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Dynamical algebras for Pöschl–Teller Hamiltonian hierarchies

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ABSTRACT

The dynamical algebras of the trigonometric and hyperbolic symmetric Pöschl–Teller Hamiltonian hierarchies are obtained. A kind of discrete–differential realizations of these algebras are found which are isomorphic to $so(3,2)$ Lie algebras. In order to get them, first the relation between ladder and factor operators is investigated. In particular, the action of the ladder operators on normalized eigenfunctions is found explicitly. Then, the whole dynamical algebras are generated in a straightforward way.

1. Introduction

An important class of solvable one-dimensional quantum systems is obtained by means of the factorization method. Indeed, Dirac [1] and Schrödinger [2] already applied it at the beginning of quantum mechanics. The basics of the method and the factorization types can be found for instance in [3], or for a deeper insight in the classical paper by Infeld and Hull [4]. A feature of the method is that the discrete spectrum and eigenfunctions of the factorizable Hamiltonians can be obtained algebraically in terms of the operators (here called "factor operators") that enter in the factorization of such Hamiltonians. However, these factor operators that link different Hamiltonians, giving rise to a hierarchy, are not the only ones. In some cases one can define lowering and raising operators (called "ladder operators") for each Hamiltonian in the hierarchy. These ladder operators are used in many contexts: to construct coherent states [5–7], to find matrix elements of some operators [8], to describe the spectrum of many physical systems like neutrons and anyons in magnetic fields [9–11], or simply to understand the underlying algebra of the full Hamiltonian hierarchy [12]. The factor operators close the so called potential algebra, and the ladder operators generate the spectrum generating algebra. If we combine both types of operators we can get a larger algebra that we call the dynamical algebra of the hierarchy (another dynamical algebras have been considered, see for instance in [13]).

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On the quantization of sectorially Hamiltonian dissipative systems

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A B S T R A C T

We present a theoretical discussion showing that, although some dissipative systems may have a sectorial Hamiltonian description, this description does not allow for canonical quantization. However, a quantum Liouville counterpart of these systems is possible, although it is not unique.

1. Introduction

In a recent paper [1], we have shown that on phase space, one-dimensional systems satisfying an equation of motion of the form $\ddot{x} + F(x, \dot{x}) = 0$ is sectorially Hamiltonian. This means that the phase space can be divided into disjoint sectors such that the behavior of this dissipative system can be obtained from a Hamiltonian function defined in each sector. These sectors may change with a change of variables, but this fact is not essential in our discussion. The methods we presented in [1] were valid for one-dimensional systems on the configuration space, or two-dimensional on phase space. However, these methods could not be extended in general for more dimensions because they were based on the existence of integrating factors for some Pfaffian equations. This investigation had its origin in a previous paper of our group in which the existence of local constants of motion for the Sinai billiard was investigated [2].

The next step in our research should be double. On one side, we should investigate if these results can be extended to arbitrary dimensions without making use of integrating factor, which restricts the number of cases in which our results can be valid.

On the other side, we should investigate when these type of systems admit quantization. This paper is one step in this direction. Previous studies have been dealt with the quantization of the one-dimensional oscillator with friction [3,4]. More recently, the problem of quantizing dissipative systems have been studied in [5,6].

A rather recent work [7] shows that the proper framework for canonical quantization of dissipative systems could be the Liouvillian formulation of quantum mechanics. In the present paper, we show that this idea is initially correct, although quantization in the Liouville space should not be unique.

This paper is organized as follows: In Section 2, we show that sectorially defined Hamiltonians do not admit in general canonical quantization, since this eventual quantization does not lead to self adjoint Hamiltonians. In Section 3, we give a rigorous argument on why this quantization should be possible on the Liouville formulation of quantum mechanics and why we do not expect uniqueness.

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Quantum infinite square well with an oscillating wall

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ABSTRACT

A linear matrix equation is considered for determining the time dependent wave function for a particle in a one-dimensional infinite square well having one moving wall. By a truncation approximation, whose validity is checked in the exactly solvable case of a linearly contracting wall, we examine the cases of a simple harmonically oscillating wall and a non-harmonically oscillating wall for which the defining parameters can be varied. For the latter case, we examine in closer detail the dependence on the frequency changes, and we find three regimes: an adiabatic behaviour for low frequencies, a periodic one for high frequencies, and a chaotic behaviour for an intermediate range of frequencies.

