \\ t_k^{(\pm)} \end{pmatrix} = -\frac{1}{(1 + ikL_+)(1 + ikL_-)} \begin{pmatrix} 1 + k^2 L_+ L_- \mp ik(L_+ - L_-)\cos\mu \\ \pm ik(L_+ - L_-)\sin\mu\, e^{\pm i\nu} \end{pmatrix} \ . \tag{4.20}$$

The amplitudes obey the unitarity conditions,

$$|r^{(-)}|^2 + |t^{(-)}|^2 = 1 \ , \qquad |r^{(+)}|^2 + |t^{(+)}|^2 = 1 \ , \tag{4.21}$$

and

$$r^{(-)^*} t^{(+)} + t^{(-)^*} r^{(+)} = 0 \ . \tag{4.22}$$

If we let k take negative values, too, and noting that $k \to -k$ implies $q \to q^{-1}$, we obtain further relations among the reflection and transmission amplitudes as

$$r_{-k}^{(-)} = r_k^{(-)^*}, \qquad r_{-k}^{(+)} = r_k^{(+)^*}, \qquad t_{-k}^{(-)} = t_k^{(+)^*}, \qquad t_{-k}^{(+)} = t_k^{(-)^*} \tag{4.23}$$

(note the relationship to time reflection).

4.3 Properties of line systems

Analysing the results we can observe that the number, the energy value and the characteristic length scale of the bound states are governed by the eigenvalues of U only, in other words, in terms of the two independent length scales $L_\pm$. Remarkably, this fact remains valid even in the case of parity invariant *singular potentials*,[3] like $V(x) \sim 1/|x|$ and $V(x) \sim 1/x^2$ [16]. Finite values of these length parameters again imply the quantum breakdown of classical scale invariance.

We can also read off that the angle ν means only a phase jump when we travel from the negative half line to the positive one. This jump is known to be related to a Dirac-delta vector potential [5] and means only an unphysical gauge freedom, since in one dimension a vector potential can be gauged away. Note however that this parameter may carry

[3] for those potentials which are limit-circle type at the location of the singularity and limit-point type in the space infinities

real physical information if the point defect we have is actually a small ring with an Aharonov-Bohm magnetic flux driven through it.

At last, the other angle μ measures the extent the wave function on one side is copied to the other side. This observation is one of the key elements in the proposal of 'abacus qubits' [18]. Namely, if we have a controllable point interaction then we can govern the rate a state is copied from one side to the other.[4]

The one-parameter gauge freedom is not the only connection between different self-adjoint domains. Indeed, there is a very rich variety of symmetries, dualities and generalized duality relationships, named as *generalized symmetries* for the point interaction systems. These relationships are strongly connected to the fact that the *boundary transformations* (C.2) which linearly mix the left and right side parts of any wave function with coefficients that are the entries of an arbitrary matrix $W \in U(2)$, map a self-adjoint domain with characteristic matrix U to a one with the conjugate matrix WUW^{-1}. These maps leave the spectrum invariant because the spectrum depends on the diagonal part of U only but transform the eigenfunctions nontrivially. These boundary transformations provide not only duality, triality or higher order discrete maps among systems but a continuous group of them. The gradually explored duality-type generalized symmetries [9, 10] (exhibiting mappings between coupling constants of two different systems — say, a Dirac delta potential and a so-called delta-prime or epsilon interaction — as $g_2 = 1/g_1$) are all covered by them. See Appendix C for a detailed introduction and investigation of the boundary transformations.

Notably, the family of 'point interaction on a line' systems admits a number of further intriguing properties, like the scale invariant subfamily, numerous other special subfamilies, supersymmetric cases, or energy anholonomy — the latter being the property that if we travel along a closed curve in the family of possible self-adjoint domains with an energy eigenstate, the energy will change gradually but, when the loop is completed, we arrive at a higher or lower energy value. This Berry-like behaviour is not only theoretically remarkable but, in case continuously tunable pointlike singularities are experimentally realized, it can become important and may provide practical application as well. The interested Reader is asked to consult [9, 10] for these details.

[4]The other key ingredient in the 'abacus' suggestion is an applied harmonic potential whose caustic property makes states to repeat their initial form after every time unit of half period. The combination of these two ideas provides the possibility to perform any $U(2)$ qubit operation, within a well-defined finite time step.

Chapter 5

Free motion on a circle with a point interaction (defect, scatterer)

In this chapter, we change the infinite and linelike configuration space to a finite, closed circular one, following [14].[1] The difference will cause three essential changes. The first one is that finiteness makes all energy eigenstates normalizable and the spectrum a discrete one. The second is that the phase jump from one side of the point interaction to the other is here definitely physical, and corresponds to the magnetic flux that is driven through the loop. For experiments that have measured the dependence of the energy spectrum on the magnetic flux, see [32, 33, 34]. The third change is that finiteness brings in a further length scale in addition to $L_{\pm}$, which, together with the now physical phase jump, reduces the range of available symmetries and generalized symmetries — the latter to a $U(1)$ group —, and, correspondingly, provides a richer variety of possible energy spectra.

Let us remark that, in case the circle is really a closed curve in a plane then the Hamiltonian is shifted by the squared curvature of the curve, as an effective remnant from the two dimensional Laplacian kinetic energy term, as the transversal width is contracted to zero. Fortunately, for circles this produces only a constant shift in the Hamiltonian which can be ignored for our purposes.

It is also worth mentioning that, in a practical realization, the width $d_{\text{transversal}}$ of such a path may also play a role. First, because the transversal motion degree of freedom can also get excited if the energy is high enough [$E_{\text{transversal}} \sim \hbar^2/(m\, d^2_{\text{transversal}})$], and, second, because in the presence of a magnetic flux driven through the circle the nonzero transversal width is expected to cause an additional quadratic magnetic field dependence of the eigenenergies [50].

[1] For earlier results, see [48, 49].

5.1 Spectral properties

There is no difference in the form of the connection condition from what we have seen for the line case:

$$(U-I)\Psi + i(U+I)L_0\Psi' = 0\,, \qquad \Psi := \begin{pmatrix} \psi(+0) \\ \psi(l-0) \end{pmatrix}, \quad \Psi' := \begin{pmatrix} \psi'(+0) \\ -\psi'(l-0) \end{pmatrix}, \tag{5.1}$$

except from some notation: the coordinate x again starts with 0 from the location of the pointlike object but arrives at its other side at $x = l$, where l is the circumference of the loop. We will also make use of the alternative formulation of (5.1) (cf. Sect. 2.2),

$$U\Psi^{(+)} = \Psi^{(-)}\,, \qquad \Psi^{(\pm)} := \Psi \pm iL_0\Psi'. \tag{5.2}$$

To study the spectral properties of the circle system, we first recall the energy eigenvalues and eigenfunctions for the various self-adjoint domains. The positive spectrum is provided by the energy eigenfunctions of the form

$$\varphi_k(x) = A_k\, e^{ikx} + B_k\, e^{-ikx}\,, \qquad k > 0\,. \tag{5.3}$$

For such a wave function, the boundary vectors are

$$\Psi = \tau_k \begin{pmatrix} A_k \\ B_k \end{pmatrix}, \qquad \Psi' = ik\sigma_3\tau_k\sigma_3 \begin{pmatrix} A_k \\ B_k \end{pmatrix}, \tag{5.4}$$

where σ_k, $k = 1, 2, 3$ denote the Pauli matrices and

$$\tau_k := \begin{pmatrix} 1 & 1 \\ e^{ikl} & e^{-ikl} \end{pmatrix}. \tag{5.5}$$

Then, the connection condition (5.1) reads

$$[(U-I)\tau_k - kL_0(U+I)\sigma_3\tau_k\sigma_3] \begin{pmatrix} A_k \\ B_k \end{pmatrix} = 0\,, \tag{5.6}$$

or, explicitly,

$$\begin{pmatrix} \alpha K_- + (\beta e^{ikl} - e^{-i\xi})K_+ & \alpha K_+ + (\beta e^{-ikl} - e^{-i\xi})K_- \\ \alpha^* e^{ikl}K_+ - (\beta^* + e^{-i\xi}e^{ikl})K_- & \alpha^* e^{-ikl}K_- - (\beta^* + e^{-i\xi}e^{-ikl})K_+ \end{pmatrix} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = 0, \tag{5.7}$$

with $K_\pm := 1 \pm kL_0$. To have a nontrivial solution for the coefficients A_k, B_k, the determinant of the matrix of the lhs of (5.7) must be zero. This gives the condition

$$[\beta_{\rm I} + \sin\xi\, \cos kl] + \left[(\cos\xi - \alpha_{\rm R}) + (\cos\xi + \alpha_{\rm R})\,(kL_0)^2\right] \frac{\sin kl}{2kL_0} = 0 \tag{5.8}$$

for the wave number k. The positive spectrum is an infinite discrete series, in which, for large k, the difference between subsequent levels is getting closer and approaches π/l (see Appendix D). For the negative spectrum one only needs to replace $ik \to \kappa$ in the formulas above to obtain the corresponding condition,

$$[\beta_{\rm I} + \sin\xi\, \cosh\kappa l] + \left[(\cos\xi - \alpha_{\rm R}) - (\cos\xi + \alpha_{\rm R})\,(\kappa L_0)^2\right] \frac{\sinh\kappa l}{2\kappa L_0} = 0\,. \tag{5.9}$$

From (5.9) one finds that at most two negative energy states can exist. Similarly, for a possible zero energy state, the $k \to 0$ limit can be used to obtain the corresponding condition

$$[\beta_{\rm I} + \sin\xi] + [\cos\xi - \alpha_{\rm R}]\,\frac{l}{2L_0} = 0\,. \tag{5.10}$$

We note that, similarly to the line system, for some special U such as $U = -\sigma_1$ the ground state may be doubly degenerate. This is not in conflict with the well-known property of nondegeneracy in energy levels of one dimensional quantum mechanics, because the premises used to prove that property do not hold here. Indeed, at the location of the singular object, neither the wave function nor its derivative are required to be continuous.

In fact, one can determine when an energy eigenstate (ground state or higher) becomes doubly degenerate[2] as follows. Observe first that, for states with positive energy $E > 0$, degeneracy occurs when all the four elements of the matrix in (5.7) are zero. From this one derives

$$\alpha_{\rm I} = \beta_{\rm R} = 0\,, \qquad\qquad \beta_{\rm I} \neq 0\,, \tag{5.11}$$

and, further, the conditions for the energy eigenvalue

$$\beta_{\rm I}\cos kl = -\sin\xi\,, \qquad \beta_{\rm I}\,kL_0\sin kl = -(\cos\xi - \alpha_{\rm R})\,, \qquad \beta_{\rm I}\sin kl = -(\cos\xi + \alpha_{\rm R})\,kL_0 \tag{5.12}$$

in addition to (5.8). Since (5.11) implies $\alpha_{\rm R}^2 + \beta_{\rm I}^2 = 1$, from (5.12) we find

$$k^2L_0^2(\cos\xi + \alpha_{\rm R}) = \cos\xi - \alpha_{\rm R}\,. \tag{5.13}$$

On can obtain the conditions for states with $E = 0$ and $E < 0$ analogously, and the result is that, in both cases, one has (5.11) and

$$\xi = \operatorname{arccot}\frac{l}{2L_0} \tag{5.14}$$

together with (5.12) with $k = 0$ for $E = 0$, or (5.12) with $k \to -i\kappa$ for $E < 0$. One then finds that degeneracy of an $E \leq 0$ eigenvalue excludes any other degeneracies, and that, unless $\cos\xi = -\alpha_{\rm R}$, (5.13) can hold for only one k. If $\cos\xi = -\alpha_{\rm R}$, one has $\cos\xi = \alpha_{\rm R}$ (see (5.13) and its $E \leq 0$ variants) and, consequently, $\xi = \pi/2$, $\alpha_{\rm R} = 0$ and $\beta_{\rm I} = \pm 1$. This shows that in the $SU(2)$ family there are only two types of singularities specified by $U = \pm\sigma_1$ that admit double degeneracy with more then one energy levels. Actually, for the cases $U = \pm\sigma_1$ all the positive energies prove to be doublets. Further, the case $U = \sigma_1$ possesses a singlet zero energy state as the ground state while $U = -\sigma_1$ does not have any nonpositive energies. This (almost) entire degeneracy of energy levels suggests that the system may be bestowed supersymmetry, which we shall confirm later.

Now we come to the point to discuss the spectral space of the circle system with a point singularity, that is, we determine the entirety of distinct spectra that can arise on the circle under the $U(2)$ family of point interactions. From the spectral conditions (5.8)–(5.10) we can see immediately that the spectrum depends at most on the three parameters,

[2]Degeneracy higher than two does not arise since the energy eigenvalue equation is a second order differential equation.

ξ, $\alpha_{\rm R}$ and $\beta_{\rm I}$, of the four of $U \in U(2)$, even though the eigenstates depend on all of the four parameters in a nontrivial way [see (5.7)]. We have also seen that the conditions for an energy to be degenerate depend only on the same three parameters. The question is thus whether these three parameters, ξ, $\alpha_{\rm R}$ and $\beta_{\rm I}$, really index different spectra. This can be answered affirmatively by a detailed examination on the possible spectra and their connection with the set of parameters. In fact, our argument presented in Appendix D.1 shows that the spectrum of a circle system uniquely determines the parameters ξ, $\alpha_{\rm R}$ and $\beta_{\rm I}$ and, consequently, the spectral space $\Sigma_{\rm circle} := \{{\rm Spec}(H_U) \,|\, U \in U(2)\}$ is given by

$$\Sigma_{\rm circle} = \Big\{(\xi, \alpha_{\rm R}, \beta_{\rm I}) \in \mathbb{R}^2 \mid \xi \in [0, \pi),\ \alpha_{\rm R}^2 + \beta_{\rm I}^2 \leq 1\Big\} \cong S^1 \times D^2, \tag{5.15}$$

which is topologically a filled torus. The disc D^2 part of $\Sigma_{\rm circle}$ can equally be realized by $SU(2)/U(1) \cong S^3/S^1$, where the $SU(2) \cong S^3$ given by

$$\{(\alpha_{\rm R}, \alpha_{\rm I}, \beta_{\rm R}, \beta_{\rm I}) \in \mathbb{R}^4 \mid \alpha_{\rm R}^2 + \alpha_{\rm I}^2 + \beta_{\rm R}^2 + \beta_{\rm I}^2 = 1\} \tag{5.16}$$

is factorized by the phase of $\alpha_{\rm I} + i\beta_{\rm R}$ which forms the $U(1) \cong S^1$. This latter identification is advantageous for when the system is discussed as a special case of a circle with two singularities [14]. It is interesting to compare the spectral space (5.15) with that of the line system which is two dimensional.

5.2 Generalized symmetries, symmetries and invariant subfamilies

Before investigating various symmetries and generalized symmetries arising for the circle systems, we start with a formula valid for a certain important class of transformations and becomes convenient in the subsequent discussions. Suppose that a transformation $\mathcal{W}$ of the wave functions, $\psi \xrightarrow{\mathcal{W}} \tilde{\psi} = \mathcal{W}\psi$, commutes with our Hamiltonian (understood on the maximal domain) and induces transformations on the boundary vectors in (5.1) as

$$\Psi \xrightarrow{\mathcal{W}} \tilde{\Psi} = M\Psi\,, \qquad\qquad \Psi' \xrightarrow{\mathcal{W}} \tilde{\Psi}' = N\Psi' \tag{5.17}$$

with some two-by-two matrices M and N. Then, in terms of $\Psi^{(+)}$ and $\Psi^{(-)} = U\Psi^{(+)}$ defined in (5.2) we have

$$\tilde{\Psi}^{(\pm)} = M\Psi \pm iL_0 N\Psi' = \frac{1}{2}\big[M(I+U) \pm N(I-U)\big]\,\Psi^{(+)}\,, \tag{5.18}$$

and hence

$$\tilde{\Psi}^{(-)} = \big[M(I+U) - N(I-U)\big]\,\big[M(I+U) + N(I-U)\big]^{-1}\,\tilde{\Psi}^{(+)} \tag{5.19}$$

as long as the inverse matrix in question exists. We thus see that if

$$U_{\mathcal{W}} := \big[M(I+U) - N(I-U)\big]\,\big[M(I+U) + N(I-U)\big]^{-1} \tag{5.20}$$

is unitary and hence belongs to $U(2)$, then $\mathcal{W}$ is a generalized symmetry. In particular, when $M = N \in U(2)$, which we will meet frequently below, (5.20) reduces to

$$U_{\mathcal{W}} = MUM^{-1}\,. \tag{5.21}$$

Since this $U_{\mathcal{W}}$ belongs to $U(2)$, such a $\mathcal{W}$ commuting with H is a generalized symmetry. If, in addition, U commutes with M, then one has $U_{\mathcal{W}} = U$ and hence such $\mathcal{W}$ is a symmetry.

Specializing to the circle system, the first example of symmetry transformations we wish to mention is the parity (or space reflection), $\mathcal{P}$, defined as

$$\psi(x) \xrightarrow{\mathcal{P}} (\mathcal{P}\psi)(x) = \psi(l-x)\,. \tag{5.22}$$

It clearly commutes with the Hamiltonian, and its action on the boundary vectors [see (5.1) and (5.2)] is found readily to be of the form (5.17) with $M = N = \sigma_1$ and, hence, the parity $\mathcal{P}$ is a generalized symmetry. Indeed, $U \xrightarrow{\mathcal{P}} U_{\mathcal{P}} = \sigma_1 U \sigma_1$ implies

$$\xi \xrightarrow{\mathcal{P}} \xi\,, \qquad \alpha \xrightarrow{\mathcal{P}} \alpha^*\,, \qquad \beta \xrightarrow{\mathcal{P}} -\beta^*\,, \tag{5.23}$$

and thus the spectral parameters ξ, $\alpha_{\rm R}$ and $\beta_{\rm I}$ remain the same, as required. Since $\sigma_1^2 = I$, the parity $\mathcal{P}$ induces *duality* in spectrum in the family Ω of singularities on a circle. Note that for systems with U satisfying $[U, \sigma_1] = 0$, the parity $\mathcal{P}$ is a symmetry, and that such a U has such parameters ξ, α, β that $\alpha_{\rm I} = 0$ and $\beta_{\rm R} = 0$. The set of those U forms the parity invariant subfamily $\Omega_{\mathcal{P}}$ which, in view of (4.5), reads

$$\Omega_{\mathcal{P}} \cong S^1 \times S^1 \subset \Omega. \tag{5.24}$$

We can consider a one-parameter family ($U(1)$ group) of generalized symmetries constructed from the parity $\mathcal{P}$ used as an infinitesimal generator,

$$\mathcal{P}_\vartheta := e^{-i\frac{\vartheta}{2}\mathcal{P}} = \cos\frac{\vartheta}{2} I - i \sin\frac{\vartheta}{2}\mathcal{P}\,, \qquad\qquad \vartheta \in [0, 2\pi)\,. \tag{5.25}$$

These transformations also commute with H and act on the boundary vectors as (5.17) with $M = N = e^{-i\frac{\vartheta}{2}\sigma_1}$, and are thus generalized symmetries. Their physical effect is incorporated through the transformations of the $U(2)$ parameters: ξ, $\alpha_{\rm R}$ and $\beta_{\rm I}$ are kept invariant, while a rotation is induced among $\beta_{\rm R}$ and $\alpha_{\rm I}$ as

$$\beta_{\rm R} + i\alpha_{\rm I} \xrightarrow{\mathcal{P}_\vartheta} e^{i\vartheta}(\beta_{\rm R} + i\alpha_{\rm I})\,. \tag{5.26}$$

This means that $\mathcal{P}_\vartheta$ furnishes a rotation among the spectrally identical point interaction systems in the parameter space, and that systems that are invariant under $\mathcal{P}_\vartheta$ are those with $\beta_{\rm R} = \alpha_{\rm I} = 0$, which, to no surprise, is the parity invariant subfamily $\Omega_{\mathcal{P}}$. Now the point is that, because of this $U(1)$ group of generalized symmetries within the family $\Omega = U(2)$, the spectral space is found to be the coset,

$$\Sigma_{\rm circle} = U(2)/U(1) = U(1) \times [SU(2)/U(1)], \tag{5.27}$$

which is precisely the result (5.16).

Another important discrete transformation worth mentioning is the time reflection,

$$\psi \xrightarrow{\mathcal{T}} \mathcal{T}\psi = \psi^*, \tag{5.28}$$

which leaves H invariant. It transforms the boundary vectors as

$$\Psi \xrightarrow{\mathcal{T}} \Psi^*\,, \qquad \Psi' \xrightarrow{\mathcal{T}} \Psi'^*\,, \qquad \Psi^{(\pm)} \xrightarrow{\mathcal{T}} \Psi^{(\mp)^*}\,, \tag{5.29}$$

and, consequently, maps the characteristic matrix to its transposed, $U \xrightarrow{\mathcal{T}} U_{\mathcal{T}} = U^T \in SU(2)$. This shows that the time reflection $\mathcal{T}$ is a generalized symmetry, although it does not belong to the class mentioned in (5.17), being actually antiunitary. In terms of the parameters, we find

$$\xi \xrightarrow{\mathcal{T}} \xi\,, \qquad \alpha \xrightarrow{\mathcal{T}} \alpha\,, \qquad \beta \xrightarrow{\mathcal{T}} -\beta^*\,, \tag{5.30}$$

and hence the spectrum is preserved. Clearly, $\mathcal{T}$ is a duality and the time reversal invariant subfamily $\Omega_{\mathcal{T}}$ consists of those U with $U = U^T$, *i.e.*, with $\beta_{\rm R} = 0$, and hence

$$\Omega_{\mathcal{T}} \cong S^1 \times S^2 \subset \Omega. \tag{5.31}$$

We also mention that the two duality transformations, $\mathcal{P}$ and $\mathcal{T}$, can be combined to give the space-time reflection operator $\mathcal{PT}$. On U it acts as $U \xrightarrow{\mathcal{PT}} U_{\mathcal{PT}} = \sigma_1 U^T \sigma_1$ and hence

$$\xi \xrightarrow{\mathcal{PT}} \xi\,, \qquad \alpha \xrightarrow{\mathcal{PT}} \alpha^*\,, \qquad \beta \xrightarrow{\mathcal{PT}} \beta\,. \tag{5.32}$$

The subfamily $\Omega_{\mathcal{PT}}$ of $\mathcal{PT}$-invariant U is determined by $\alpha_{\rm I} = 0$, and hence

$$\Omega_{\mathcal{PT}} \cong S^1 \times S^2 \subset \Omega. \tag{5.33}$$

Clearly, from neither $\Omega_{\mathcal{P}}$ nor $\Omega_{\mathcal{PT}}$ one can define a one-parameter family of generalized symmetries analogous to $\mathcal{P}_\vartheta$.

5.3 Supersymmetry

We have encountered in Sect. 5.1 two cases in the $\Omega = U(2)$ family where all the positive energy states are doubly degenerate. These cases are characterized by $U = \pm\sigma_1$, and we examine now if these can be interpreted as supersymmetric.

One might think that this is trivial, since the Hamiltonian is the same differential operator as of the free system, and hence the supercharges,

$$Q_1 := \frac{\hbar}{2i\sqrt{m}}\frac{\mathrm{d}}{\mathrm{d}x}\,, \qquad\qquad Q_2 := i\mathcal{P}Q_1, \tag{5.34}$$

will clearly fulfill the algebraic relation of supersymmetry

$$\{Q_i, Q_j\} = H_U\,\delta_{ij}\,, \qquad\qquad i,j = 1,2\,. \tag{5.35}$$

However, the point is that the algebra (5.35) should hold also in the sense of domains, not just in the differential operator relation, and it is a nontrivial question if the domains $\mathcal{D}(Q_i)$ of the supercharges Q_i for $i = 1, 2$ can be given so that they can meet this demand.[3] To see that this is indeed the case, we first note that, for the two cases in question, $U = \varepsilon\sigma_1$ with $\varepsilon = \pm 1$, the domains of the Hamiltonian read

$$\mathcal{D}(H_{\varepsilon\sigma_1}) = \{\psi \in \mathcal{H} \,|\, \psi,\, \psi' \in \mathrm{AC}(0,l),\ \psi(l) = \varepsilon\psi(0),\, \psi'(l) = \varepsilon\psi'(0)\}. \tag{5.36}$$

Now, if we provide the domains $\mathcal{D}(Q_i)$ as

$$\mathcal{D}(Q_i) = \{\psi \in \mathcal{H} \,|\, \psi \in \mathrm{AC}(0,l),\, \psi(l) = \varepsilon\psi(0)\}\,, \tag{5.37}$$

we can readily confirm that Q_i are self-adjoint on these domains. Moreover, by using the formulae

$$\mathcal{D}(A+B) = \mathcal{D}(A) \cap \mathcal{D}(B), \qquad \mathcal{D}(AB) = \{\psi \in \mathcal{D}(B) \,|\, B\psi \in \mathcal{D}(A)\}, \tag{5.38}$$

for the domains of the sum and the product of any two linear operators A and B, we see immediately that the domain of the lhs of (5.35) coincides with the domain (5.36). We therefore conclude that the systems $U = \pm\sigma_1$ indeed possess an $N = 2$ supersymmetry.

Note that for $U = \sigma_1$ the ground state is unique and hence the supersymmetry is unbroken (or 'good'), whereas for $U = -\sigma_1$ the ground state is doubly degenerate and supersymmetry is broken.[4] Due to the topology of the circle, the possibility of supersymmetry is limited compared to the line system where a richer variety of supersymmetric systems have been found [51, 54], under a slightly generalized supercharges.

5.4 More subfamilies and the WKB exactness

We have seen in Sect. 5.2 that generalized symmetries can be used to define various subfamilies, such as $\Omega_{\mathcal{T}}$, $\Omega_{\mathcal{P}}$, $\Omega_{\mathcal{PT}}$ as the set of the singularities for which the respective generalized symmetry is actually a symmetry. There are, however, some other subfamilies which are defined without using the generalized symmetries and admit salient properties in the spectrum and the WKB exactness. In this section we discuss these properties in some detail, providing a fuller account of our earlier result in [55] (from which we adopt the notations for the subfamilies).

We begin our discussion with the separating subfamily, $\Omega_1 \subset \Omega = U(2)$, which is the set of singular objects that prohibit the transmission of probability current. This condition is fulfilled by diagonal Us, *i.e.,* by those with $\beta = 0$, and the connection conditions split into two separate ones of half-line type, with length parameters $L_\pm$. Obviously, the cutoff of physical contact at $x = 0$ allows us to regard such a system effectively an interval $(0, l)$, in other words, a box or infinite potential well system. Among this subfamily Ω_1 are four

[3] The question of domain in the supersymmetry algebra is a nontrivial mathematical problem and has been answered only partially for simple systems such as lines/intervals [51, 52].

[4] Incidentally, we point out that here the Witten parity operator [53] is played by the parity $\mathcal{P}$.

special cases $(L_+, L_-) = (0,0)$, (∞,∞), $(0,\infty)$, $(\infty,0)$, in which the theory is explicitly solvable [55]. For example, the Feynman kernel is found to be

$$K(b,T;a,0) = \sqrt{\frac{m}{2\pi i\hbar T}} \sum_{n=-\infty}^{\infty} \epsilon^n \left(e^{\frac{i}{\hbar}\frac{m}{2T}\{(b-a)+2nl\}^2} \mp e^{\frac{i}{\hbar}\frac{m}{2T}\{(b+a)+2nl\}^2} \right) , \tag{5.39}$$

where the '$-$'-sign is for $L_- = 0$ and the '$+$'-sign is for $L_- = \infty$, and ϵ is 1 for $(L_+, L_-) = (0,0)$ and (∞,∞), and is -1 for the two other cases. This propagator is WKB-exact in the sense that it is a sum of free WKB amplitudes contributed by all possible classical paths that lead from $(a,0)$ to (b,T), including those that perform bouncing motion, hitting the left wall n times and the right one n or $n \pm 1$ times (depending on the initial direction of the particle). Even the appearing ± 1 factors allow a WKB interpretation since one can observe that any -1 factor belongs to a bouncing on a reflecting wall with $L = 0$ and the 1 ones to bouncing on a wall with $L = \infty$, in view of the fact that, based on some appropriate realizing potential sequences for a reflecting wall, an $L = 0$ wall picks up a WKB factor -1, while an $L = \infty$ wall has the WKB factor 1 (Sect. 3.4)

The second subfamily we mention is the *scale independent* subfamily Ω_2 consisting of systems for which the coefficients A, B in the eigenfunctions [cf. (5.3)] are k-independent. This happens for the characteristic matrices U with $\xi = \frac{\pi}{2}$ and $\alpha_{\rm R} = 0$ [which form a sphere $S^2 \subset \Omega$], and for $U = \pm I$ [two isolated points in Ω] (see Appendix D.2). These are the cases where the boundary conditions do not mix the boundary values of ψ with values of ψ'. More explicitly, in these cases L_+ and L_- are zero and hence the scale constant L_0 does not appear in the boundary conditions, leaving l as the only scale parameter. One may therefore expect that, in the limit $l \to \infty$, the system becomes a scale invariant 'point interaction on a line' system. Indeed, it has been known [10] that, on the line, systems belonging to the subfamily Ω_2 are those which are invariant under the dilatation symmetry $(\mathcal{W}_\lambda \psi)(x) = \lambda^{\frac{1}{2}} \psi(\lambda x)$. As for Ω_1, the systems belonging to Ω_2 can be solved [55],[5] and the Feynman kernel can be obtained explicitly [55]. For a generic $U \in \Omega_2$, using the notations

$$C_\pm = \frac{(1+\alpha_{\rm I}) + (\beta_{\rm I} - i\beta_{\rm R})e^{\pm i\theta}}{2\sqrt{(1+\alpha_{\rm I})(1-\beta_{\rm I}^2)}} , \qquad \theta = \arg(\beta) , \tag{5.40}$$

one finds

$$K(b,T;a,0) = \sqrt{\frac{m}{2\pi i\hbar T}} \sum_{n=-\infty}^{\infty} \left\{ M_n e^{\frac{i}{\hbar}\frac{m}{2T}\{(b-a)+nl\}^2} - N_n e^{\frac{i}{\hbar}\frac{m}{2T}\{(b+a)+nl\}^2} \right\} , \tag{5.41}$$

with

$$M_n = |C_+|^2 e^{-i\theta n} + |C_-|^2 e^{i\theta n}, \qquad N_n = C_-^* C_+ e^{-i\theta n} + C_+^* C_- e^{i\theta n} \tag{5.42}$$

Unlike in the previous subfamily Ω_1, however, the factors M_n, N_n do not admit a semi-classical interpretation, as one can readily confirm by using (5.42) and (5.40) together

[5]The intersection of the subfamilies Ω_1 and Ω_2 consists of the two special cases $U = \pm\sigma_3$, which are the box systems $(L_+, L_-) = (0,\infty)$, $(\infty,0)$. Two other important special cases in Ω_2 are $U = \pm\sigma_1$, which have already been discussed in Sect. 5.3. Note that the energy eigenfunctions of $U = \sigma_1$ provide just the basis $\{\cos nx, \sin nx\}$ that is used in the classic Fourier expansion.

with $|\alpha|^2+|\beta|^2=1$ that, *e.g.*, $|M_n|<1$ for generic n. The situation is similar to the half line systems with a wall that have a finite L, for which the bounce factors are not phase factors [13]. Consequently, we can apply the result found there, that is, such bounce factors cannot be given a semiclassical realization. Hence, generically, the WKB exactness is not perfect in the subfamily Ω_2.

However, there is a subfamily within the family Ω_2 where the WKB exactness holds perfectly. It is the *smooth* subfamily Ω_3, containing the cases in Ω_2 with $\alpha_{\rm I}=0$. Ω_3 is a one-parameter U(1) subfamily, parametrized solely by the θ of above. The boundary conditions here read

$$\psi(0)=e^{i\theta}\psi(l)\,,\qquad \psi'(0)=e^{i\theta}\psi'(l)\,, \tag{5.43}$$

which are nothing but the boundary conditions for the smooth circle [43], *i.e.,* for the circle with no singularity. As mentioned in sect.2, the phase parameter θ is regarded as the flux of a magnetic field penetrating through the circle. In this subfamily, the propagator (5.41) simplifies to the well-known kernel of the smooth circle

$$K(b,T;a,0)=\sqrt{\frac{m}{2\pi i\hbar T}}\sum_{n=-\infty}^{\infty}e^{i\theta n}e^{\frac{i}{\hbar}\frac{m}{2T}[(b-a)+nl]^2}\,, \tag{5.44}$$

which is readily seen to be WKB exact — the nth term belongs to a classical path on which the particle takes n turns before reaching the point b, without acquiring any additional action contribution each time when it crosses the point $x=l\equiv 0$.

Another subfamily worth mentioning is the *isospectral* subfamily Ω_4, comprising those U with $\xi=0$ and $\beta_{\rm I}=0$. These systems are peculiar in that they possess the same positive energy spectrum, $k=n\pi/l\quad(n=1,2,\ldots)$, independently of U, although the possible zero or negative energy is U dependent. This subfamily admits a generalization to the *semi-isospectral* subfamily Ω_5, characterized by the condition $\sin\xi=\pm\beta_{\rm I}$, where the positive spectrum consists of two infinite sequences, one that is equidistant and U-independent and another one that is U-dependent and given by transcendental roots of (5.8).

Chapter 6

Quantum pressure induced by distinct boundary conditions

Here, a case study is presented to demonstrate how remarkable differences can be caused by having different contact conditions. We consider a box system with Dirichlet boundary conditions at both ends, and place an infinitely thin still separating wall. The two half boxes are populated by the same type and number of particles, kept at the same temperature — the only difference is that on one side of the separating wall the boundary condition is chosen to be Dirichlet and on the other side the Neumann one. Because of the difference in the energy levels, the quantum statistical average pressure will be different in the two containers and a net force acting on the separating wall will emerge. We calculate this net force (as the function of temperature and particle number) both numerically and via analytical approximations and find that this quantity illustrates nicely the considerably different physical circumstances in the two subsystems.[1]

Approximately half of the results presented here have been published in [15], the other half is later development. The paper [19] also presents an extract of the earlier findings.

6.1 The considered system

The arrangement we wish to consider is visualized and explained in Fig. 6.1. The particles are considered identical and noninteracting, and thus to follow the Bose-Einstein or Fermi-Dirac distribution, depending on the spin s of the particles. The number of particles on both sides, is arbitrary, and is not necessarily macroscopically large. Our numerical results will be presented for $N = 100$ particles in each spin degree of freedom, which is a realistic population number in nanoscale quantum experiments [34].

The two half wells are two special — separating — cases of 'circle' systems, and admit

[1]We note that an investigation of quantum pressure acting on a Dirichlet boundary is presented in [56]. The energy distribution (level occupation distribution) considered there is not a thermal one but is concentrated on one energy level only.

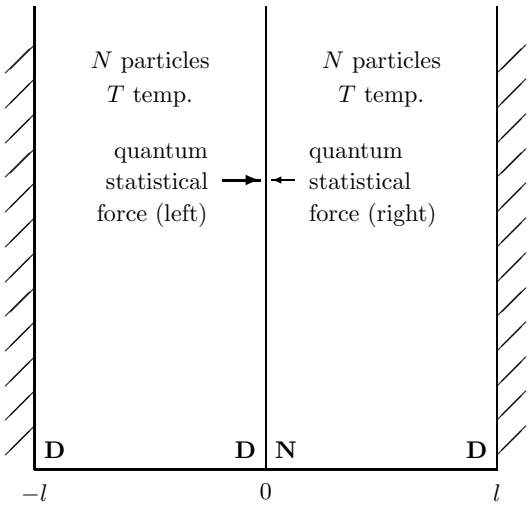

Figure 6.1: The two boxes of the same size l, with Dirichlet (**D**, $\psi = 0$) and Neumann (**N**, $\psi' = 0$) boundary conditions at the walls. Both sides are kept at the same temperature T and contain particles of the same mass m, the same spin s, and the same number of particles N in each spin degree of freedom. (The total number of particles on each side is $(2s+1)N$.)

the energy levels $E_n = e_n\mathcal{E}$, $n = 1, 2, 3, \ldots$, with

$$e_n^+ = \left(n - \frac{1}{2}\right)^2, \qquad e_n^- = n^2, \qquad \mathcal{E} = \frac{\hbar^2}{2m}\left(\frac{\pi}{l}\right)^2. \tag{6.1}$$

The superscripts $+$ and $-$ refer to the positive and negative half wells, respectively. Formulas in which these superscripts are omitted are valid on each side.

The equilibrium distribution of the particles, and the normalization condition for it reads

$$N_n = \frac{1}{e^{\alpha+be_n} - \eta}, \qquad N = \sum_n N_n, \tag{6.2}$$

where we have introduced $b = 1/t = \beta\mathcal{E}$, the dimensionless version of the inverse temperature $\beta = 1/kT$, which suits our problem conveniently, and

$$\eta = (-1)^{2s} \tag{6.3}$$

is 1 or -1 according to whether the particles are bosons or fermions, respectively. It is this normalization condition which determines α for a given temperature and particle number.

The force (or pressure — in one dimension, the two coincide) acting on the partition from one side is given by

$$F = -(2s+1)\sum_n N_n \frac{\partial E_n}{\partial l} = (2s+1)\frac{2\mathcal{E}}{l}\sum_n N_n e_n, \qquad f = \sum_n N_n e_n \tag{6.4}$$

with the similarly appropriately defined dimensionless equivalent $f = \frac{1}{2s+1}\frac{l}{2\mathcal{E}}F$ of the force F. Our aim will be to determine

$$\Delta f = f^- - f^+ \tag{6.5}$$

as a function of the temperature variable t. Since these sums cannot be summed up exactly, and an analytical solution for α which has to be determined is also not available, we are forced to apply approximations. The standard attitude, to approximate the sum with an integral and perform the integration is unfortunately not satisfactory in the present situation. Namely, the resulting Fermi-Dirac integral (for the fermionic case), which is related to the Lerch transcendent, can be expressed via an asymptotic series. This series is thus not summable but its truncations can be good approximations to the original quantity in a given region for the temperature. Unfortunately, as we have checked, these truncations do not provide enough preciseness for that the force difference, which, like any difference, is rather sensitive to errors. Hence, we need to work out methods for the present problem by ourselves. For bosons the situation is even worse.

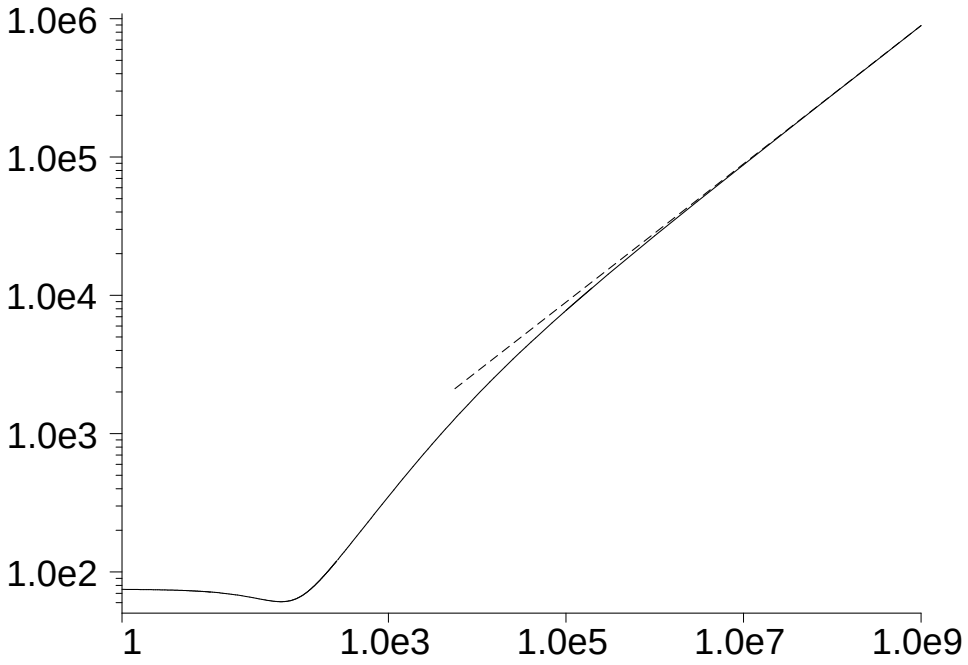

Figure 6.2: The net force Δf as the function of the temperature variable t, for bosons, at $N = 100$, obtained by a numerical computation (solid line). The high-temperature approximation (6.12) is also displayed (dashed line). The figure is double logarithmic. For fermions, the curve is qualitatively similar and its high-energy part coincides with that of the bosonic case.