1. Introduction

Solution of the Schrödinger equation subject to moving boundary conditions has been studied for many years and a small number of exactly solvable cases, in one spatial dimension, are known [1–11]. The simplest of these describes a particle in an infinite square well with one wall moving at constant speed. For the most part, the other solved cases are found by starting from the Schrödinger equation for a harmonic oscillator with a time-dependent "frequency". By transforming the spatial coordinate to eliminate the wall motion, new time-dependent terms are introduced into the potential. By selecting the wall motion suitably, one can cancel inconvenient terms and end up with a solvable problem. A supersymmetry approach has recently been proposed to extend the list of solvable cases [12].

One situation which apparently cannot be studied in this way is the so-called quantum Fermi accelerator: an infinite square well with one oscillating wall. In 1949, Fermi [13] suggested that cosmic ray protons might have been accelerated to high energy by colliding with moving galactic magnetic fields. He proposed no specific model, but merely provided some estimates based on contemporary data. It appears to have been Ulam [14] who modeled this as a classical particle in a square well with a moving wall. His numerical studies displayed both regular and stochastic motion and the model has been popular in chaos studies. The quantum mechanical version soon emerged in the area of quantum chaos. In 1986, José and Cordery [15] formulated the solution to the Schrödinger equation for sawtooth motion of the moving wall and examined the statistical features of the energy spectrum. This was followed in 1990 by Seba's work [16] on the absolute continuity of the spectrum. In these papers, dealing with a saw-tooth profile, the particle is subject to a periodic sequence of force discontinuities and subsequently this version of the model was shown to be equivalent to the periodically kicked rotator and many aspects of its dynamics have been investigated (several references are provided in [17]).

Our aim in this article is to examine features of the wave function and the variation of the energy when the particle is initially in a given instantaneous eigenstate. We assume that the wall oscillates smoothly. The paper is organized as follows: in Section 2 the theoretical foundations are presented, in Section 3 some examples are developed, paying especial attention to the change in the frequency of the oscillations of the wall, and finally, Section 4 ends the paper with some conclusions.

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Travelling wave solutions of the generalized Benjamin–Bona–Mahony equation

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Abstract

A class of particular travelling wave solutions of the generalized Benjamin–Bona–Mahony equation is studied systematically using the factorization technique. Then, the general travelling wave solutions of Benjamin–Bona–Mahony equation, and of its modified version, are also recovered.

1. Introduction

The generalized Benjamin–Bona–Mahony (BBM) equation has a higher order nonlinearity of the form

$$u_t + u_x + au^n u_x + u_{xxt} = 0, \quad n \geqslant 1, \tag{1}$$

where a is constant. The case $n = 1$ corresponds to the BBM equation, which was first proposed in 1972 by Benjamin et al. [1]. This equation is an alternative to the Korteweg–de Vries (KdV) equation, and describes the unidirectional propagation of small-amplitude long waves on the surface of water in a channel. The BBM equation is not only convenient for shallow water waves but also for hydromagnetic and acoustic waves, and therefore it has some advantages compared with the KdV equation. When $n = 2$, Eq. (1) is called the modified BBM equation. When looking for travelling wave solutions, the BBM and modified BBM equations can be reduced to ordinary differential equations that possess the Painlevé property and which are integrable in terms of elliptic functions [2,3]. The generalized BBM equation is also integrable in terms of elliptic functions, provided that some restrictions on the parameters are imposed. Recently many methods have been presented to obtain the travelling wave solutions of the generalized BBM equation: the tanh–sech [4,5] and the sine–cosine methods [4–6], an approach based on balancing principle to obtain some explicit solutions in terms of elliptic function [7], and an extended algebraic method with symbolic computation [8]. These techniques are presently very popular in the analysis of other related equations, like the KP-BBM and the ZK-BBM equations [9–11].