6.2 High temperature regime

The high-temperature asymptotic behaviour can be calculated completely analogously for bosons and fermions.

For increasing temperature, we expect N_1 to decrease so [see (6.2) for $n = 1$] we expect α to increase to higher positive values. Inspired by this, let us expand N_n in $q := e^{-\alpha}$ as

$$N_n = \frac{q\mathrm{e}^{-be_n}}{1 - \eta q \mathrm{e}^{-be_n}} = \eta^{-1} \sum_{k=1}^{\infty} (\eta q)^k \mathrm{e}^{-kbe_n} , \tag{6.6}$$

which is valid for any positive α. Thus

$$\eta N = \eta \sum_{n=1}^{\infty} N_n = \sum_{k=1}^{\infty} (\eta q)^k \sum_{n=1}^{\infty} \mathrm{e}^{-kbe_n} = \sum_{k=1}^{\infty} (\eta q)^k \left[-\frac{\sigma}{2} + \frac{1}{2} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-kbe_n} \right] , \tag{6.7}$$

with the constants $\sigma^+ = 0$, $\sigma^- = 1$ corresponding to the $\pm$ half wells, where we have extended the meaning of the notation e_n [see (6.1)] to negative ns, too. Applying the Poisson summation formula

$$\sum_{n=-\infty}^{\infty} y(n) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}u \, y(u) \, e^{2\pi i m u} , \tag{6.8}$$

we obtain

$$\eta N = \sum_{k=1}^{\infty} (\eta q)^k \left[-\frac{\sigma}{2} + \sqrt{\frac{\pi}{4kb}} \sum_{m=-\infty}^{\infty} (\tau)^m e^{-\frac{\pi^2}{kb} m^2} \right] \tag{6.9}$$

with $\tau^{\pm} = \mp 1$. Similarly, for the force quantity f, one can find

$$f = \sum_{n=1}^{\infty} N_n e_n = \eta^{-1} \sum_{k=1}^{\infty} (\eta q)^k \sqrt{\frac{\pi}{16 k^3 b^3}} \sum_{m=-\infty}^{\infty} (\tau)^m \left(1 - \frac{2\pi^2}{kb} m^2 \right) e^{-\frac{\pi^2}{kb} m^2} . \tag{6.10}$$

For the high-temperature asymptotic behaviour ($q \to 0$), it suffices to consider only the first some terms in the sums over k [both in (6.9) and (6.10)], and within each term to keep only the $m = 0$ term in the sums over m (the $m \neq 0$ terms being exponentially suppressed). Now, the leading, $k = 1$ term in (6.9) gives that $q = 2N \left(\frac{b}{\pi} \right)^{1/2} + \mathcal{O}(b)$. Since this leading behaviour of q is independent of σ, inserting it into (6.10) gives that the leading, $\mathcal{O}(b^{-1})$ term of f (coming from $k = 1$, $m = 0$) is also σ-independent. Hence, this term will drop out from the net force. Therefore, to have the first nonvanishing term in the net force we need the first subleading term in q, too. Incorporating the $k = 2$ term as well for q, we find[2]

$$q = 2N \left(\frac{b}{\pi} \right)^{1/2} + 2N \left[\sigma - \eta \sqrt{2} N \right] \frac{b}{\pi} + \mathcal{O}\left(b^{3/2} \right) . \tag{6.11}$$

[2]The result confirms the expectation that, for high temperatures, α tends to infinity — although logarithmically slowly.

Plugging this into (6.10) and then calculating the net force yields

$$\Delta f = \frac{N}{2}\left(\frac{t}{\pi}\right)^{1/2} + \mathcal{O}\left(t^0\right) . \tag{6.12}$$

We can see in Fig. 6.2 how the net force actually reaches this square-root asymptotic behaviour at high temperatures.

By incorporating higher orders, the approximation can be improved easily. For example, in the next order, one finds

$$\Delta f = \frac{N}{2}\left(\frac{t}{\pi}\right)^{1/2} - \frac{N}{\pi}\left[(\sqrt{2}-1)\eta N - \frac{1}{2}\right] + \mathcal{O}\left(t^{-1/2}\right) . \tag{6.13}$$

Nevertheless, being a high-temperature expansion, it may not be expected to be able to explain the low and medium temperature part of the force curve.

6.3 Low temperature regime

Next, let us approach from the low-temperature direction. At exactly zero temperature, all the particles sit on the lowest available level. For bosons this means the ground state, from which we can immediately conclude

$$\Delta f(0) = f^-(0) - f^+(0) = Ne_1^- - Ne_1^+ = \frac{3}{4}N \tag{6.14}$$

which is apparently nonzero and is proportional to N. For fermions, the lowest N levels will be occupied, and we find

$$\Delta f(0) = \sum_{n=1}^{N} e_n^- - \sum_{n=1}^{N} e_n^+ = \frac{N(N+1)(2N+1)}{6} - \frac{N(4N^2-1)}{12} = \frac{N(2N+1)}{4} , \tag{6.15}$$

which (roughly) is proportional to N^2, instead.

Since the subsequent energy levels have a bigger difference on the Dirichlet side than on the Neumann side, at the same energy height, we can guess that, for a little bit increased temperature, the particles start to occupy the first empty level more early on the Neumann half. Consequently, the force difference will decrease a bit.

Indeed, in the two-level approximation for bosons, where the higher levels are treated as still completely unoccupied, the force difference is found

$$\Delta f \approx \frac{3}{4}N + \left(3\,e^{-3/t} - 2\,e^{-2/t}\right) , \tag{6.16}$$

which accounts for decrease: see Fig. 6.3. We mention that, for α, the low temperature behaviour is

$$\alpha \approx -be_1 + \ln\left(1 + \frac{1}{N}\right) , \tag{6.17}$$

which is a straightforward consequence of the approximation $N_1 \approx N$.

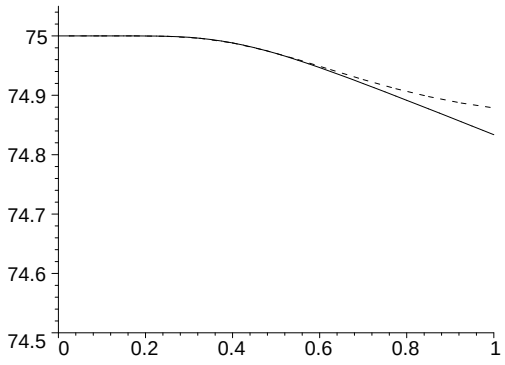

Figure 6.3: The temperature dependence of the net force Δf for bosons, $N = 100$, in the region $t < 1$, obtained by a numerical computation (solid line), and in the two-level approximation (6.16) (dashed line).

Unfortunately, this result, and even its improvement by incorporating an approximate participation of a few higher levels as well, does not prove satisfying to describe the further behaviour of the force curve. We will need different methods to discuss the medium temperature domain.

For fermions, the analogue of the bosonic two-level approximation is when only the occupation of the Nth and $N+1$th levels differ from the zero temperature value. Assuming this, one easily finds

$$\alpha \approx -\frac{b}{2}\,(e_N + e_{N+1}) \tag{6.18}$$

and

$$\Delta f \approx \Delta f(0) + \Delta\left(\frac{e_{N+1} - e_N}{e^{\frac{b}{2}(e_{N+1}-e_N)} + 1}\right). \tag{6.19}$$

This is able to describe the decreasing to the similar extent as for bosons: it gives correctly where and how the force curve starts to decrease but is unable — and, again, unable even if a few higher levels are also taken into account — to explain the subsequent

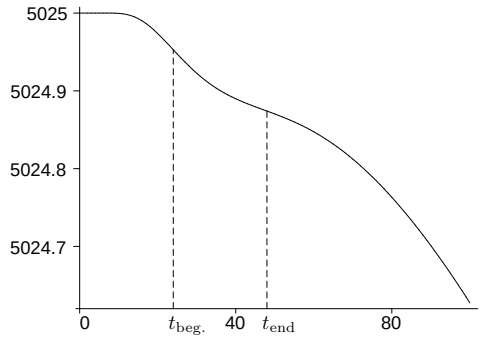

Figure 6.4: The low-temperature behaviour of the net force for fermions, $N = 100$. Observe the steplike shape, characterized by the temperature values at the two points of inflection.

behaviour. Namely, there is a qualitative difference between the fermionic curve and the bosonic one. The fermionic curve exhibits a 'steplike' pattern, but only one step independently of N, during the initial decrease (Fig. 6.4). This step is already a rather complex feature, an interplay of at least $\mathcal{O}(N)$ levels (effectively). Numerically, one finds that this step occurs at a temperature proportional to N (Fig. 6.5).

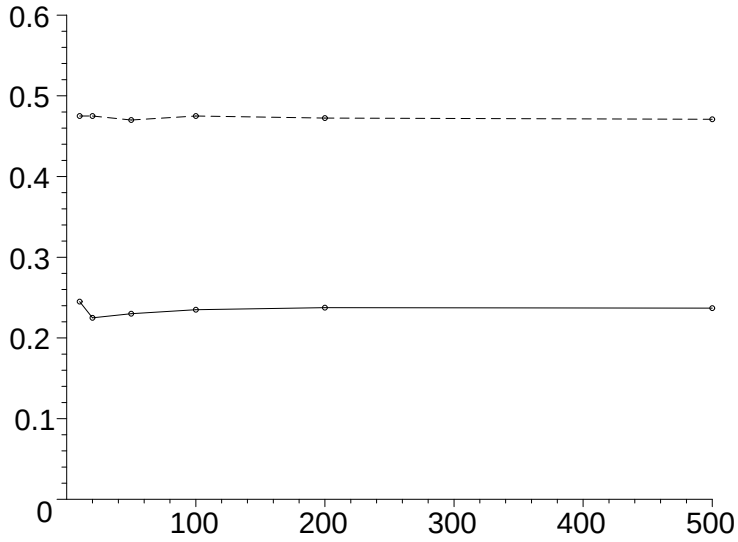

Figure 6.5: $t_{\mathrm{beg.}}/N$ and t_{end}/N, as the function of N, determined numerically. They appear to tend to constants that are approximately .237 and .472, respectively. Within error, the second number is just the double of the first one.

6.4 Medium temperature regime

The qualitative shape of the force curve agrees for bosons and fermions not only in the start at a nonzero value and that the initial constant plateau is followed by decrease, and not only in the (even quantitatively coinciding) high-temperature increase but also in that there is only one minimum between the two limiting domains. It is this medium temperature part where the job to calculate the force is the toughest. For bosons, the place and value of the minimum is proportional to N when $N \gg 1$ and can be determined as follows.

We start with that the trapezoid approximation of integrals, applied for a function g behaving "peacefully" in $[y_1, \infty)$ with $\lim_{\infty} g = 0$, gives

$$\sum_{n=1}^{\infty} g(y_n) \approx \frac{g(y_1)}{2} + \frac{1}{\Delta y} \int_{y_1}^{\infty} g(y)\,\mathrm{d}y \qquad \left(\Delta y = y_{n+1} - y_n = \sqrt{b}\right). \tag{6.20}$$

This approximation is better and better for smaller and smaller Δy — and, in our case, $\Delta y = \sqrt{b} \sim N^{-1/2}$. Remarkably, the trapezoid approach provides an approximation one

order better (in Δy) than the simple rectangular one. If g is "peaceful" even in $[0,\infty)$, which will always be the case in our applications, then, further,

$$\approx \frac{g(y_1)}{2} - \frac{y_1}{\Delta y}\, g(0) + \frac{1}{\Delta y}\int_0^\infty g(y)\,\mathrm{d}y \approx \left(\frac{1}{2} - \frac{y_1}{\Delta y}\right) g(0) + \frac{1}{\Delta y}\int_0^\infty f(y)\,\mathrm{d}y\,. \qquad (6.21)$$

Next, we argue that, at $t \sim 1$, $\alpha + be_1$ is $\ll 1$ and increases only slowly with t from its $t = 0$ value:

$$\alpha + be_1 = \ln\left(1 + \frac{1}{N_1}\right) = \ln\left(1 + \frac{1}{N - \sum\limits_{n=2}^{\infty} N_n}\right) = \ln\left(1 + \frac{1}{N - \sum\limits_{n=2}^{\infty} \frac{1}{e^{\alpha+be_1} e^{b(e_n-e_1)} - 1}}\right)$$

$$\approx \ln\left(1 + \frac{1}{N}\right) \qquad \text{(zeroth iteration)}, \qquad (6.22)$$

$$\approx \ln\left(1 + \frac{1}{N - \sum\limits_{n=2}^{\infty} \frac{1}{(1+\frac{1}{N})\underbrace{e^{b(e_n-e_1)}}_{>1 \text{ or } \gg 1} - 1}}\right) \qquad \text{(first iteration)}.$$

Therefore, it is reasonable to conjecture that, for some $t \gg 1$, $\alpha + be_1$ is still $\ll 1$. (And then $b \ll 1$, $|\alpha| \ll 1$.) The high-t asymptotics also supports this idea since there α increases only logarithmically with t. So, let us assume $b \ll 1$, $|\alpha| \ll 1$ in what follows. The validity of this assumption will be confirmed later.

Let us now derive an expression for the net force, under the conditions $b \sim 1/N \ll 1$; $|\alpha^-|, |\alpha^+| \ll 1$. For the force on one side, we can write

$$f = \sum_{n=1}^{\infty} \frac{e_n}{e^{\alpha+be_n} - 1}\,, \qquad bf + N\alpha = \sum_{n=1}^{\infty} \frac{\alpha + be_n}{e^{\alpha+be_n} - 1} = \sum_{n=1}^{\infty} \frac{z_n}{e^{z_n} - 1} \qquad (6.23)$$

with $z_n = \alpha + be_n$. Fortunately, we are actually interested in the difference of the two forces, $\Delta f = f^- - f^+$, which, a sum of differences, will be possible to evaluate as an integral of a derivative, in the leading order. This can be done as follows.

$$\Delta(bf + N\alpha) = b\,\Delta f + N\Delta\alpha = \sum_{n=1}^{\infty} \Delta\left(\frac{z_n}{e^{z_n} - 1}\right), \qquad (6.24)$$

and note that $\frac{z}{e^z-1}$ and its derivative (by z) are both "peaceful" functions in $z \in [0,\infty)$. Furthermore,

$$\Delta z_n = z_n^- - z_n^+ = \Delta\alpha + b\Delta(n-\tau)^2 = \Delta(\alpha + b\tau^2) - 2b\,\Delta\tau\, n \qquad (6.25)$$

where τ is the constant appearing in $e_n = (n-\tau)^2$, *i.e.*, $\tau^- = 0$ and $\tau^+ = 1/2$. Thus, up to $n = \mathcal{O}\left(t^{1/2}\right)$, $\Delta z_n = \mathcal{O}\left(t^{-1/2}\right) = \mathcal{O}\left(N^{-1/2}\right)$. Hence, for increasing N (and a fixed such n), the approximation

$$\Delta\left(\frac{z_n}{e^{z_n} - 1}\right) \approx \left(\frac{\mathrm{d}}{\mathrm{d}z}\,\frac{z}{e^z - 1}\right)_{z=z_n} \cdot \Delta z_n \qquad (6.26)$$

gets valid better and better. Here, $\left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{z}{e^z-1}\right)_{z=z_n}$ can either be the Dirichlet or the Neumann one, or, for increased preciseness, the average of the two. As it happens, the relevant, leading, order is the same for the two sides so we don't have to specify a choice, actually. Note also that it is harmless to write the approximation (6.26) for higher ns as well, since the higher n terms are exponentially suppressed.

To proceed, let us express Δz_n as

$$\Delta z_n = [\Delta\alpha + b(\Delta\tau^2 - 2\tau\,\Delta\tau)] - 2\Delta\tau\sqrt{b}\,y_n \tag{6.27}$$

(still a form valid on both sides). Then, putting everything together,

$$b\Delta f + N\Delta\alpha \approx \sum_{n=1}^{\infty}\left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{z}{e^z-1}\right)_{z=z_n}\cdot\Delta z_n \tag{6.28}$$

$$= \underbrace{[\Delta\alpha + b(\Delta\tau^2 - 2\tau\,\Delta\tau)]}_{\text{both terms } \mathcal{O}(N^{-1})}\sum_{n=1}^{\infty}\left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{z}{e^z-1}\right)_{z=z_n} - 2\Delta\tau\sqrt{b}\sum_{n=1}^{\infty}\left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{z}{e^z-1}\right)_{z=z_n}\cdot y_n \tag{6.29}$$

$$\approx \mathcal{O}\left(N^{-1}\right)\left[\mathcal{O}\left(b^0\right) + \frac{1}{\sqrt{b}}\underbrace{\int_{y_1}^{\infty}\left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{z}{e^z-1}\right)_{z=\alpha+y^2}\mathrm{d}y}_{\mathcal{O}(b^0)\ \text{(see below)}}\right] \tag{6.30}$$

$$-2\Delta\tau\sqrt{b}\Big[\mathcal{O}\left(b^0\right) + \frac{1}{\sqrt{b}}\int_{y_1}^{\infty}\left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{z}{e^z-1}\right)_{z=\alpha+y^2}\cdot\underbrace{y\,\mathrm{d}y}_{\frac{1}{2}\mathrm{d}z}\Big], \tag{6.31}$$

where we utilized the trapezoid approximation. The integral in the third line here is $\mathcal{O}\left(b^0\right)$ since, by $|\alpha| \ll 1$ and $y_1 \sim \sqrt{b}$, it is near to

$$\int_0^{\infty}\left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{z}{e^z-1}\right)_{z=y^2}\mathrm{d}y \tag{6.32}$$

(the integrand is a "peaceful" function!), which is a numerical constant.

The leading term among the $2+2=4$ obtained terms in (6.30) is the last one, and can be evaluated as

$$-2\Delta\tau\sqrt{b}\frac{1}{\sqrt{b}}\frac{1}{2}\int_{z_1}^{\infty}\left(\frac{\mathrm{d}}{\mathrm{d}z}\frac{z}{e^z-1}\right)\mathrm{d}z = -\Delta\tau\left[\frac{z}{e^z-1}\right]_{z=z_1}^{\infty} \tag{6.33}$$

$$= \Delta\tau\frac{\alpha+y_1^2}{e^{\alpha+y_1^2}-1} = \Delta\tau\,[\,1 + \mathcal{O}\underbrace{(\alpha+y_1^2)}_{\text{both terms } \mathcal{O}(N^{-1})}\,] = -\frac{1}{2} + \mathcal{O}\left(N^{-1}\right). \tag{6.34}$$

Hence,

$$b\Delta f + N\Delta\alpha \approx -\frac{1}{2} + \mathcal{O}\left(N^{-1/2}\right), \tag{6.35}$$

from which

$$\frac{\Delta f}{N} \approx -\frac{1}{2}\frac{t}{N} - \Delta(t\alpha). \tag{6.36}$$

Now our task is to provide some approximation for $\Delta\alpha$ under the assumptions $b \ll 1$, $|\alpha| \ll 1$. We can do it the following way:

$$N = \sum_{n=1}^{\infty} \frac{1}{e^{\alpha+be_n} - 1} \approx \sum_{n=1}^{\infty} \frac{1}{\alpha + be_n}\,, \tag{6.37}$$

the approximation being surely good at least for the lower — the most — relevant levels. (N_n falls rapidly with n.) Let us write this in the rearranged form

$$\frac{N}{t} \approx \sum_{n=1}^{\infty} \frac{1}{t\alpha + e_n}\,. \tag{6.38}$$

The solution of this for $t\alpha$ will be a function of $\frac{t}{N}$. From [57],

$$S(t\alpha) := \sum_{n=1}^{\infty} \frac{1}{t\alpha + (n-\tau)^2} = \begin{cases} \frac{\pi\sqrt{t\alpha}\coth\pi\sqrt{t\alpha}-1}{2t\alpha} & (\text{Dir};\ \tau = 0\,) \\ \frac{\pi\tanh\pi\sqrt{t\alpha}}{2\sqrt{t\alpha}} & (\text{Neu};\ \tau = \frac{1}{2}\,) \end{cases}\,. \tag{6.39}$$

Both formulas are valid for negative α as well, and are a smooth function of $t\alpha$ at zero, see Fig. 6.6.

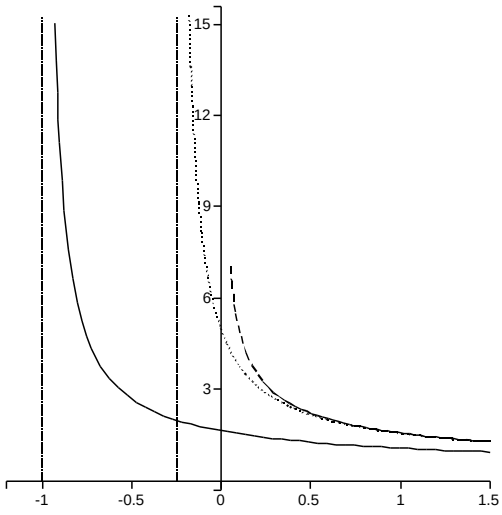

Figure 6.6: The functions S^- (solid line) and S^+ (dash-dotted line) as defined in (6.39). They are smooth at zero and diverge at $-e_1^-$ resp. $-e_1^+$, see (6.17) why. The dashed line depicts the approximation (6.47) for S^+ around 1.

It is a reasonable first choice to investigate the temperatures where either α^- or α^+ becomes zero. From (6.38) and (6.39), we have to solve

$$\frac{N}{t} \approx \begin{cases} S^-(0) = \pi^2/6 & (\text{if } \alpha^- = 0) \\ S^+(0) = \pi^2/2 & (\text{if } \alpha^+ = 0) \end{cases}\,, \tag{6.40}$$

from which

$$t_0^- \approx (6/\pi^2)N\,, \tag{6.41}$$

$t_0^+ \approx (2/\pi^2)N$. These are really $b \sim 1/N \ll 1$ cases.[3] In addition, the relative error of (6.37) tends to zero with $N \to \infty$: *e.g.,* for a t with $\alpha = 0$, the error of (6.37) is

$$\sum_{n=1}^{\infty} \frac{1}{e^{y_n^2}-1} - \frac{1}{y_n^2} \qquad \text{with} \quad y_n = \sqrt{be_n} = \sqrt{b}\,(n-\tau)\,. \tag{6.42}$$

Thus

$$\sum_{n=1}^{\infty}\left(\frac{1}{e^{y_n^2}-1} - \frac{1}{y_n^2}\right) \approx \mathcal{O}\left(b^0\right) + \frac{1}{\sqrt{b}}\int_0^{\infty}\left(\frac{1}{e^{y^2}-1} - \frac{1}{y^2}\right)\mathrm{d}y \tag{6.43}$$
$$= (N\text{- and } t\text{-independent constant}) - 1.29420\sqrt{t}\,.$$

$\left[\frac{1}{e^{y^2}-1} - \frac{1}{y^2}\right.$ is "peaceful" in $[0,\infty)$ so we could apply the trapezoid approximation on it.$\big]$ With $t \sim N$, this $\sqrt{t}$ error (this $\sqrt{N}$ error) gets negligible with respect to N, the lhs in (6.37).

Now let us choose a t in the vicinity of t_0^-. There, $|t\alpha^-| \ll 1$, and the equation we wish to solve is

$$\frac{N}{t} = \frac{\pi\sqrt{t\alpha^-}\coth\pi\sqrt{t\alpha^-} - 1}{2t\alpha^-} = \frac{\pi^2}{6} - \frac{\pi^4}{90}t\alpha^- + \frac{\pi^6}{945}(t\alpha^-)^2 + \mathcal{O}\left((t\alpha^-)^3\right)\,, \tag{6.44}$$

inverting which we can obtain its solution as

$$t\alpha^- = \frac{5}{2}\left(\frac{t}{N} - \frac{6}{\pi^2}\right) + \frac{5\pi^2}{28}\left(\frac{t}{N} - \frac{6}{\pi^2}\right)^2 + \mathcal{O}\left(\left(\frac{t}{N} - \frac{6}{\pi^2}\right)^3\right)\,. \tag{6.45}$$

For $t\alpha^-$ around 0, the equations we wish to solve can be combined as

$$S^+(t\alpha^+) = N/t = S^-(t\alpha^-) \approx S^-(0)\,, \tag{6.46}$$

and from 6.6 we can read off that the $t\alpha^+$ corresponding to $S^+(t\alpha^+) \approx S^-(0)$ is roughly 1, where $\tanh\pi\sqrt{t\alpha^+}$ already almost saturates to its large-variable asymptotic value, 1. Taking this asymptotical approximation

$$\tanh\pi\sqrt{t\alpha^+} \approx 1\,, \tag{6.47}$$

$t\alpha^+$ is provided by the solution of $N/t = \pi/(2\sqrt{t\alpha^+})$, which is

$$t\alpha^+ = \frac{\pi^2}{4}\left(\frac{t}{N}\right)^2\,. \tag{6.48}$$

Note that this solution satisfies $t_0^-\alpha^+ = \mathcal{O}(1)$, $\alpha^+ = \mathcal{O}(1/N) \ll 1$, so here our initial assumption $b \ll 1$, $|\alpha| \ll 1$ has been validated.

[3] In addition, one of the αs is zero. However, we don't know yet whether the other $|\alpha|$ is also much smaller than 1 or not. That will come later.

Now let us insert the obtained solutions (6.45), (6.48) in (6.36) to see the net force in the temperature region around t_0^-. We obtain

$$\frac{\Delta f}{N} \approx \frac{\pi^2}{14}\left(\frac{t}{N} - \frac{6}{\pi^2}\right)^2 + \frac{6}{\pi^2}\,. \tag{6.49}$$

We thus find that, in our approximation, the force difference possesses a parabolic minimum, at the temperature where, incidentally, $\alpha^- = 0$ (and α^+ is some corresponding positive, nonspecial value), with

$$\frac{t_{\min}}{N} \approx \frac{\Delta f_{\min}}{N} \approx \frac{6}{\pi^2} = 0.6079\ldots\,. \tag{6.50}$$

In spite of the various approximations made, the result is fairly reliable, as can be seen for $N = 100$ in Fig. 6.7, and from the true N-dependence of $t_{\min}$ and $\Delta f_{\min}$ displayed in Fig. 6.8. Actually, this result fits better for $N \sim 100$ than in the limit $N \to \infty$: the high-N limits of $t_{\min}/N$ and $\Delta f_{\min}/N$ are predicted with a bit too big error.

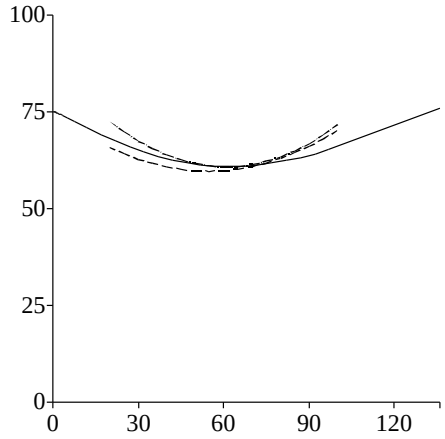

Figure 6.7: The minimum of the force curve, for bosons, with $N = 100$. Solid line: numerical computation; dash-dotted line: the approximation (6.49); dashed line: the approximation (6.53).

For an approximation better than (6.47), we can apply

$$\tanh x \approx \frac{\tanh x_* + (x - x_*)}{1 + \tanh x_* \cdot (x - x_*)}\,, \tag{6.51}$$

a formula precise up to the quadratic Taylor term at x_*, and behaving much better than the quadratic Taylor polynomial approximation in a larger neighbourhood. From 6.6 we can read off that, at the t/N where $t\alpha^-$ is zero, $t\alpha^+$ is near 0.9 and $\pi\sqrt{t\alpha^+}$ is near 3. Thus we choose the expansion point (x_*) simply to be 3. Denoting the corresponding t/N as t_*/N (which is, naturally, close to t_0^-/N) and assuming an expansion

$$t\alpha^+ - (t\alpha^+)_* = c_1\left(\frac{t}{N} - \frac{t_*}{N}\right) + c_2\left(\frac{t}{N} - \frac{t_*}{N}\right)^2 + \mathcal{O}\left(\left(\frac{t}{N} - \frac{t_*}{N}\right)^3\right)\,, \tag{6.52}$$

we obtain a quadratic approximation for $t\alpha^+$ that is better than (6.48). Correspondingly, the approximation of the force difference improves to

$$0.51211 \cdot (t/N - 0.54648)^2 + 0.59672\,. \tag{6.53}$$

These $t_{\min}/N$ and $\Delta f_{\min}/N$ values are really very close to the real ones, see Fig. 6.7. Accidentally, for $N \sim 100$ this latter parabola is less good than (6.49), as can be seen in Fig. 6.7 but for increasing N it becomes more and more reliable.

At last, for an even better approximation of the $N \to \infty$ limiting values of $\frac{t_{\min}}{N}$ and $\frac{\Delta f_{\min}}{N}$, we can solve

$$S^-(t\alpha^-) = \frac{N}{t} = S^+(t\alpha^+) \tag{6.54}$$

numerically at many t/N-s in favour of $t\alpha^-$ and $t\alpha^+$, and put those solutions into (6.36). Choosing the temperature where the force difference (6.36) is minimal, we find

$$\frac{t_{\min}}{N} = 0.54805\,, \qquad \frac{\Delta f_{\min}}{N} = 0.5967\,. \tag{6.55}$$

These values differ only very slightly from the ones in (6.53).

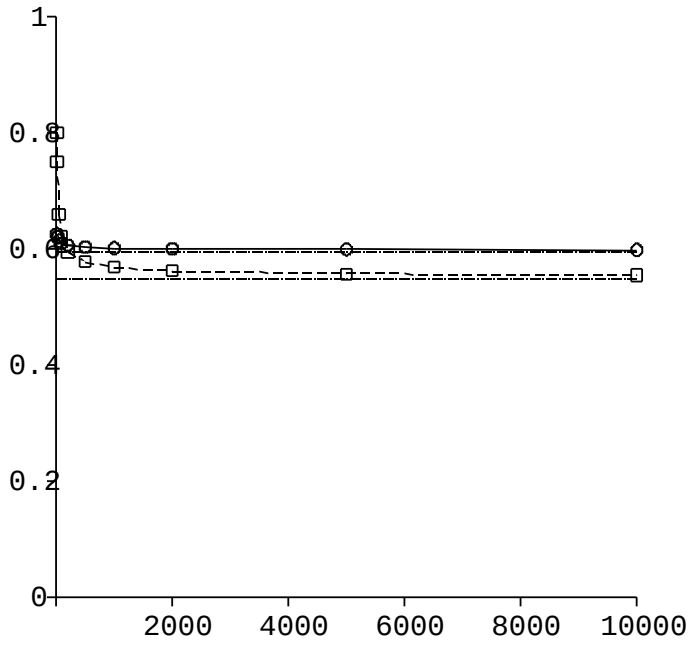

Figure 6.8: $t_{\min}/N$ (dashed line) and $\Delta f_{\min}/N$ (solid line), as the function of N, for bosons. The constants (6.55) to which they tend are also displayed (dash-dotted lines).

We can see that the parabolic approximation is, naturally, not able to describe the whole medium temperature domain. Expanding at other values and/or using approximate formulas for the other parts of the functions S, a local description is available at the other

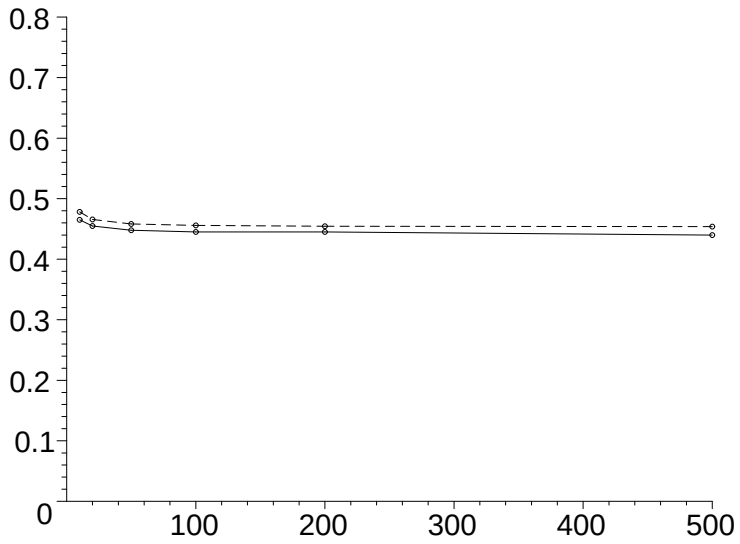

Figure 6.9: $t_{\min}/N^2$ (solid line) and $\Delta f_{\min}/N^2$ (dashed line), as the function of N, for fermions. The constants to which they appear to tend are approximately 0.45 and 0.46, respectively.

parts of the force curve. To derive a more universally valid approximate description of the medium temperature region seems hard.

For the case of fermions, the minimum in the medium temperature region is qualitatively similar to the bosonic one but quantitatively not: both $t_{\min}$ and $\Delta f_{\min}$ appear to be proportional to N^2 rather than to N (see Fig. 6.9). For fermions, an approximation like (6.37) is not available, and the "mechanism" that creates the minimum seems be different. Unfortunately, determining the location and value of the minimum for the fermionic case is still an open problem.

6.5 Ideas to improve the results

During studying the medium temperature domain, we have introduced various technics for treating the medium temperature domain. They can actually be listed as follows.

- One such method is an improvement of the trapezoid integral approximation, where the sum is approximated by two intergrals based on the one order more precise Simpson integral approximation.
- Another is the adaptation of partial intergration for sums.
- A third approach uses an idea similar to the one applied in (6.26), to express the difference of forces, and, more generally, the difference of two similar sums, expanding in terms of the parameters in which they differ slightly.

- A fourth possible way is to "factorize" the two-parameter sums[4] into two one-parameter ones, like done in (6.6), then approximating the inner one-parameter sum with a simple enough function that admits the same asymptotics for small and large values of the parameter and interpolates well in between, and finally to somehow sum up the remaining outer sum.

- A fifth is to approximate arising functions with "less transcendental" and more easily integrable and summable ones, like

$$\frac{z^2 e^{-kz}}{2(\cosh z - 1)} = \left[1 - \frac{z^2}{12} + \mathcal{O}\left(z^4\right)\right] e^{-kz} \qquad (k = 1, 2, \ldots)\,, \tag{6.56}$$

$$\begin{aligned} \frac{z}{e^z - 1} &= e^{-\frac{z}{2}} \left[1 + \mathcal{O}\left(z^2\right)\right] = \left(1 + z/\sqrt{12}\right) e^{-\left(1/2 + 1/\sqrt{12}\right) z} \left[1 + \mathcal{O}\left(z^3\right)\right] \\ &= \left[1 + \frac{z}{2} + \frac{z^2}{12} + \mathcal{O}\left(z^3\right)\right] e^{-z}\,, \end{aligned} \tag{6.57}$$

$$\frac{z}{1 - e^{-z}} e^{-kz} = \left(\frac{5}{6} + \frac{2}{3} z + \frac{1}{6} e^{-z}\right) e^{-kz} \left[1 + \mathcal{O}\left(z^3\right)\right] \qquad (k = 1, 2, \ldots)\,, \tag{6.58}$$

  which are chosen to reproduce the first some Taylor terms around $z = 0$ as well as to follow the approximated function faithfully enough for large values of z, too.

- A sixth is to differentiate the sums with respect to one of its parameters and to derive, approximate and solve a differential equation in the parameter from a known special case.

- A seventh is to expand an two-parameter sum around some special value of one parameter, like $\alpha = 0$.

Naturally, these ideas can also be combined. Still, it is found hard to reach reasonable analytic results. What is easier is to derive a good approximation of the force difference that contains the αs explicitly, even globally from $t = 0$ to $t \to \infty$. It is harder to reach such version that contains the αs in a simple enough form so that if we have an approximation for the αs then the result is a not too complicated and reasonably usable one. What is the hardest is to achieve an approximation for the αs to enough preciseness, since a generally observed feature about the α-containing force approximations is that the force difference is extremely sensitive to the error of α.

6.6 Some remarks concerning the numerical calculation of the net force

The numerical computation of the net force for a given N and t is, naturally, based on a finite truncation of the infinite sums involved. The solution of (6.2) for α also happens

[4] the two parameters being α and b, or $\hat{\alpha} = \alpha + be_1$ and b — the advantage of the latter is that $\hat{\alpha}$ is always non-negative, and $e^{-\hat{\alpha}} \leq 1$

numerically. Since the force difference is very sensitive to the error in the αs, a great care is to be taken of the errors of the truncations and of the determined αs. To this end, estimates, and wherever it is available, upper estimates are needed for these errors. The dependence of a sum on α can be estimated by the derivative of the sum with respect to α, and then an upper estimate can be used for the derivative sum. A practical way to work out a first estimate of the sum when summed up to a given index n_1, to really sum up to an appropriately chosen n_1, and then to overestimate the omitted further part of the sum using both another estimate formula and the numerically obtained sum, as an additional information. For sum estimates, one can use different ones for low and for high temperature. The useful technics include upper estimate by a geometric series and considering the sum as a lower estimate of an integral. The floating-point precision of the computations must also be chosen by hand, according to the error estimates. For higher N and higher t, the precision may need to be increased. The calculations presented here, and throughout the dissertation, have been performed using the mathematical computer software Maple (©Maplesoft, Waterloo Maple Inc.).

6.7 Analysis of the results

We have found that the net force acting on the separating wall is nonzero at low temperatures, being practically constant for very small temperatures and starting to decrease when temperature is increased. Knowing that the energy spectrum is different on the two halves this property is not very surprising. What is surprising, however, is that this decrease stops at a certain temperature and the net force starts to increase above this value. Furthermore, a remarkable fact is that this increase does not stop nor converges to some finite high-temperature limit but increases to infinity, as the square root of the temperature. From the naive expectation that such quantum effects coming from the different boundary conditions should vanish at high temperatures where the classical picture would be available, this result seems quite unusual. However, this may be understood by the fact that, contrary to most quantum systems, one dimensional boxes have such energy spectra that the level spacing is not decreasing but increasing for higher energy levels (which is actually valid not only for boxes with Dirichlet and/or Neumann boundary conditions but for all other boxes as well, as has been seen in Sect. 5.1). In other words, quantum boxes can be distinguished by their high-temperature behaviour, too.

We mention that the calculation presented here could be repeated for boxes with other boundary conditions, too. We note however that, for most box systems, the energy values are determined by a transcendental equation [(5.8), (5.9) and (5.10)], and hence a certain additional difficulty for carrying out calculations, especially analytical ones, will arise there. Our intuition says that the Dirichlet and Neumann conditions represent two very different, probably most different, cases so the effect can be reliably demonstrated already via them. Nevertheless, some details may vary depending on which types of boxes we choose, especially the low and medium temperature ones (since, asymptotically, the energy levels follow an n^2 pattern so the high-temperature part may be more universal).

It is not only this net force that can be determined from the calculations. One can

also ask what an equilibrium position would be for the separating wall, with appropriate unequal box sizes $l^{(+)} \neq l^{(-)}$, $l^{(+)} + l^{(-)} = 2l$. Another similar question is when the box sizes are kept fixed and equilibrium is achieved by choosing appropriate unequal particle numbers on the two sides, $N^{(+)} \neq N^{(-)}$, $N^{(+)} + N^{(-)} = 2N$. Calculations not presented here show that, for bosons, these equilibrial values at zero temperature are $l^{(-)}/l^{(+)} \cong 4.404$, $N^{(+)}/N^{(-)} = 4$. This shows that for achieving equilibrium one needs $\mathcal{O}(1)$ changes in the parameters, *i.e.,* changes comparable to the initial values. For fermions, these required changes prove to be less significant, $\mathcal{O}(1/N)$. In other words, for fermions the amount of unbalancedness is smaller — at least at zero temperature. In the future, we plan to repeat the same calculations in the medium and high temperature regimes as well.

Chapter 7

The deuteron and proton-neutron scattering

This chapter reports about a work that investigates the relevance of contact conditions in the description of certain nuclear physical systems. We wish here to give account of the proton-neutron scattering experimental results and of the deuteron. Since the nuclear force that acts between the two particles is short-range, and is strongly repulsive if the interparticle distance is within a given range, the idea is to assume that, seen from the outside, the nuclear force can be modelled by some contact condition. Nuclear physics says [58] that the $S = 1\,,\ L = J \pm 1$ channels[1] are coupled (due to the spin dependence of the nuclear force); and here we will be interested in the $J = 1$ case — the coupling between the $L = 0$ and $L = 2$ channels —, the case the deuteron bound state belongs to. The interaction is assumed to possess time reversal invariance.