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Supertwistors, massive superparticles and κ-symmetry

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Abstract: We consider a $D = 4$ two-twistor lagrangian for a massive particle that incorporates the mass-shell condition in an algebraic way, and extend it to a two-supertwistor model with $N = 2$ supersymmetry and central charge identified with the mass. In the purely supertwistorial picture the two $D = 4$ supertwistors are coupled through a Wess-Zumino term in their fermionic sector. We demonstrate how the κ-gauge symmetry appears in the purely supertwistorial formulation and reduces by half the fermionic degrees of freedom of the two supertwistors; a formulation of the model in terms of κ-invariant degrees of freedom is also obtained. We show that the κ-invariant supertwistor coordinates can be obtained by dimensional (D=6→D=4) reduction from a $D = 6$ supertwistor. We derive as well by 6→4 reduction the $N = 2$, D=4 massive superparticle model with Wess-Zumino term introduced in 1982. Finally, we comment on general superparticle models constructed with more than two supertwistors.

Keywords: p-branes, Extended Supersymmetry, Superspaces.

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Exchange energy density in density-functional theory via the Dirac density matrix for a nonrelativistic 10-electron atomic ion compared with Becke's proposal for a gradient-corrected local-density-approximation result

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Especially in atomic systems, it is now well established that exchange energy generally dominates correlation effects. Therefore we focus here on the exchange energy density $\varepsilon_x(r)$ as given in terms of the idempotent Dirac density matrix. This is then brought into contact with the one-parameter form of Becke's functional, which corrects the local-density-approximation form $-c_x[n(r)]^{4/3}$ with $n(r)$ as the ground-state electron density, $c_x=(3/4)e^2(3/\pi)^{1/3}$, by terms involving the dimensionless gradient ratio $|\nabla n(r)|/n^{4/3}(r)$. A particular nonrelativistic model of the 10-electron Ne-like atomic ions, with large atomic number Z, is then compared to Becke's approximation to $\varepsilon_x(r)$.

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I. BACKGROUND

It is now well established for neutral atoms that the exchange energy generally dominates, numerically, the correlation contribution [1]. Therefore there has been lately a resurgence of interest in the exchange energy E_x and the corresponding exchange potential $V_x(\boldsymbol{r})$ in density-functional theory (DFT).

A notable contribution in the above context is that of Della Sala and Görling [2], referred to here as DG who, on the basis of the somewhat drastic assumption that the Hartree-Fock determinant equaled its Kohn-Sham counterpart, derived an integral equation for the exchange potential $V_x(\boldsymbol{r})$. Howard and March [3] subsequently gave a formally exact generalization of the DG result, but it involved a function they denoted by $P(\boldsymbol{r})$, for which only the sum rule

$$\int P(\boldsymbol{r})d\boldsymbol{r}=0 \tag{1}$$

is known.

II. EXCHANGE ENERGY IN TERMS OF THE IDEMPOTENT DIRAC DENSITY MATRIX

In terms of the Slater-Kohn-Sham (SKS) [4,5] orbitals $\psi_i(\boldsymbol{r})$ of DFT, one defines the ground-state Dirac density matrix $\gamma(\boldsymbol{r},\boldsymbol{r}')$ as [6]

$$\gamma(\boldsymbol{r},\boldsymbol{r}')=\sum_{\text{occ}}\psi_i^*(\boldsymbol{r})\psi_i(\boldsymbol{r}'), \tag{2}$$

which is clearly related to the (formally exact) ground-state electron density $n(\boldsymbol{r})$ by

$$n(\boldsymbol{r})=\gamma(\boldsymbol{r},\boldsymbol{r}')|_{r=r'}. \tag{3}$$

Then, as was first written by Dirac [6], the total exchange energy, E_x say, is given by

$$E_x=-\frac{e^2}{4}\int\frac{[\gamma(\boldsymbol{r},\boldsymbol{r}')]^2}{|\boldsymbol{r}-\boldsymbol{r}'|}d\boldsymbol{r}d\boldsymbol{r}'. \tag{4}$$