The standard way to describe such nuclear interactions is to use some model potentials with (usually numerous) free parameters that have to be fitted to the experimental data. According to our experience gained in the previous chapters, such an approach may introduce too many parameters compared to the few essential contact-type parameters that are provided by boundary/connection conditions. In addition, some of the boundary parameters may be hard to expressed via a potential realization. Therefore, here we test the idea how the formalism of contact conditions can give account of the nuclear force.

7.1 Formulating the model

We will consider a channel L as an effective quantum subsystem on a positive half line with Hamiltonian

$$H_L\psi_L = \frac{\hbar^2}{2m}\left(-\frac{\mathrm{d}^2\psi_L}{\mathrm{d}r^2} + \frac{L(L+1)}{r^2}\psi_L\right)\,, \qquad \psi_L \in L^2((\rho,\infty),\mathrm{d}r) \tag{7.1}$$

with m being the reduced mass (see Appendix E). Here, $\rho > 0$ is introduced as the range outside which the nuclear force is considered zero; [58] indicates that $\rho \geq 0.5$ fm.

[1] angular momentum sectors of the relative motion of the two particles

For $L \geq 1$, $r = 0$ would be a limit-point singularity, and thus we would have no free fitting parameter nor mixing. That's why the original idea of the Fermi-potential leads only to the one-parameter delta-potential. However, here we will impose our fitting at the positive radius value $r = \rho$.

Note that connecting two half lines at a common positive value with connection condition means the continuity of the probability current at ρ from one channel to the other, not entering the excluded core region. Therefore, the physical essence of our present model is that we don't allow the probability to be nonzero in the core region while, via the $U(2)$ variety of connection conditions we allow probability flow from angular momentum one channel to the other, in other words, we are able to incorporate spherically nonsymmetric interactions as well. The known repulsion for very short distances supports this concept. Nevertheless, our model means a simplification which may or may not prove to be realistic. On the other side, if our idea works then it means that there is no need — and room — for so many free parameters that are usually used in nuclear potentials for connection: the language of connection conditions would provide an economically small family of the necessary, and physically really distinct, parameters.

The experimental input we will use is the binding energy of the deuteron and the large-distance asymptotic ratio of the deuteron wave function in the $L = 2$ channel with respect to the $L = 0$ channel. This ratio, η_{D}, is a relatively easily measurable quantity (see Appendix E) and its small nonzero value indicates the mixing of the two angular momentum channels, in other words, the nonsphericalness (spin dependence) of the proton-neutron interaction. The output of our calculation is the proton-neutron scattering phase shifts, as a function of the few free parameters allowed by the family of connection conditions. Then we can do fitting with our parameters and check whether some appropriate values of them fall close enough the experimentally known phase shifts or not. That will be the test of our model.

The configuration space for our effective system is two positive half lines (the radial coordinate $r \in [\rho, \infty)$ running on them is positive and outward oriented), connected at one point (at the effective endpoints $r = \rho$). Topologically, this two-legged star graph setting is the same as the line system in Chapter 4, a positive and a negative half line connected at their endpoints, so we can utilize the formulation of the connection condition from there. What we need to change in those formulas is that the negative half line has to be reverted to a positive one (and the endpoint coordinates have to be shifted from 0 to ρ).

For the time reversal invariance of the nuclear force, we are interested in time reversal invariant connection conditions, and because of the nonzero coupling of the two channels, in the nonseparating ones. The latter will allow us to use the transit matrix (4.10). Now, the characteristic matrix of a nonseparating and time reversal invariant pointlike singularity at $x = 0$ on a line $x \in (-\infty, \infty)$ is

$$U = e^{i\xi} \begin{pmatrix} \alpha_{\mathrm{R}} + i\alpha_{\mathrm{I}} & \beta_{\mathrm{R}} + i\beta_{\mathrm{I}} \\ -\beta_{\mathrm{R}} + i\beta_{\mathrm{I}} & \alpha_{\mathrm{R}} - i\alpha_{\mathrm{I}} \end{pmatrix} \tag{7.2}$$

with $\beta \neq 0$ (nonseparating) and $\beta_{\mathrm{R}} = 0$ (time reversal invariant), and the corresponding

transit matrix is

$$\Lambda = \frac{-1}{\beta_{\rm I}} \begin{pmatrix} \sin\xi - \alpha_{\rm I} & -L_0(\cos\xi + \alpha_{\rm R}) \\ L_0^{-1}(\cos\xi - \alpha_{\rm R}) & \sin\xi + \alpha_{\rm I} \end{pmatrix} \tag{7.3}$$

(see Sect. 4.1). This Λ has real[2] entries and its determinant is found one; and any Λ with these two properties is allowed (gives a nonseparating, time reversal invariant self-adjoint Hamiltonian). In terms of Λ, the connection condition reads

$$\Lambda \begin{pmatrix} \psi(-0) \\ \mathrm{d}\psi/\mathrm{d}x(-0) \end{pmatrix} = \begin{pmatrix} \psi(+0) \\ \mathrm{d}\psi/\mathrm{d}x(+0) \end{pmatrix} . \tag{7.4}$$

If we revert the negative half line ($x \in (-\infty, 0)$, x increasing inward) into positive ($y \in (0, \infty)$, y increasing outward) then

$$\begin{pmatrix} \psi \\ \mathrm{d}\psi/\mathrm{d}x \end{pmatrix} = \begin{pmatrix} \psi \\ -\mathrm{d}\psi/\mathrm{d}y \end{pmatrix} = \sigma_3 \begin{pmatrix} \psi \\ \mathrm{d}\psi/\mathrm{d}y \end{pmatrix} , \tag{7.5}$$

and correspondingly

$$\Lambda\sigma_3 \begin{pmatrix} \psi \\ \mathrm{d}\psi/\mathrm{d}y \end{pmatrix}_{y\searrow 0} = \begin{pmatrix} \psi \\ \mathrm{d}\psi/\mathrm{d}x \end{pmatrix}_{x\searrow 0} . \tag{7.6}$$

This connection condition is now easily adapted for our two channels:

$$\Lambda\sigma_3 \begin{pmatrix} \psi_0 \\ \mathrm{d}\psi_0/\mathrm{d}r \end{pmatrix}_{r\searrow \rho} = \begin{pmatrix} \psi_2 \\ \mathrm{d}\psi_2/\mathrm{d}r \end{pmatrix}_{r\searrow \rho} , \tag{7.7}$$

where $\Lambda\sigma_3 =: \Lambda_3$ is any real[3] matrix with determinant -1.

7.2 Solving the problem

Next, let us introduce notations for the negative and positive energy eigenfunctions of the differential operators H_L, which can be given in terms of the (spherical) Bessel (or Hankel) functions, and can be expressed with exact and compact formulas. For negative energies, a convenient choice for two linearly independent solutions is

$$\varphi_L^{(\mp)}(r) = \mp\sqrt{\kappa/2}\; r\; h_L^{(\mp)}\left(\frac{\kappa r}{i}\right) = \begin{cases} \frac{1}{\sqrt{2\kappa}} e^{\mp\kappa r} & (L=0) \\ \frac{1}{\sqrt{2\kappa}} \left[-\left(1 + \frac{3}{(\kappa r)^2}\right) \mp \frac{3}{\kappa r} \right] e^{\mp\kappa r} & (L=2) \end{cases} \tag{7.8}$$

(for our needs only the negative bound state energy $E = -E_{\rm D}$ and the corresponding $\kappa = \sqrt{2mE_{\rm D}/\hbar^2}$ — see Appendix E for their actual values — will be interesting). In parallel, for positive energies $E = k^2/(2m)$ a practical choice is

$$\chi_L^{(\mp)}(r) = i^{L+1} k r h_L^{(\mp)}(kr) = \begin{cases} \mp e^{\mp ikr} & (L=0) \\ \left[\mp\left(1 - \frac{3}{(kr)^2}\right) + \frac{3i}{kr} \right] e^{\mp ikr} & (L=2) . \end{cases} \tag{7.9}$$

[2]Real in the sense that the diagonal elements are real numbers while the offdiagonal ones are real but dimensionful quantities, with length (resp. inverse length) dimension.

[3]Again, up to dimensions.

We can observe that, for large r, the solutions in the two channels have identical asymptotic behaviour (in case of negative and positive energies both).

In addition to the known $E_{\rm D}$, we have another experimental input for our investigation, which is the mixing $\eta_{\rm D}$ of the two channels in the deuteron bound state. A first and naive approach to our problem could be that, for any possible value of the three free parameters in our connection condition, we numerically check whether the bound state arises with the required energy and mixing, and whether the scattering parameters are also satisfactorily reproduced or not. However, the numerical scanning of a three dimensional region is practically very tedious — as well as conceptually somewhat simple-minded. In the following method we will be able to directly express how the two bound state parameters restrict the three fitting parameters to one remaining free parameter. Thus only a one-dimensional scanning will be needed.[4]

The normalizable bound state eigenfunction can be written as the following composite two-row wave function:

$$\begin{pmatrix}\psi_0\\ \psi_2\end{pmatrix} = \begin{pmatrix}c_0\varphi_0^{(-)}\\ c_2\varphi_2^{(-)}\end{pmatrix} \tag{7.10}$$

(*i.e.,* containing only the decreasing solutions). We know that $\left|\frac{c_2}{c_0}\right| = \eta_{\rm D}$. According to our assumption, it has to satisfy the connection condition (7.7). Thus the connection condition will determine the ratio of c_1 and c_2. If we introduce the auxiliary matrices

$$W_L := \begin{pmatrix}\varphi_L^{(-)}(\rho) & \varphi_L^{(+)}(\rho)\\ \varphi_L^{(-)\prime}(\rho) & \varphi_L^{(+)\prime}(\rho)\end{pmatrix} \qquad (W_L \text{ real, } \det W_L = 1) \tag{7.11}$$

(prime means derivative) then

$$W_L \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}\varphi_L^{(-)}(\rho)\\ \varphi_L^{(-)\prime}(\rho)\end{pmatrix}, \tag{7.12}$$

and using the connection condition we can write

$$\begin{aligned} c_2\begin{pmatrix}1\\0\end{pmatrix} &= c_2 W_2^{-1}\begin{pmatrix}\varphi_2^{(-)}(\rho)\\ \varphi_2^{(-)\prime}(\rho)\end{pmatrix} = W_2^{-1}\begin{pmatrix}\psi_2(\rho)\\ \psi_2'(\rho)\end{pmatrix} = W_2^{-1}\Lambda_3\begin{pmatrix}\psi_0(\rho)\\ \psi_0'(\rho)\end{pmatrix} \\ &= c_0 W_2^{-1}\Lambda_3\begin{pmatrix}\varphi_0^{(-)}(\rho)\\ \varphi_0^{(-)\prime}(\rho)\end{pmatrix} = c_0 W_2^{-1}\Lambda_3 W_0\begin{pmatrix}1\\0\end{pmatrix}. \end{aligned} \tag{7.13}$$

Hence, the matrix $\Lambda_W = W_2^{-1}\Lambda_3 W_0$ (which is also real matrix with determinant -1) has $\binom{1}{0}$ as an eigenvector with eigenvalue $\frac{c_2}{c_0}$. Consequently, Λ_W is of the form

$$\begin{pmatrix}a & b\\ 0 & \frac{-1}{a}\end{pmatrix} \tag{7.14}$$

where a, b are real, and $\frac{c_2}{c_0} = a = \pm\eta_{\rm D}$, while b is unrestricted.

[4] If we are able to pick out a characteristic parameter in the scattering data as well then we may aspire to determine from it the last remaining free parameter as well. For example, the energy where δ_0 [see (7.25), (7.26)] becomes zero seems to be a good candidate.

Therefore, we learn that we can express the connection matrix Λ_3 in the form

$$\Lambda_3 = W_2 \Lambda_W W_0^{-1} = W_2 \begin{pmatrix} a & b \\ 0 & \frac{-1}{a} \end{pmatrix} W_0^{-1}\,, \tag{7.15}$$

containing now only one free parameter (b), plus a free sign (the sign of a). This is the form we will use subsequently, for the scattering state solutions.

According to the conventions for the S-matrix for two channels, the 0-incoming and the 2-incoming solutions must asymptotically ($r \to \infty$) behave as

$$\Phi_0^{\rm inc}(r) \approx \begin{pmatrix} -e^{-ikr} + S_{00} e^{ikr} \\ S_{20} e^{ikr} \end{pmatrix}, \qquad \Phi_2^{\rm inc}(r) \approx \begin{pmatrix} S_{02} e^{ikr} \\ -e^{-ikr} + S_{22} e^{ikr} \end{pmatrix} \tag{7.16}$$

(the minus sign preceding the incoming term comes from the general multiplier $(-1)^{L+1}$).[5] Therefore, the two incoming solutions are the following linear combinations of $\chi_L^{(\mp)}$:

$$\Phi_0^{\rm inc} = \begin{pmatrix} -\chi_0^{(-)} + S_{00}\chi_0^{(+)} \\ S_{20}\chi_2^{(+)} \end{pmatrix}, \qquad \Phi_2^{\rm inc}) = \begin{pmatrix} S_{02}\chi_0^{(+)} \\ -\chi_2^{(-)} + S_{22}\chi_2^{(+)} \end{pmatrix}. \tag{7.17}$$

It is again beneficial to introduce "the positive energy version of the matrices W_L",

$$\Omega_L := \begin{pmatrix} \chi_L^{(-)}(\rho) & \chi_L^{(+)}(\rho) \\ \chi_L^{(-)\prime}(\rho) & \chi_L^{(+)\prime}(\rho) \end{pmatrix}. \tag{7.18}$$

Then

$$\begin{pmatrix} \left(\Phi_0^{\rm inc}\right)_0(\rho) \\ \left(\Phi_0^{\rm inc}\right)_0'(\rho) \end{pmatrix} = \Omega_0 \begin{pmatrix} 1 \\ S_{00} \end{pmatrix}, \qquad \begin{pmatrix} \left(\Phi_0^{\rm inc}\right)_2(\rho) \\ \left(\Phi_0^{\rm inc}\right)_2'(\rho) \end{pmatrix} = \Omega_2 \begin{pmatrix} 0 \\ S_{20} \end{pmatrix},$$

$$\begin{pmatrix} \left(\Phi_2^{\rm inc}\right)_0(\rho) \\ \left(\Phi_2^{\rm inc}\right)_0'(\rho) \end{pmatrix} = \Omega_0 \begin{pmatrix} 0 \\ S_{02} \end{pmatrix}, \qquad \begin{pmatrix} \left(\Phi_2^{\rm inc}\right)_2(\rho) \\ \left(\Phi_2^{\rm inc}\right)_2'(\rho) \end{pmatrix} = \Omega_2 \begin{pmatrix} 1 \\ S_{22} \end{pmatrix}, \tag{7.19}$$

from which we derive

$$\begin{aligned} \begin{pmatrix} 0 \\ S_{20} \end{pmatrix} &= \Omega_2^{-1} W_2 \begin{pmatrix} a & b \\ 0 & \frac{-1}{a} \end{pmatrix} W_0^{-1} \Omega_0 \begin{pmatrix} 1 \\ S_{00} \end{pmatrix}, \\ \begin{pmatrix} 1 \\ S_{22} \end{pmatrix} &= \Omega_2^{-1} W_2 \begin{pmatrix} a & b \\ 0 & \frac{-1}{a} \end{pmatrix} W_0^{-1} \Omega_0 \begin{pmatrix} 0 \\ S_{02} \end{pmatrix}. \end{aligned} \tag{7.20}$$

With the notation

$$\Omega_2^{-1} W_2 \begin{pmatrix} a & b \\ 0 & \frac{-1}{a} \end{pmatrix} W_0^{-1} \Omega_0 =: T = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \tag{7.21}$$

(fulfilling $\det T = -1$), the solution of this linear system of equations for the S-matrix components is

$$S_{00} = -\frac{T_{11}}{T_{12}}\,, \quad S_{02} = \frac{1}{T_{12}}\,, \quad S_{20} = \frac{1}{T_{12}}\,, \quad S_{22} = -\frac{T_{22}}{T_{12}}\,. \tag{7.22}$$

[5] The order of the indices of S is according to the general convention $S_{\rm fi}$.

Explicitly, we find

$$
\begin{aligned}
T_{11} &= \frac{i}{4k^3\kappa^3\rho^3}\left\{\left[b(k^2+\kappa^2)e^{-2\kappa\rho} - a(k-i\kappa)^2\right](f_+ + g_+) - \frac{(k+i\kappa)^2}{a}(f_- + g_-)\right\}, \\
T_{12} &= \frac{i}{4k^3\kappa^3\rho^3}e^{2ik\rho}\left\{\left[b(k-i\kappa)^2e^{-2\kappa\rho} - a(k^2+\kappa^2)\right](f_+ + g_+) - \frac{(k^2+\kappa^2)}{a}(f_- + g_-)\right\}, \\
T_{21} &= \frac{i}{4k^3\kappa^3\rho^3}e^{-2ik\rho}\left\{\left[-b(k+i\kappa)^2e^{-2\kappa\rho} + a(k^2+\kappa^2)\right](f_+ - g_+) + \frac{(k^2+\kappa^2)}{a}(f_- - g_-)\right\}, \\
T_{22} &= \frac{i}{4k^3\kappa^3\rho^3}\left\{\left[-b(k^2+\kappa^2)e^{-2\kappa\rho} + a(k+i\kappa)^2\right](f_+ - g_+) + \frac{(k-i\kappa)^2}{a}(f_- - g_-)\right\}, \qquad (7.23)
\end{aligned}
$$

where

$$
\begin{aligned}
f_\pm &= \rho[3(k^2-\kappa^2) + k^2\kappa^2\rho^2] \pm 3\kappa(-1+k^2\rho^2), \\
g_\pm &= 3ik(1\pm\kappa\rho)^2 \qquad (7.24)
\end{aligned}
$$

The last step is to write the S-matrix in terms of the "nuclear bar" phase shifts [58] introduced by Stapp, which are the quantities depicted in [58] as experimental results:

$$
S = \begin{pmatrix} S_{00} & S_{02} \\ S_{20} & S_{22} \end{pmatrix} = \begin{pmatrix} \cos 2\varepsilon e^{2i\delta_0} & i\sin 2\varepsilon e^{i(\delta_0+\delta_2)} \\ i\sin 2\varepsilon e^{i(\delta_0+\delta_2)} & \cos 2\varepsilon e^{2i\delta_2} \end{pmatrix} \qquad (7.25)
$$

($S_{02} = S_{20}$ is actually a consequence of time reversal invariance). From S, these phases can be identified, *e.g.,* as

$$
\delta_0 = \arg(S_{00}/|S_{00}|)/2\,, \quad \delta_2 = \arg(S_{22}/|S_{22}|)/2\,, \quad \varepsilon = \arcsin(S_{02}/(ie^{i(\delta_0+\delta_2)}))/2\,. \qquad (7.26)
$$

Some ambiguities (uncertainties up to π) arise, which are allowed to be fixed to follow the conventions how they are plotted in [58].

Thus we have obtained the predictions of the model for the scattering phase shifts, as the function of the parameters ρ, b and the sign of a). For a comparison of the model with the experimentally measured phase shifts, see Fig. 7.1. The parameters used for the comparison are $b = 0$, the + sign for a, and $\rho = 0.56$ fm, the last value chosen to ensure that δ_0 becomes zero at the experimentally known energy value. The agreement is apparently quite good for this simple set of parameters, and may be improved further by tuning the parameters.

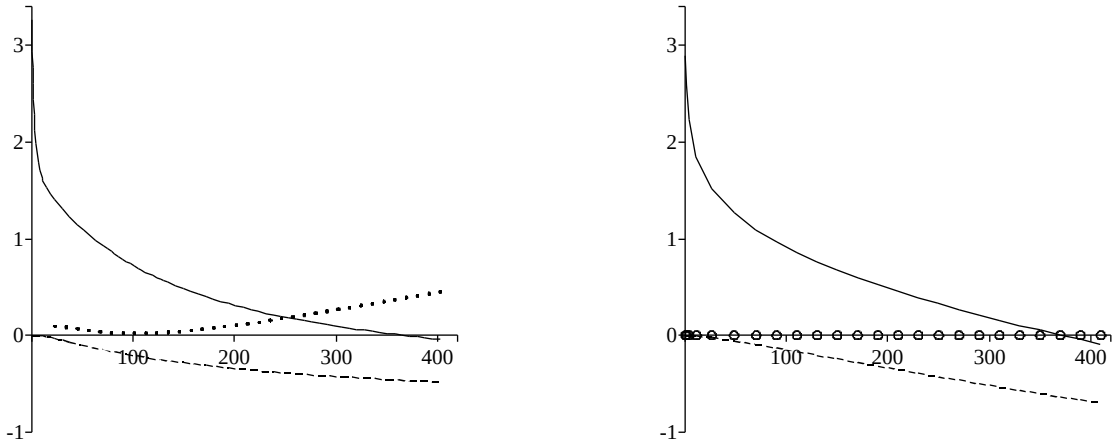

Figure 7.1: The proton-neutron scattering phase shifts for $S = 1\,,\ \ J = 1$ in the coupled channels $L = 0$ and $L = 2\,,$ as the function of the energy $E_{\rm LAB}$ (in MeV): δ_0 (solid line), δ_2 (dashed line) and ϵ (left: dotted line, right: circles). Left: experimental results reproduced from [58]. Right: the present model, at $a = +\eta_{\rm D}\,,\ \ b = 0$ and $\rho = 0.56$ fm.