Below, we shall focus most attention on the exchange energy density, denoted by $\varepsilon_x(\boldsymbol{r})$. Although its definition is not unique, all choices must clearly satisfy the relation

$$E_x=\int\varepsilon_x(\boldsymbol{r})d\boldsymbol{r}. \tag{5}$$

The most natural choice for exchange energy density is then, from Eqs. (4) and (5), given by

$$\varepsilon_x(\boldsymbol{r})=-(e^2/4)\int\frac{|\gamma(\boldsymbol{r},\boldsymbol{r}')|^2}{|\boldsymbol{r}-\boldsymbol{r}'|}d\boldsymbol{r}', \tag{6}$$

which Slater [4] adopted (also see Kleinman [7]). We will mainly use this in the present paper; however, in Appendix A an alternative form is given which can be shown to be a functional of the electron density $n(r)$.

Let us consider now a 10-electron "atomic ion" model in the nonrelativistic limit of large nuclear charge. The exchange energy density $\varepsilon_x(\boldsymbol{r})$ in exact analytical form for an atomic model studied by Howard *et al.* [8] will be exten-

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Poisson–Hopf limit of quantum algebras

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Abstract
The Poisson–Hopf analogue of an arbitrary quantum algebra $U_z(g)$ is constructed by introducing a one-parameter family of quantizations $U_{z,\hbar}(g)$ depending explicitly on $\hbar$ and by taking the appropriate $\hbar \to 0$ limit. The q-Poisson analogues of the $su(2)$ algebra are discussed and the novel $su_q^{\mathcal{P}}(3)$ case is introduced. The q–Serre relations are also extended to the Poisson limit. This approach opens the perspective for possible applications of higher rank q-deformed Hopf algebras in semiclassical contexts.

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1. Introduction

Quantum groups were initially introduced as quantizations of Poisson–Lie groups associated with certain solutions of the classical Yang–Baxter equation. In this context, the deformation parameters were taken as $q = e^z$, where z is the constant that governs the noncommutativity of the algebra of observables given by the quantum group entries, and quantum algebras were obtained as the Hopf algebra dual of quantum groups (for a detailed discussion, see [1–5] and references therein). In the case of the transition from classical to quantum physical models, the deformation parameter z was interpreted as the Planck constant $\hbar$.

However, in more general contexts z is a parameter whose geometric/physical meaning has to be elucidated for each particular case. In fact, quantum groups and quantum algebras were soon considered as 'abstract' Hopf algebras (being both noncommutative and non-co-commutative) in order to explore whether these new objects can be considered as new symmetries of some physically relevant systems. The keystone of this approach was the discovery of the $su_q(2)$ invariance of the Heisenberg spin XXZ chain [6, 7], that was followed by a number of results exploiting quantum algebra symmetries in two-dimensional models [8]. Indeed, in the XXZ chain the 'quantum' deformation parameter q is clearly identified

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A delta well with a mass jump

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Abstract

In this paper, it is shown that a one-dimensional Hamiltonian with an attractive delta potential at the origin plus a mass jump at the same point cannot have a bound state, as is the case with the ordinary attractive delta potential with constant mass, unless another term is added into the potential in the form of a derivative of the Dirac delta at the origin. The consistency of this singular potential with two terms is guaranteed by choosing suitable matching conditions at the singular point for the wavefunctions. Furthermore, it is proved that the self-adjointness of the Hamiltonian with both singular interactions determines the coefficient of the derivative of the delta in a unique manner. Under these conditions, the bound state and its energy are obtained and it is checked that the correct results in the limit of equal masses are obtained.

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1. Introduction

The consideration of Hamiltonians with variable mass in non-relativistic quantum mechanics is an old problem that has recently attracted a lot of attention [1]. When the mass is not a constant, but depends on the position, $m(x)$, it has to be considered as a position-dependent operator not commuting with the momentum operator p. Therefore, the kinetic term K of the Hamiltonian cannot be written in the usual way, being the most generally accepted form of $H = K + V$ [2]:

$$H = K + V = \tfrac{1}{2}\, m^{\alpha}(x)\, p\, m^{\beta}(x)\, p\, m^{\alpha}(x) + V(x), \tag{1}$$

with $2\alpha + \beta = -1$. Note that the usual form of the kinetic energy is recovered for constant mass.