Chapter 8

Conclusion

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.[1]

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

[1]To put it very simplified: life is much richer than only the Dirichlet boundary condition.

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.

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Appendix A

Mathematical background

This appendix contains the necessary mathematical definitions, theorems and notes, compiled from the references [20, 21, 22, 23, 59]. For further information, the Reader is asked to consult these sources.

Throughout this appendix, we will treat operators (linear maps) mapping from a subset of a separable Hilbert space $\mathcal{H}$ to $\mathcal{H}$. For the purposes of quantum mechanics, we will need to deal with unbounded symmetric operators, which cannot have the whole $\mathcal{H}$ as their domain of definition (Hellinger-Toeplitz theorem). We will assume the domains to be dense in $\mathcal{H}$. $\mathcal{D}(A)$ will denote the domain of an operator A. A and B will always denote densely defined operators. The scalar product on $\mathcal{H}$ is denoted by $(\cdot,\cdot)$.

A.1 Self-adjointness

Definition B is an *extension* of A if $\mathcal{D}(A) \subset \mathcal{D}(B)$ and $B|_{\mathcal{D}(A)} = A$. Notation: $A \subset B$.

Note The definition includes the trivial case $\mathcal{D}(A) = \mathcal{D}(B)$, $A = B$.

Definition The *adjoint* A^+ of A is defined on the domain $\mathcal{D}(A^+)$ which is the set of functions $\chi \in \mathcal{H}$ for which there is a $\widetilde{\chi} \in \mathcal{H}$ such that

$$(A\psi, \chi) = (\psi, \widetilde{\chi}) \qquad \text{for all} \quad \psi \in \mathcal{D}(A)\,; \tag{A.1}$$

and maps each such χ to the corresponding $\widetilde{\chi}$.

Note For χ, the corresponding $\widetilde{\chi}$ is uniquely determined, which is ensured by the denseness of $\mathcal{D}(A)$.

Note The adjoint always exists, but its domain may not be dense. It is even possible to have $\mathcal{D}(A^+) = \{0\}$.

Theorem $A \subset B$ implies $B^+ \subset A^+$.

Definition A is *symmetric* if $A \subset A^+$. Equivalently, A is symmetric if and only if

$$(A\psi, \chi) = (\psi, A\chi) \qquad \text{for all} \quad \psi, \chi \in \mathcal{D}(A)\,. \tag{A.2}$$

Definition A is *self-adjoint* if $A = A^+$, that is, if and only if A is symmetric and $\mathcal{D}(A) = \mathcal{D}(A^+)$.

Note We avoid to use the term *Hermitian* because different authors assign different meaning to it (some use them for symmetric operators and others for self-adjoint ones).

Definition A is *closed* if the ordered pairs of ψ and $A\psi$ form a closed subset in $\mathcal{H} \times \mathcal{H}$ as ψ takes all values in $\mathcal{D}(A)$. An operator is *closable* if it admits a closed extension. The smallest closed extension of a closable A is called its *closure* and is denoted by $\overline{A}$.

Theorem A symmetric A is always closable, and, as such, satisfies $A^{++} = \overline{A}$ and $(\overline{A})^+ = A^+$.

Definition A symmetric A is called *essentially self-adjoint* if $\overline{A}$ is self-adjoint.

Definition For a nonreal λ, the *deficiency subspaces* $\mathcal{E}_\lambda$ and $\mathcal{E}_{\lambda^*}$ are defined as the eigensubspace of A^+ with respect to the eigenvalue λ and the complex conjugate eigenvalue λ^*, respectively. The *deficiency indices* n_λ , n_{λ^*} are defined as the dimension of $\mathcal{E}_\lambda$, resp. $\mathcal{E}_{\lambda^*}$.

Definition A closed symmetric A is *maximal symmetric* if at least one of its deficiency indices is zero.

Theorem A closed symmetric A is self-adjoint if and only if both deficiency indices are zero.

Theorem A closed symmetric A admits self-adjoint extensions if and only if its deficiency indices are equal. With an arbitrarily fixed nonreal λ, the self-adjoint extensions of A are in a one-to-one correspondence with the unitary maps of $\mathcal{E}_\lambda$ to $\mathcal{E}_{\lambda^*}$. Each unitary $\mathcal{U} : \mathcal{E}_\lambda \to \mathcal{E}_{\lambda^*}$ assigns a self-adjoint domain

$$\mathcal{D}(A_\mathcal{U}) = \{\psi_0 + \psi_\lambda + \mathcal{U}\psi_\lambda \,|\, \psi_0 \in \mathcal{D}(A),\, \psi_\lambda \in \mathcal{E}_\lambda\}\,. \tag{A.3}$$

Note In an equivalent form, $\psi \in \mathcal{D}(A^+)$ belongs to the self-adjoint domain $\mathcal{D}(A_\mathcal{U})$ if and only if

$$\mathcal{U}P_\lambda\psi = \mathcal{P}_{\lambda^*}\psi\,, \tag{A.4}$$

where P_λ and $\mathcal{P}_{\lambda^*}$ are the projectors projecting into $\mathcal{E}_\lambda$ and $\mathcal{E}_{\lambda^*}$, respectively, in $\mathcal{H}$.

Note Denoting the equal deficiency indices of such an A by n, the family of all possible self-adjoint domains is an n^2-parameter $U(n)$ family.

Note This characterization of the self-adjoint extensions has been provided by Neumann.

Definition An antilinear map $C : \mathcal{H} \to \mathcal{H}$ [that is, satisfying $C(c_1\psi_1 + c_2\psi_2) = c_1^*\psi_1 + c_2^*\psi_2$] is a *conjugation* if it is norm-preserving and $C^2 = I_{\mathcal{H}}$ (the identity operator on $\mathcal{H}$).

Note Complex conjugation on an L^2 Hilbert space is an example for conjugation.

Theorem If a conjugation C maps the domain of a symmetric A into itself and commutes with A then A has equal deficiency indices.

Definition For an operator A, a *boundary value space* is a triple $(\mathcal{H}_{\text{boundary}}, \Gamma_1, \Gamma_2)$, where $\mathcal{H}_{\text{boundary}}$ is a Hilbert space with its scalar product denoted by $\langle \cdot, \cdot \rangle$ and Γ_1, Γ_2 are linear mappings of $\mathcal{D}(A^+)$ into $\mathcal{H}_{\text{boundary}}$, if

1) for any $\psi, \chi \in \mathcal{D}(A^+)$,
$$(A^+\psi, \chi) - (\psi, A^+\chi) = \langle \Gamma_1\psi, \Gamma_2\chi \rangle - \langle \Gamma_2\psi, \Gamma_1\chi \rangle ; \tag{A.5}$$

2) for any $\Psi_1, \Psi_2 \in \mathcal{H}_{\text{boundary}}$ there exists a $\psi \in \mathcal{D}(A^+)$ such that $\Gamma_1\psi = \Psi_1$, $\Gamma_2\psi = \Psi_2$.

Note With the notations $\Gamma^{(\pm)} := \Gamma_1 \pm i\Gamma_2$, the rhs of (A.5) reads
$$\frac{1}{2i}\left[\langle \Gamma^{(+)}\psi, \Gamma^{(+)}\chi \rangle - \langle \Gamma^{(-)}\psi, \Gamma^{(-)}\chi \rangle \right] , \tag{A.6}$$
and condition 2) is equivalent to that, for any $\Psi^{(+)}, \Psi^{(-)} \in \mathcal{H}_{\text{boundary}}$, there exists a $\psi \in \mathcal{D}(A^+)$ such that $\Gamma^{(+)}\psi = \Psi^{(+)}$, $\Gamma^{(-)}\psi = \Psi^{(-)}$.

Theorem A closed symmetric A with equal deficiency indices n always admits a boundary value space, with an n dimensional $\mathcal{H}_{\text{boundary}}$.

Note Indeed, a boundary value space is provided by the choice $\mathcal{H}_{\text{boundary}} = \mathcal{E}_\lambda$, $\Gamma^{(+)} = 2\sqrt{\text{Im}\lambda}\, P_\lambda$ and $\Gamma^{(-)} = 2\sqrt{\text{Im}\lambda}\, U_{\lambda,\lambda^*}\mathcal{P}_{\lambda^*}$, where U_{λ,λ^*} is an arbitrary unitary mapping of $\mathcal{E}_{\lambda^*}$ to $\mathcal{E}_\lambda$ and, without loss of generality, we have assumed $\text{Im}\lambda > 0$.

Note The name "boundary value space" of this abstract notion comes from that, in the important special case of differential operators, it can be chosen to be constructed from the boundary values (or the asymptotic boundary behaviours) of the square integrable functions and its derivatives.

Theorem The self-adjoint extensions of a closed symmetric A with equal deficiency indices are, for an arbitrarily fixed boundary value space $(\mathcal{H}_{\text{boundary}}, \Gamma_1, \Gamma_2)$, in a one-to-one correspondence with the unitary operators of $\mathcal{H}_{\text{boundary}}$. The self-adjoint domain $\mathcal{D}(A_U)$ corresponding to such a unitary U is formed by those $\psi \in \mathcal{D}(A^+)$ which satisfy
$$(U - I)\Gamma_1\psi + i(U + I)\Gamma_2\psi = 0 , \tag{A.7}$$
where I is the identity operator of $\mathcal{H}_{\text{boundary}}$.

Note An equivalent form of (A.7) is
$$U\,\Gamma^{(+)}\psi = \Gamma^{(-)}\psi . \tag{A.8}$$

Note This latter characterization of self-adjoint extensions, via a boundary value space, is presented, *e.g.,* in [59]. The unitary operator U in this description is in a one-to-one correspondence with $\mathcal{U}$ appearing in the Neumann approach. The mentioned example for boundary value space ($\mathcal{H}_{\text{boundary}} = \mathcal{E}_\lambda$, *etc.*) shows that Neumann's approach can be considered as a special case of the boundary value space characterization.

Note With appropriate modifications, the boundary value space approach is able to describe the maximal symmetric extensions of symmetric operators with unequal deficiency indices, too.

A.2 Application for ordinary differential operators (*i.e.,* on a one dimensional configuration space)

In this section, the question of self-adjoint domains of a differential operator H of the form

$$H\psi = -(p\psi')' + q\psi\,, \tag{A.9}$$

acting on appropriate square integrable functions $\psi \in L^2(a,b)$, is addressed. The one dimensional interval (a,b) may be finite or infinite. The functions p and q are required to be real, measurable in (a,b), and $1/|p|$, $|q|$ to be locally[1] Lebesgue-integrable. If a is finite and $1/|p|$, $|q|$ are integrable on a subinterval (a,c) then the endpoint a is called *regular,* and is *singular* otherwise. The other endpoint b is classified analogously.

In what follows, we will discuss the case of a regular a and a singular b. The other possibilities, as well as configuration spaces formed by more than one interval, can be treated by analogous means.

Definition A (real or complex) function f on a closed interval $[\alpha,\beta]$ is *absolutely continuous* if, for any positive ε, there is a positive δ so that

$$\sum_{k=1}^{n} |f(y_k) - f(x_k)| < \varepsilon \tag{A.10}$$

for every finite collection of disjoint intervals $[x_k, y_k]$ satisfying

$$\sum_{k=1}^{n} |y_k - x_k| < \delta\,. \tag{A.11}$$

Theorem If f is absolutely continuous on $[\alpha,\beta]$ then f is differentiable almost everywhere, $f' \in L^1[\alpha,\beta]$, and f is the indefinite integral of f'. Conversely, if $g \in L^1[\alpha,\beta]$ then its indefinite integral G is absolutely continuous, and $G' = g$ almost everywhere.

Note It is this property why absolutely continuous functions will play a distinguished role for the self-adjoint domains of ordinary differential operators. For partial differential

[1] *i.e.,* on every finite closed subinterval

operators, it is not some higher dimensional generalization of absolute continuity that can be used as a general concept to derive the self-adjoint domains. It is an alternative formulation, treating differentiation in the distributional sense and imposing some Sobolev space-like properties that admits a natural higher dimensional generalization.

Notation Let $\mathcal{D}_{\max}$ denote the class of those functions $\psi \in L^2(a,b)$ such that $\psi, p\psi'$ are locally absolutely continuous and $-(p\psi')' + q\psi \in L^2(a,b)$, and let $H_{\max}$ be the operator acting on this domain as (A.9).

Notation Let Ω denote the antisymmetric sesquilinear form

$$\Omega[\psi_1, \psi_2] = p(\psi_1^* \psi_2' - \psi_1^{*\prime} \psi_2)\,, \qquad \psi_1, \psi_2 \in \mathcal{D}_{\max}\,. \tag{A.12}$$

Theorem For any $\psi_1, \psi_2 \in \mathcal{D}_{\max}$, $\Omega[\psi_1, \psi_2](x)$ has a finite limit when x approaches either endpoint. In addition, when approaching the regular endpoint a, for any $\psi \in \mathcal{D}_{\max}$ both ψ and $p\psi'$ have a finite limit.

Notation Let $\mathcal{D}_{\min}$ denote the class of those functions $\psi \in \mathcal{D}_{\max}$ which, for any $\chi \in \mathcal{D}_{\max}$, satisfy

$$\lim_{x\to a} \Omega[\psi, \chi](x) = \lim_{x\to b} \Omega[\psi, \chi](x) = 0\,, \tag{A.13}$$

and let $H_{\min}$ be the corresponding restriction of $H_{\max}$.

Note For all these ψs, $\lim_{x\to a} \psi(x) = \lim_{x\to a}(p\psi')(x) = 0$.

Note $\mathcal{D}_{\min}$ is dense in $\mathcal{H}$, since it contains all functions with compact support.

Theorem $H_{\min}$ is symmetric and has equal deficiency indices.

Note For the first statement in this theorem, note that integration by parts yields

$$(H_{\max}\psi_1, \psi_2) - (\psi_1, H_{\max}\psi_2) = \Omega[\psi_1, \psi_2](b) - \Omega[\psi_1, \psi_2](a) \tag{A.14}$$

for any $\psi_1, \psi_2 \in \mathcal{D}_{\max}$, and the analogous formula holds for $H_{\min}$ within $\mathcal{D}_{\min}$. For the second statement, we can use the invariance of $H_{\min}$ under complex conjugation as a conjugation.

Theorem $H_{\min}$ is closed, and $H_{\min}^+ = H_{\max}$.

Note Neither that $\mathcal{D}(H_{\min}^+)$ is formed by such "smooth enough" functions as the ones in $\mathcal{D}_{\max}$ nor that $H_{\min}^+$ acts on them as the differential operator $H_{\max}$ is trivial.

Theorem The deficiency index of $H_{\min}$ is either 1 or 2. If it is 1 then $\lim_{x\to b} \Omega[\psi_1, \psi_2](x) = 0$ for all $\psi_1, \psi_2 \in \mathcal{D}_{\max}$. If it is 2 then any eigenfunction of (A.9) with any real eigenvalue is locally square integrable near b [that is, in an interval (c, b) with some finite c].

Note The first interesting fact here is that the deficiency index cannot be 0. It means that, approaching the singular endpoint, not all eigenfunctions of the eigenvalue problem of H in (A.9) for a nonreal eigenvalue "blow up", at least some behave square integrably.

The second is that if the deficiency index is 1 then the singular endpoint produces a zero surface term in (A.14) so it does not generate multiple self-adjoint extensions for $H_{\min}$. (The two endpoints really decouple in this respect, since it is only local square integrability that plays a role in this question.)

Note In the case of deficiency index 1, the singular endpoint is called a limit-point singularity, and in the other case, a limit-circle singularity. These names do not refer to some geometric aspect of the configuration space but are of technical origin. They express whether, in the complex plane, a disk — where a certain auxiliary quantity connected to this classification is nonpositive — contracts to one point or into a disk of nonzero radius, as x approaches the singular endpoint b.

Theorem Let $\chi^{(1)}, \chi^{(2)} \in \mathcal{D}_{\max}$ be real functions, with $\omega := \Omega[\chi^{(1)}, \chi^{(2)}]$ tending to a nonzero limit when approaching a limit-circle endpoint b. Then, for any $\psi_1, \psi_2 \in \mathcal{D}_{\max}$, we have

$$\Omega[\psi_1, \psi_2] = \frac{1}{\omega} \Big(\Omega[\chi^{(1)}, \psi_1]^* \, \Omega[\chi^{(2)}, \psi_2] - \Omega[\chi^{(2)}, \psi_1]^* \, \Omega[\chi^{(1)}, \psi_2] \Big) \tag{A.15}$$

at any x where $\omega(x) \neq 0$, and in the limit $x \to b$.

Note An example for such $\chi^{(1)}, \chi^{(2)}$ is

$$\chi^{(k)} := \varphi^{(k)} , \qquad k = 1, 2 , \tag{A.16}$$

where $\varphi^{(k)}$ are two linearly independent eigenfunctions of (A.9) for an arbitrary real eigenvalue. In this case, ω is constant. The eigenfunctions $\varphi^{(k)}$ are locally square integrable near the limit-circle endpoint b so they belong to $\mathcal{D}_{\max}$.

Note If a is also singular then a possible choice is

$$\chi^{(k)} := \eta \varphi^{(k)} , \qquad k = 1, 2 , \tag{A.17}$$

where $\varphi^{(k)}$ are as before, and η is a smooth function that is nonzero only in an interval (c_1, b) with some finite c_1 and is one in an interval (c_2, b) with $c_1 < c_2 < b$. Then, ω is constant in (c_2, b). The function η here is applied only to ensure global square integrability, and it can be ignored as long as we are interested in the limit $x \to b$ only.

Note The formula (A.15) makes it easy to set a boundary value space for $H_{\min}$. Although ψ and $p\psi'$ may diverge around b for $\psi \in \mathcal{D}_{\max}$, the limit numbers $\Omega[\chi^{(k)}, \psi](b)$ are finite and can be used to construct a boundary value space. Such limit numbers are naturally finite when approaching a regular endpoint a as well, but for a regular endpoint the finite limiting values of ψ and $p\psi'$ are the simplest and most natural candidates to be used for a boundary value space.

Note For a configuration space that consists of more than one interval, the generalization of these results is simple. From the practical aspect, (A.14) will contain just more surface terms, and those of these terms which are not identically zero (that is, those belonging to a limit-circle or regular endpoint) have to be taken into account when constructing the boundary value space.

Note We can see the advantage of the boundary space value approach over the Neumann one since, for the latter, generally we need to solve the eigenvalue problem for a nonreal eigenvalue. On the contrary, in the former characterization, we need to know only two real eigenfunctions to an arbitrary real eigenvalue (for example, 0), and, what's more (what's less), typically we need to know them only approximately (the leading and subleading asymptotic behaviour of them) so that the limiting values $\Omega[\chi^{(k)}, \psi](b)$ can be determined. (Actually, we need to know only one real eigenfunction because a linearly independent second one can be determined from that their ω must be constant.)

Note The literature provides various criteria to decide whether a singular endpoint is limit-point or limit-circle, without the need to investigate by hand the local square integrability of any eigenfunctions. Many criteria are also available about the qualitative properties of the spectra of the various possible self-adjoint extensions. The following theorem is just one such result to quote.

Theorem All self-adjoint extensions of an operator with equal and finite deficiency indices have the same continuous spectrum.

Note Partial differential operators, on more than one dimensional configuration spaces, are harder to treat than ordinary differential operators (as usual...). The separation of the variables may help us to reduce the problem to one dimensional ones, and then we can apply the one dimensional arsenal we have at hand.

Appendix B

Weak classical realization of the time delay for walls with negative L

Here, we outline how a weaker classical realization of the quantum time delay, namely, as the $x_0 \to \infty$ limit of the classical time delay $\tau_{\mathrm{cl},\,x_0}(E)$, can be determined for the walls $L < 0$. Let us assume that we have a strictly decreasing positive potential such that, for a fixed finite x_0 and all energies E above $V(x_0)$, $\tau_{\mathrm{cl},\,x_0}(E) = \tau(E)$. We use the 'Landau trick' again, dividing this equation by $\sqrt{W-E}$, integrating now between $V(x_0)$ and W, and evaluating the left hand side by changing the variable to V. From the result we can express $x(W)$ to find

$$x(W) = \frac{x_0}{\pi}\arccos\left[1-\frac{2V(x_0)}{W}\right] - \frac{2|L|/\pi}{\sqrt{1+\frac{2mL^2}{\hbar^2}W}}\arccos\sqrt{\frac{1+\frac{2mL^2}{\hbar^2}W}{1+\frac{2mL^2}{\hbar^2}V(x_0)}\frac{V(x_0)}{W}}\,. \tag{B.1}$$

Now we perform the limit $x_0 \to \infty$, with a fixed W. The second term on the rhs of (B.1) remains finite no matter how $V(x_0)$ changes correspondingly. Consequently, to have a finite $x(W)$ in the limit, $\arccos\left[1-\frac{2V(x_0)}{W}\right]$ has to tend to zero. This means $V(x_0) \to 0$, and from $\cos\varepsilon \approx 1-\frac{\varepsilon^2}{2}$ $(\varepsilon \approx 0)$ we have the asymptotics $\arccos\left[1-\frac{2V(x_0)}{W}\right] \approx 2\sqrt{\frac{V(x_0)}{W}}$ so to reach a finite limit of (B.1) $x_0\sqrt{V(x_0)}$ has to converge to a constant. Introducing

$$c := \lim_{x_0\to\infty} \tfrac{2\sqrt{2m}}{\pi\hbar}\, x_0\sqrt{V(x_0)}\,, \tag{B.2}$$

which will be a free parameter in the realizing potential, the limit of (B.1) is

$$x(W) = \tfrac{\hbar}{\sqrt{2m}}\left(c/\sqrt{W} \,-\, 1\Big/\sqrt{\tfrac{\hbar^2}{2mL^2}+W}\right). \tag{B.3}$$

One can check that the inverse of this $x(W)$ is really a strictly decreasing potential tending to zero if $c \geq 1$, and that the time delay corresponding to it is

$$\tau_{\mathrm{cl},\,x_0}(E) = \hbar\left[c\,\frac{\sqrt{1-\frac{V(x_0)}{E}}-1}{\sqrt{V(x_0)E}} + \frac{1}{\sqrt{\frac{\hbar^2}{2mL^2}+V(x_0)}}\left(\frac{1}{\sqrt{E}} - \frac{\sqrt{E-V(x_0)}}{\frac{\hbar^2}{2mL^2}+E}\right)\right], \tag{B.4}$$

whose $x_0 \to \infty$ limit is really the desired quantum time delay (3.40) (independently of c). The potential itself is obtained by solving the biquadratic equation that follows from (B.3), and reads, for example, for $c = 1$,

$$V(x) = \frac{2\hbar^2}{mL^2} \left(\frac{x}{|L|}\right)^{-\frac{2}{3}} \left[\left(\frac{x}{|L|}\right)^{\frac{2}{3}} + \eta(x)^{-1} + 2\sqrt{\eta(x) - \eta(x)^4}\right]^{-2} \tag{B.5}$$

with

$$\eta(x) = \frac{1}{\sqrt{2}} \left[\left(\sqrt{1 + \frac{1}{27}\left(\frac{x}{|L|}\right)^4} + 1\right)^{\frac{1}{3}} - \left(\sqrt{1 + \frac{1}{27}\left(\frac{x}{|L|}\right)^4} - 1\right)^{\frac{1}{3}}\right]^{\frac{1}{2}} . \tag{B.6}$$

Appendix C

Symmetries, dualities and other generalized symmetries for the line system

Here, the boundary transformations for the 'point interaction on a line' systems are introduced and investigated, in a systematic sequence of gradual technical mathematical steps.

C.1 On parity-type operators

Parity-type operator (on an arbitrary vector space $\mathcal{V}$): a $P : \mathcal{V} \to \mathcal{V}$ linear map such that $P^2 = \mathrm{id}_{\mathcal{V}}$ but $P \neq \pm\mathrm{id}_{\mathcal{V}}$.

In other words, an operator whose eigenvalues are $+1$ and -1.

$\mathcal{V} = \mathcal{V}_1 \oplus \mathcal{V}_2$, where $\mathcal{V}_1$ and $\mathcal{V}_2$ are the eigenspaces corresponding to the eigenvalues $+1$ and -1, respectively. Any $x \in \mathcal{V}$ can be decomposed uniquely as $x = x_1 + x_2 = \frac{1+P}{2}x + \frac{1-P}{2}x$.

C.2 On $U(2)$-matrices

Notations: In the sequel D and X are always diagonal matrices, Y is offdiagonal ($Y = \begin{pmatrix} 0 & Y_{12} \\ Y_{21} & 0 \end{pmatrix}$), P is parity-type, Z is parity-type and offdiagonal, V and T are $SU(2)$-matrices, U and W are $U(2)$-matrices, I is the identity matrix, σ_j are the Pauli matrices. U, D and V will always be in the relationship $U = VDV^{-1}$ with each other.
Further notations: Indices like j are $j = 1, 2$ or $j = 1, 2, 3$, always according to the sense.

$D = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix}$, $\tilde{D} = \begin{pmatrix} d_2 & 0 \\ 0 & d_1 \end{pmatrix}$, $X = \begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix}$, $W = \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix}$, $Uv_j = d_j v_j$ (for the eigenvalues and eigenvectors of U); $\sigma = c_j \sigma_j$ $(c_j c_j = 1)$ .The parametrization

$$W = e^{i\eta} \begin{pmatrix} \gamma & \delta \\ -\delta^* & \gamma^* \end{pmatrix} = e^{i\eta}(\gamma_{\mathrm{R}} I + i\delta_{\mathrm{I}}\sigma_1 + i\delta_{\mathrm{R}}\sigma_2 + i\gamma_{\mathrm{I}}\sigma_3)$$

of $U(2)$-matrices (with $\eta \in [0, \pi)$, $|\gamma|^2 + |\delta|^2 = 1$) will also be used.

Ds are of the form $e^{i\xi}e^{i\rho\sigma_3}$, where $\xi \in [0, \pi), \rho \in [0, 2\pi)$.

Ys are of the form $e^{i\tau}(\cos\omega\sigma_1 + \sin\omega\sigma_2)$, where $\tau \in [0, \pi)$, $\omega \in [0, 2\pi)$. $Y \in SU(2)$s are the ones $i(\cos\omega\sigma_1 + \sin\omega\sigma_2)$. Parity-type Ys are the ones $Z = \cos\omega\sigma_1 + \sin\omega\sigma_2$.

For conjugations WUW^{-1}s, TUT^{-1}s are enough, since $\det W$ drops out from WUW^{-1}.

In the diagonalization $U = VDV^{-1}$, D contains the eigenvalues of U, and V the corresponding eigenvectors. The first column of the matrix V is v_1, the other is v_2.

If $d_1 \neq d_2$ then WDW^{-1} is diagonal only if W is diagonal (in which case $WDW^{-1} = D$) or if W is offdiagonal (in which case $WDW^{-1} = \tilde{D}$).
Proof: For example, by computing directly the product

$$\begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix} \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix} \frac{1}{\det W} \begin{pmatrix} W_{22} & -W_{12} \\ -W_{21} & W_{11} \end{pmatrix}.$$

Corollaries: If $d_1 \neq d_2$ then:
1) The matrices commuting with U are the VXV^{-1} ones.
2) In the diagonalization $U = VDV^{-1}$, V is uncertain exactly up to $V' = VX$, if $D' = D$ is required. This corresponds to that v_1 obtains a phase factor x_1, and v_2 obtains a phase factor x_2. If we allow $D' = \tilde{D}$ as well, the further uncertainties are the $V' = VY$ ones. In these cases the columns v_j are interchanged as well.
3) The $W = VYV^{-1}$s are the ones with which $WUW^{-1} = V\tilde{D}V^{-1}$, in other words, which preserve V but flip D.

Only $W = wI$s commute with each $U \in U(2)$. (See Corollary 1 above.)

WUW^{-1} and U have the same eigenvalues.

All Us that have the same pair of eigenvalues can be connected by conjugation, $(\exists W)\, U' = WUW^{-1}$. As a special case, D and $\tilde{D}$ can be connected by the conjugations $\tilde{D} = YDY^{-1}$.

The Ws with diagonal W^2 are: the ones with $\gamma_{\mathrm{R}} = 0$, in other words, the $W = e^{i\eta}i\sigma$ ones (in which case $W^2 = \text{const.}\, I$), and the ones with $\delta = 0$, in other words, the $W = e^{i\eta}(\gamma_{\mathrm{R}} I + i\gamma_{\mathrm{I}}\sigma_3)$ ones.
Proof: For example, by computing the square of W directly, where W is written in the form with η, γ, δ.

As special cases, Ps are the σs.

Another aspect: Ps are the $T\sigma_3T^{-1}$s (since, in the diagonalization $P = TXT^{-1}$, X must be σ_3, as X carries the eigenvalues of P).

For example, a diagonalization of a Z is: $T = \frac{1}{\sqrt{2}}[\cos\frac{\omega}{2}I + i\sin\frac{\omega}{2}\sigma_1 - i\cos\frac{\omega}{2}\sigma_2 - i\sin\frac{\omega}{2}\sigma_3]$.

The matrices anticommuting with σ_3 are the Ys.
Proof: For example, by computing directly the product

$$\begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix} \sigma_3 \frac{1}{\det W} \begin{pmatrix} W_{22} & -W_{12} \\ -W_{21} & W_{11} \end{pmatrix} . \tag{C.1}$$

Corollary: The matrices anticommuting with a $V\sigma_3V^{-1}$ are the VYV^{-1} ones.

C.3 Boundary transformations and their properties

In the sequel, $\psi \in \mathcal{H}$ and $W \in U(2)$, however, the definition and most of the results below will be valid for arbitrary functions $\psi : \mathbb{R} \setminus \{0\} \to \mathbb{C}$ and matrices W (with $\det W \neq 0$).

$$\begin{aligned}(\mathcal{F}_W\psi)(x) &:= \begin{cases} W_{11}\psi(x) + W_{12}\psi(-x) & x > 0 \\ W_{21}\psi(-x) + W_{22}\psi(x) & x < 0 \end{cases} \\ &= W_{11}\psi_+(x) + W_{12}\psi_-(-x) + W_{21}\psi_+(-x) + W_{22}\psi_-(x)\,,\end{aligned} \tag{C.2}$$

where we have used the decomposition

$$\psi = \psi_+ + \psi_-\,, \qquad \psi_+(x) = \Theta(x)\psi(x)\,, \qquad \psi_-(x) = \Theta(-x)\psi(x)\,. \tag{C.3}$$

The $\mathcal{P}_j$s of the paper [12] are the cases $W = \sigma_j$.

$\mathcal{F}_{\lambda_1W_1+\lambda_2W_2} = \lambda_1\mathcal{F}_{W_1} + \lambda_2\mathcal{F}_{W_2} \qquad (\forall\lambda_1,\lambda_2 \in \mathbb{C})\,.$

$\mathcal{F}_{W_1W_2} = \mathcal{F}_{W_1}\mathcal{F}_{W_2}\,, \qquad \mathcal{F}_{W^{-1}} = \mathcal{F}_W^{-1}\,, \qquad \mathcal{F}_{W^+} = \mathcal{F}_W^+\,.$

$\mathcal{F}_W$ is unitary iff W is unitary.

Proposition: A w is an eigenvalue of $\mathcal{F}_W$ iff it is an eigenvalue of W. Further, if w is a nondegenerate eigenvalue of W then the corresponding eigenvector, $t = \begin{pmatrix} (t)_1 \\ (t)_2 \end{pmatrix}$, determines the form of the eigenfunctions of $\mathcal{F}_W$ belonging to the eigenvalue w, in the following way: The eigenfunctions are the $\psi(x) = (t)_1\psi_0(x) + (t)_2\psi_0(-x)$ ones where $\psi_0 \in \mathcal{H}$ is such an arbitrary function that is zero on the negative half line of $\mathbb{R}$.
Proof: $\mathcal{F}_W\psi = w\psi$ means the conditions

$$(\forall x > 0) \qquad W_{11}\psi_+(x) + W_{12}\psi_-(-x) = \psi_+(x)\,, \tag{C.4}$$

$$(\forall x<0)\qquad W_{21}\psi_+(-x)+W_{22}\psi_-(x)=\psi_-(x)\,. \tag{C.5}$$

In compact form,

$$(\forall y>0)\qquad \begin{pmatrix} W_{11} & W_{12}\\ W_{21} & W_{22}\end{pmatrix}\begin{pmatrix}\psi_+(y)\\ \psi_-(-y)\end{pmatrix}=w\begin{pmatrix}\psi_+(y)\\ \psi_-(-y)\end{pmatrix}\,. \tag{C.6}$$

There must exist such a y_0 for which $\begin{pmatrix}\psi_+(y_0)\\ \psi_-(-y_0)\end{pmatrix}\neq\begin{pmatrix}0\\0\end{pmatrix}$ (since an eigenfunction ψ cannot be the identically zero function) so we can see that w must be an eigenvalue of W and that $\begin{pmatrix}\psi_+(y_0)\\ \psi_-(-y_0)\end{pmatrix}$ must be a corresponding eigenvector of W.
If w is a nondegenerate eigenvalue of W then, denoting a corresponding normed eigenvector by t, $\begin{pmatrix}\psi_+(y_0)\\ \psi_-(-y_0)\end{pmatrix}=\text{const.}\,t$. For different y_0s this factor can be different: let us therefore denote it by $\psi_0(y_0)$. Let us extend the function ψ_0 for the ys where $\begin{pmatrix}\psi_+(y)\\ \psi_-(-y)\end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix}$ as well, in the way $\psi_0(y):=0$, ψ_0 becomes defined on the whole positive line. Let us extend it further, to the negative half line as well, in the way $\psi_0:=0$. Then we can write that $\psi(x)=(t)_1\psi_0(x)+(t)_2\psi_0(-x)\quad(\forall x)$. Since ψ is normalizable, ψ_0 is also normalizable. Remark: From ψ, ψ_0 can be determined as $\psi_0(x)=\Theta(x)[(t)_1^*\psi(x)+(t)_2^*\psi(-x)]$.

If W has two nondegenerate eigenvalues then the eigenfunctions of $\mathcal{F}_W$ corresponding to the eigenvalue w_1 (*i.e.,* the elements of the eigensubspace $\mathcal{H}_1$) are of the form $\psi_1(x)=(t_1)_1(\psi_1)_0(x)+(t_1)_2(\psi_1)_0(-x)$, and the eigenfunctions belonging to w_2 are $\psi_2(x)=(t_2)_1(\psi_2)_0(x)+(t_2)_2(\psi_2)_0(-x)$, where t_j $(j=1,2)$ are normed eigenvectors of W corresponding to w_j, in other words, the two columns of the matrix T in the diagonalization $W=T\begin{pmatrix}w_1&0\\0&w_2\end{pmatrix}T^{-1}$, $\quad T=\begin{pmatrix}t_1 & t_2\end{pmatrix}=\begin{pmatrix}(t_1)_1 & (t_2)_1\\ (t_1)_2 & (t_2)_2\end{pmatrix}$. $\mathcal{H}_1$ and $\mathcal{H}_2$ are orthogonal to each other (since $\mathcal{F}_W$ is unitary).

Proposition: The decomposition $\mathcal{H}=\mathcal{H}_1\oplus\mathcal{H}_2$ is, in concrete terms, $\psi=\psi_1+\psi_2$ $(\psi_j\in\mathcal{H}_j)$, where the $(\psi_j)_0$s belonging to the ψ_js are

$$\begin{pmatrix}(\psi_1)_0(x)\\ (\psi_2)_0(x)\end{pmatrix}=\Theta(x)\,T^{-1}\begin{pmatrix}\psi(x)\\ \psi(-x)\end{pmatrix}\,.$$

Proof: Let us observe that the decomposition $\psi=\psi_1+\psi_2$ is equivalent to the equation

$$(\forall y>0)\qquad \begin{pmatrix}\psi_+(y)\\ \psi_-(-y)\end{pmatrix}=\begin{pmatrix}(t_1)_1(\psi_1)_0(y)+(t_2)_1(\psi_2)_0(y)\\ (t_1)_2(\psi_1)_0(y)+(t_2)_2(\psi_2)_0(y)\end{pmatrix}=T\begin{pmatrix}(\psi_1)_0(y)\\ (\psi_2)_0(y)\end{pmatrix}\,. \tag{C.7}$$

Multiplying this equation by T^{-1} we reach the stated result.

If the eigenvalues of W coincide then $W=wI$, and therefore $\mathcal{F}_W=w\mathrm{id}_{\mathcal{H}}$. In this case any function is the eigenfunction of $\mathcal{F}_W$. (No $\mathcal{H}_1$ and $\mathcal{H}_2$ in this case.)

The parity-type $\mathcal{F}_W$s are the ones $\mathcal{F}_{T\sigma_3T^{-1}}$, in other words, the $\mathcal{F}_\sigma$s.

All $\mathcal{F}_{VXV^{-1}}$s commute with each other. Further, their eigensubspaces $\mathcal{H}_1$, $\mathcal{H}_2$ are the same (since the V determining them is the same). Among the $\mathcal{F}_{VXV^{-1}}$s, the ones with

$X = \pm\sigma_3$ take the eigenvalue 1 on one of $\mathcal{H}_1$ and $\mathcal{H}_2$, and take the eigenvalue -1 on the other.

The generalized symmetries (see the definition below in section 4) mapping $\mathcal{H}_1$ (of a fixed V) to $\mathcal{H}_2$ and mapping $\mathcal{H}_2$ to $\mathcal{H}_1$ are the ones that flip the eigenvalue of an arbitrary $\psi \in \mathcal{H}_j$ taken under the operator $\mathcal{F}_{V\sigma_3 V^{-1}}$ from 1 to -1 and vice versa.

In other words, the ones that anticommute with $\mathcal{F}_{V\sigma_3 V^{-1}}$.

In other words, the $\mathcal{F}_W$s mapping $\mathcal{H}_1$ to $\mathcal{H}_2$ and vice versa are the ones with $W = VYV^{-1}$.

C.4 Definition of some important maps within the family Ω

Notation: $\mathcal{X}$ is always a unitary or antiunitary $\mathcal{H} \to \mathcal{H}$ operator.

$\mathcal{X}$ is a *generalized symmetry of* U if there exists such a $U_{\mathcal{X}} \in U(2)$ that $\mathcal{X} H_U \mathcal{X}^{-1} = H_{U_{\mathcal{X}}}$.

Remark: Here $U_{\mathcal{X}}$ is necessarily unique, since the different self-adjoint extensions of H are indexed by the Us in a one-to-one way.

$\mathcal{X}$ is a *generalized symmetry of* Ω if it is a generalized symmetry of all $U \in U(2)$.

$\mathcal{X}$ is a *symmetry of* U if $U_{\mathcal{X}} = U$.

$\mathcal{X}$ is a *symmetry of* Ω if it is a symmetry of all $U \in U(2)$.

$\mathcal{X}$ is a *trivial* generalized symmetry of U if it is a symmetry of it; *nontrivial* if not.

$\mathcal{X}$ is a *trivial* generalized symmetry of Ω if it is a symmetry of it; *nontrivial* if not, *i.e.,* if there exists such a U that $U_{\mathcal{X}} \neq U$.

$\mathcal{X}$ is a *trivial* symmetry of U, as well as of Ω, if $\mathcal{X} = \text{const.}\, \mathrm{id}_{\mathcal{H}}$.

$\mathcal{X}$ is a *duality transformation of* U if it is such a nontrivial generalized symmetry of it that $(U_{\mathcal{X}})_{\mathcal{X}} = U$.

$\mathcal{X}$ is a *duality transformation of* Ω if it is such a nontrivial symmetry of it that $(U_{\mathcal{X}})_{\mathcal{X}} = U$ $(\forall U \in U(2))$. In other words, if $(U_{\mathcal{X}})_{\mathcal{X}} = U$ for all U but $\exists U$ that $U_{\mathcal{X}} \neq U$.

C.5 The role of boundary transformations in the family Ω

If ψ satisfies the boundary condition corresponding to U then $\mathcal{F}_W\psi$ satisfies the boundary condition corresponding to $U_{\mathcal{F}_W} = WUW^{-1}$. Some possible names for $\mathcal{F}_W$s: boundary transformations, boundary condition transformations, boundary conjugations.

Remark: If we are interested only in $U_{\mathcal{F}_W} = WUW^{-1}$ but not $\mathcal{F}_W$ directly, it is enough to use $W \in SU(2)$s only.

$\mathcal{F}_W H_U \mathcal{F}_W^{-1}$ remains a differential operator.

Putting the two things together, $\mathcal{F}_W$s are generalized symmetries, with $U_{\mathcal{F}_W} = WUW^{-1}$.

$\mathcal{F}_W$ is a nontrivial generalized symmetry of Ω if $W \neq wI$, while it is a trivial symmetry of it if $W = wI$.

If the eigenvalues of U coincide then all $\mathcal{F}_W$s are symmetries of U.

If the eigenvalues of U differ then the $\mathcal{F}_W$-type symmetries of U are the ones with $W = VXV^{-1}$. These symmetries actually depend on V only but not on D. Among these symmetries the parity-type ones are those with $X = \pm\sigma_3$.

If the eigenvalues of U coincide then U has no $\mathcal{F}_W$-type duality transformations, all the $\mathcal{F}_W$-type duality transformations of Ω leave such an U invariant. These Us are called the *self-dual* Us.

If the eigenvalues of U differ then the $\mathcal{F}_W$-type duality transformations of U are the ones with $W = Ve^{i\eta}i\sigma V^{-1}$, where $\sigma \neq \pm\sigma_3$. These also do not depend on D but on V only. The square of any duality transformation of this kind is of the form $\text{const.}\,\mathrm{id}_{\mathcal{H}}$.
Proof: Introducing $W' := V^{-1}WV$, the requirement is that $(W')^2$ has to commute with D, therefore, that it has to be diagonal. However, W' itself must not commute with D, therefore, W' must not be diagonal.

The $\mathcal{F}_W$s anticommuting with $\mathcal{F}_{V\sigma_3V^{-1}}$ are the ones with $W = VYV^{-1}$.

Remark: These are just the $\mathcal{F}_W$s that flip D (to $\tilde{D}$) but preserve V (in other words, the ones doing $VDV^{-1} \mapsto V\tilde{D}V^{-1}$).

The $\mathcal{F}_W$-type duality transformations of U anticommuting with $\mathcal{F}_{V\sigma_3V^{-1}}$ (the so-called *strict duality transformations*) are the ones with $W = VZV^{-1}$.

$U = VDV^{-1}$ and $U' = V'D'(V')^{-1}$ can be connected by an $\mathcal{F}_W$ (*i.e.,* $(\exists W)\ U' = U_{\mathcal{F}_W}$), if $D' = D$ or $D' = \tilde{D}$ (*e.g.,* with $W = V'V^{-1}$, respectively with $W = V'V^{-1}Y$), and cannot be connected by an $\mathcal{F}_W$ otherwise.

C.6 Application for the spectral properties of H_Us

If U and U' have the same pair of eigenvalues then H_U and $H_{U'}$ have the same spectrum, since they can be connected by a generalized symmetry (by an $\mathcal{F}_W$-type one).

The spectrum of H_Us belonging to the same $\Omega(D)$ are the same.

Us having different pairs of eigenvalues cannot be connected by $\mathcal{F}_W$s.

In general, different $\Omega(D)$s correspond to different elements of Σ.

Conjecture: Not always. For example, systems with negative L_+ and L_- are expected to be connected to the free system by an appropriate generalized symmetry. Also, *e.g.,* systems with the same positive L_+ but different negative L_- are expected to be connected, too.

However, those appropriate generalized symmetries will not be $\mathcal{F}_W$-type.

If the eigenvalues of U differ then a nondegenerate eigenfunction of H_U is either in $\mathcal{H}_1$ or $\mathcal{H}_2$, where the $\mathcal{H}_j$s are the ones belonging to V.

Conjecture: In case of degenerate eigenfunctions, one of them can be chosen to be in $\mathcal{H}_1$ and the other in $\mathcal{H}_2$.

If the eigenvalues of U differ then the $\mathcal{F}_W$-type duality transformations that map $\mathcal{H}_1$ (of V) to $\mathcal{H}_2$ and vice versa are the ones with $W = VZV^{-1}$. (The strict ones.)

The duality transformation found earlier (*e.g.,* in [10], in the parity invariant subfamily) is the special case $V = \frac{i}{\sqrt{2}}(\sigma_1 + \sigma_3)$, $Z = \sigma_1$. (In which case $v_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$, $v_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$, $\omega = 0$.)

If the eigenvalues of U coincide then U has noncommuting $\mathcal{F}_W$-type symmetries (belonging to noncommuting Ws), even such ones as well that $[\mathcal{F}_{W_1}, \mathcal{F}_{W_2}]$ is an injective map, *i.e.,* it maps any nonzero ψ to a nonzero ψ'. Example: the $W_j = \sigma_j$s. Thus in this case the eigenvalues of H_U are degenerate: even if an eigenfunction ψ of H_U is an eigenfunction of $\mathcal{F}_{W_1}$, it cannot be an eigenfunction of a $\mathcal{F}_{W_2}$ noncommuting with $\mathcal{F}_{W_1}$. Therefore, either $\mathcal{F}_{W_1}$ or $\mathcal{F}_{W_2}$ will map ψ to a ψ' that is linearly independent of ψ. However, ψ' is also in the same eigensubspace of H_U as ψ is in, hence this subspace is more than one dimensional.

Appendix D

Point interaction on a circle: spectra and the scale independent subfamily

D.1 The family of distinct spectra

To prove that a spectrum uniquely determines ξ, α_{R} and β_{I}, first we study the dependence of the spectrum on these parameters. When doing this, it is useful to recall that $\xi \in [0, \pi)$, and $\alpha_{\mathrm{R}}^2 + \beta_{\mathrm{I}}^2 \leq 1$.

To start with, if $\xi = \beta_{\mathrm{I}} = 0$ (let us call this case 'case I') then the positive energies satisfy

$$[(1 - \alpha_{\mathrm{R}}) + (1 + \alpha_{\mathrm{R}})(kL_0)^2] \sin kl = 0\,. \tag{D.1}$$

Since $|\alpha_{\mathrm{R}}| \leq 1$, $1 - \alpha_{\mathrm{R}}$ and $1 + \alpha_{\mathrm{R}}$ are non-negative, and only one of them can be zero, therefore $[(1-\alpha_{\mathrm{R}})+(1+\alpha_{\mathrm{R}})(kL_0)^2]$ is always positive. Consequently, the positive energies fulfil $\sin kl = 0$, with the solutions $k_n = \frac{\pi}{l} n$, $n = 1, 2, \ldots$

If at least one of ξ and β_{I} is nonzero then let us first consider the subcase $\alpha_{\mathrm{R}} = -\cos\xi$ (called 'case II'). Here, $\sin\xi \neq 0$, since $\sin\xi = 0 \Rightarrow \xi = 0 \Rightarrow \alpha_{\mathrm{R}} = -1 \Rightarrow \beta_{\mathrm{I}} = 0$, and this case is now excluded. Thus we can write (5.8) in the form

$$\frac{\beta_{\mathrm{I}}}{\sin\xi} + \cos kl + \frac{\cot\xi}{kL_0} \sin kl = 0\,. \tag{D.2}$$

On the left hand side, if $k \to \infty$ then the third term tends to zero so $\frac{\beta_{\mathrm{I}}}{\sin\xi} + \cos kl \to 0$, $\cos kl \to -\frac{\beta_{\mathrm{I}}}{\sin\xi}$. This means that the large roots k will get closer and closer to the values of the form $\frac{1}{l}(\arccos\frac{-\beta_{\mathrm{I}}}{\sin\xi} + 2\pi n)$, respectively, $\frac{1}{l}(-\arccos\frac{-\beta_{\mathrm{I}}}{\sin\xi} + 2\pi n)$, in an alternating sequence.

In the remaining case — *i.e.,* when $\alpha_{\mathrm{R}} \neq -\cos\xi$ and at least one of ξ and β_{I} is nonzero 'case III') — (5.8) can be written as

$$\frac{a_1}{kl} + \frac{a_2}{kl}\cos kl + \left[\frac{a_3}{(kl)^2} + 1\right] \sin kl = 0\,, \tag{D.3}$$

with

$$a_1 = \frac{2\beta_{\mathrm{I}}}{\cos\xi + \alpha_{\mathrm{R}}} \frac{l}{L_0}\,, \qquad a_2 = \frac{2\sin\xi}{\cos\xi + \alpha_{\mathrm{R}}} \frac{l}{L_0}\,, \qquad a_3 = \frac{\cos\xi - \alpha_{\mathrm{R}}}{\cos\xi + \alpha_{\mathrm{R}}} \left(\frac{l}{L_0}\right)^2 . \tag{D.4}$$

If $k \to \infty$ then the terms proportional to a_1, a_2 and a_3 tend to zero so $\sin kl \to 0$. Now the large roots k are getting closer and closer to the values of the form $\frac{\pi}{l}n$, $n = 1, 2, \ldots$.

Now we will determine more details about the asymptotic behaviour of the roots k. For this reason, we make the following Ansatz:

$$k_n l = \pi n + \varepsilon_n\,, \qquad \text{where} \qquad \varepsilon_n = \frac{c_1}{n} + \frac{c_2}{n^2} + \frac{c_3}{n^3} + \cdots . \tag{D.5}$$

The coefficients c_i can be determined iteratively from (D.3). For our purposes the first three coefficients will be the interesting ones. To be up to this order, it is enough to use the formulae

$$\cos k_n l = \cos(\pi n)\cos\varepsilon_n = (-1)^n[1 - \frac{1}{2}\varepsilon_n^2] + \mathcal{O}\left(\varepsilon_n^4\right)\,, \tag{D.6}$$

$$\sin k_n l = \cos(\pi n)\sin\varepsilon_n = (-1)^n[\varepsilon_n - \frac{1}{6}\varepsilon_n^3] + \mathcal{O}\left(\varepsilon_n^5\right)\,, \tag{D.7}$$

$$(k_n l)^2 = \pi^2 n^2 + 2\pi c_1 + \mathcal{O}\left(\frac{1}{n}\right)\,, \tag{D.8}$$

$$\varepsilon_n^2 = \frac{c_1^2}{n^2} + \mathcal{O}\left(\frac{1}{n^3}\right) \qquad\qquad \varepsilon_n^3 = \frac{c_1^3}{n^3} + \mathcal{O}\left(\frac{1}{n^4}\right)\,. \tag{D.9}$$

Inserting these into the condition (D.3) multiplied, for convenience, by $(kl)^2$, and grouping the terms as decreasing powers of n, the vanishing of the coefficients of n^1, n^0 and n^{-1} lead to

$$c_1 = -\frac{1}{\pi}[(-1)^n a_1 + a_2]\,, \qquad c_2 = 0\,, \qquad c_3 = \frac{-c_1}{\pi^2}a_3 + \frac{c_1^2}{6\pi}(c_1 + 3a_2 - 6)\,, \tag{D.10}$$

respectively. We can see that there is a sequence $c_1^{(+)}, c_2^{(+)}, c_3^{(+)}, \ldots$ for even ns, and another sequence $c_1^{(-)}, c_2^{(-)}, c_3^{(-)}, \ldots$ for odd ns. Note that at least one of a_1 and a_2 is nonzero, because $\xi = \beta_{\mathrm{I}} = 0$ is now excluded. Therefore, at least one of $c_1^{(+)}$ and $c_1^{(-)}$ is nonzero. Thus in case III the roots do not *exactly* fulfil $\sin kl = 0$, they are only getting closer and closer to it, $\sin kl$ only *tends to* zero.

In the possession of this collected knowledge, we can turn to the inverse problem we wish to solve, *i.e.,* to identify the parameters ξ, α_{R} and β_{I} from a given spectrum.

If all the positive energies satisfy $\sin kl = 0$ *exactly* then we can know that we are in case I. This determines ξ and β_{I} (namely, $\xi = \beta_{\mathrm{I}} = 0$) but α_{R} is yet unknown. Let us see whether the possible zero and negative energies determine α_{R}. The condition for a zero energy state (5.10) reads in this case simply $\alpha_{\mathrm{R}} = 1$. Therefore, if the spectrum contains a zero energy state then $\alpha_{\mathrm{R}} = 1$. If not, then let us see the possibility for negative energies: (5.9) is now

$$[(1 - \alpha_{\mathrm{R}}) - (1 + \alpha_{\mathrm{R}})(\kappa L_0)^2]\sinh\kappa l = 0\,, \tag{D.11}$$

which gives that there exists one negative energy state with

$$\kappa = \frac{1}{L_0}\sqrt{\frac{1-\alpha_{\rm R}}{1+\alpha_{\rm R}}} \tag{D.12}$$

if $\alpha_{\rm R} \neq -1$ and no negative energy state if $\alpha_{\rm R} = -1$. Consequently, from the absence of negative energy states we learn $\alpha_{\rm R} = -1$, and from one negative energy state with κ we can identify $\alpha_{\rm R}$ as

$$\alpha_{\rm R} = \frac{1-(\kappa L_0)^2}{1+(\kappa L_0)^2}\,. \tag{D.13}$$

If we see that $\cos kl$ tends to a definite value as k increases then we know that we face at case II [since in case I $\cos kl$ oscillates between 1 and -1, and in case III $\cos(k_{n=2j}l) \to 1$ and $\cos(k_{n=2j+1}l) \to -1$]. From $\lim(\cos kl)$ we obtain $\beta_{\rm I}/\sin\xi$, and then, from (D.2), using any root k from the known spectrum for which $\sin kl \neq 0$, we determine $\cot\xi$, which uniquely tells ξ.

In the end, if we find that the positive spectrum is such that the values of $\sin kl$ tend to zero but are not exactly zero then we know we are in case III. For large enough ks we can determine which integer n belongs to a k (by rounding kl/π to the nearest integer). Then, we can identify the coefficients $c_1^{(+)}$ and $c_3^{(+)}$ as

$$c_1^{(+)} = \lim_{\substack{n\to\infty,\\ n\,\text{even}}} n(k_n l - \pi n)\,, \qquad c_3^{(+)} = \lim_{\substack{n\to\infty,\\ n\,\text{even}}} n^3\left[k_n l - \pi n - \frac{c_1^{(+)}}{n}\right], \tag{D.14}$$

and $c_1^{(-)}$ and $c_3^{(-)}$ in a similar way. From $c_1^{(+)}$ and $c_1^{(-)}$ we can obtain a_1 and a_2 [cf. (D.10)] as

$$a_1 = -\frac{\pi}{2}\left[c_1^{(+)} - c_1^{(-)}\right], \qquad a_2 = -\frac{\pi}{2}\left[c_1^{(+)} + c_1^{(-)}\right], \tag{D.15}$$

and then, corresponding to that which of $c_1^{(+)}$ and $c_1^{(-)}$ is nonzero — we know that at least one of them is nonzero —, a_3 can be determined from $c_3^{(+)}$ or $c_3^{(-)}$, respectively [cf. (D.10)].

From a_1, a_2 and a_3 the parameters ξ, $\alpha_{\rm R}$ and $\beta_{\rm I}$ are calculated as follows [all steps will be based on (D.4)]. If $a_3 = -(l/L_0)^2$ then $\cos\xi = 0 \quad\Rightarrow\quad \xi = \pi/2$, and $\alpha_{\rm R} = 2/[(L_0/l)a_2]$ and $\beta_{\rm I} = a_1/a_2$. If $a_3 \neq -(l/L_0)^2$ then, observing that

$$\frac{(L_0/l)\,a_2}{1+(L_0/l)^2 a_3} = \tan\xi, \tag{D.16}$$

ξ is determined uniquely. Then, we have

$$\alpha_{\rm R} = \frac{1-(L_0/l)^2 a_3}{1+(L_0/l)^2 a_3}\cos\xi\,, \qquad \beta_{\rm I} = \frac{a_1}{a_2}\sin\xi\,. \tag{D.17}$$

We can summarize the above considerations with that the spectrum of a circle system uniquely determines its parameters ξ, $\alpha_{\rm R}$ and $\beta_{\rm I}$.

D.2 The scale independent boundary conditions

On dimensional grounds, the coefficients A, B in the eigenfunctions (5.3) will be k-independent if L_0 actually drops out from the boundary conditions expressed by (5.1). This happens if both lines of the matrix equation (5.1) — or, two appropriate linear combinations of them — contain only one of the two boundary value vectors Ψ, Ψ'.

First, suppose that neither of the rows of the matrices $U-I$ and $U+I$ are identically zero. Then an appropriate linear combination of the two lines of (5.1) is needed to drop Ψ out from, say, the first line. In this case, any other linear combination will leave some Ψ in the second line so the goal of another linear combination will be to drop Ψ' out from the second line. This is possible only if both matrices $U-I$ and $U+I$ are such that their first row is a multiple of their second row. Then we have

$$\det(U-I)=\det(U+I)=0\,, \tag{D.18}$$

which tells that the two eigenvalues of U are ±1. Therefore, $U=P_+-P_-$, where P_+ is the projector projecting onto the eigensubspace of U corresponding to the eigenvalue 1, and P_- projecting onto the other eigensubspace. From this we see that U is self-adjoint, and this property leads to the requirements $\xi=\frac{\pi}{2}$, $\alpha_{\rm R}=0$.

Second, if some of the rows of $U-I$ and $U+I$ are identically zero then first we observe that this can happen to at most two of the four rows in question: Otherwise at least one of the matrices $U-I$, $U+I$ would be zero, but then the other one should be $\pm2I$, which has only nonzero rows. Now, if two rows of the four are zero then it is easy to see that one of these rows must be an upper row and the other a lower row (the difference of $U+I$ and $U-I$ is $2I$, which makes the other cases impossible). This means four possibilities, the matrices $U=\begin{pmatrix}\pm1 & 0\\ 0 & \pm1\end{pmatrix}$, which give the two isolated scale independent systems $U=\pm I$ (the two other cases, $U=\pm\sigma_3$, are included in the Us with $\xi=\frac{\pi}{2}$, $\alpha_{\rm R}=0$). At last, if one of the four rows is zero — say, a row of $U-I$ —, then one of the two lines of (5.1) is already Ψ independent. The other line will then necessarily contain Ψ so, to make it Ψ' independent, a suitable multiple of the Ψ independent line has to be added to it. This means that the two rows of $U+I$ has to be each other's multiple, consequently, $\det(U+I)=0$. However, $U-I$ has a zero row so $\det(U-I)=0$, too. Thus we arrive again back to (D.18), and hence to $\xi=\frac{\pi}{2}$, $\alpha_{\rm R}=0$.

Appendix E

Constants used in the treatment of the proton-neutron system

We have found that $\text{fm} = 10^{-15}$ m and MeV are convenient units for length, respectively energy, quantities in this problem.

Masses:

$$\begin{aligned} m_{\text{p}} &= 938.272 \text{ MeV}/c^2 \qquad \text{(source: [60])}, \\ m_{\text{n}} &= 938.565 \text{ MeV}/c^2 \qquad \text{(source: [61])}, \qquad \text{(E.1)} \\ m &= 2m_{\text{p}}m_{\text{n}}/(m_{\text{p}} + m_{\text{n}}) = 938.918 \text{ MeV}/c^2 \,; \qquad \text{(E.2)} \end{aligned}$$

Fundamental constants:

$$\begin{aligned} c &= 299792458 \text{ m/s} \qquad \text{(source: [60])}, \\ \hbar &= 6.582119 \times 10^{-22} \text{ MeVs} \qquad \text{(source: [60])}; \qquad \text{(E.3)} \end{aligned}$$

Deuteron constants:

$$\begin{aligned} E_{\text{D}} &= 2.2246 \text{ MeV} \qquad \text{(source: [62])}, \\ \kappa &= \sqrt{2mE_{\text{D}}/\hbar^2} = .327543 \text{ fm}^{-1} \,; \qquad \text{(E.4)} \\ \eta_{\text{D}} &= \lim_{r\to\infty} \left| \frac{\psi_2}{\psi_0}(r) \right| = 0.0256 \pm 0.0004 \qquad \text{(source: [63])}. \end{aligned}$$

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