Physical systems with an abrupt discontinuity of the mass at one point are modeling the behavior of a quantum particle, i.e. an electron, moving in a media formed up by two different materials. On each of the materials the particle behaves as if it had a different mass. The

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Exact analytic solutions for a Dirac electron moving in graphene under magnetic fields

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Abstract
Exact analytical solutions for the bound states of a graphene Dirac electron in various magnetic fields with translational symmetry are obtained. In order to solve the time-independent Dirac–Weyl equation the factorization method used in supersymmetric quantum mechanics is adapted to this problem. The behavior of the discrete spectrum, probability and current densities are discussed.

1. Introduction

The discovery of graphene [1, 2], a two-dimensional layer of graphite, and the massless Dirac character of the low energy electrons moving has attracted much interest in physics due to its important electronic properties. In particular, it is a scenario where some fundamental aspects of relativistic quantum mechanics can be addressed, such as the Klein–Gordon paradox or the anomalous Landau–Hall effect [2, 3]. Also, graphene is an appropriate material to develop electronic devices. Recently a series of studies concerning the interaction of graphene electrons in perpendicular magnetic fields (sometimes including electrostatic fields parallel to the layer surface) have been carried out in order to find a way for confining the charges [4–12]. In these works the Dirac–Weyl equation for massless electrons with a Fermi velocity v_F is considered, where a minimal coupling with the vector potential describes the interaction with the external field. In general, some kinds of numerical computation were needed to find the energy levels of confined states or transmission coefficients for scattering states.

In this paper our interest is to consider interactions under perpendicular magnetic fields invariant under translations in one direction, and at the same time allowing for exact analytical solutions of the Dirac–Weyl equation. In order to achieve this goal we will adapt the factorization method and the techniques of supersymmetric quantum mechanics (SUSY-QM) to this situation [13–18]. This will allow us to gather here a number of problems where the results can be easily discussed, and at the same time we can interpret them in light of other situations previously considered in the literature. Let us mention that some SUSY-QM methods have been applied to graphene to obtain the exact and numerical solutions of Dirac electron Hamiltonians [19, 20] and also to describe the quantum Hall effect [21–23].

The organization of this paper is as follows. In section 2 we introduce the factorization method in the framework of the Dirac–Weyl equation for a massless electron in a magnetic field. Section 3 supplies a list of cases that can be solved using this method and with some figures describing basic properties. We end with some comments on the obtained results in section 4.

2. The Dirac–Weyl equation and SUSY partner Hamiltonians

In graphene a Dirac electron moves with an effective Fermi velocity $v_F = c/300$, where c is the velocity of light, and behaves as a massless quasi-particle. The effective Hamiltonian around a Dirac point for a Dirac electron has the form [2]

$$H = v_F(\boldsymbol{\sigma} \cdot \mathbf{p}), \tag{2.1}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are the Pauli matrices and $\mathbf{p} = -i\hbar(\partial_x, \partial_y)$ is the two-dimensional momentum operator. The

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A one-dimensional model of resonances with a delta barrier and mass jump

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ABSTRACT

In this Letter, we present a one-dimensional model that includes a hard core at the origin, a Dirac delta barrier at a point in the positive semiaxis and a mass jump at the same point. We study the effect of this mass jump in the behavior of the resonances of the model. We obtain an infinite number of resonances for this situation, showing that for the case of a mass jump the imaginary part of the resonance poles tend to a fixed value depending on the quotient of masses, and demonstrate that none of these resonances is degenerated.

1. Introduction

The concept of resonance plays a central role in Quantum Mechanics and therefore, for this reason, it is important the search for models with resonances. Some of them are based on the Friedrichs model [1] and its variants [2,3]. In addition to be exactly solvable, the Friedrichs model has the most important and basic features for the description of resonance phenomena. A second type of solvable models are those one-dimensional with a hard core at the origin. This means that the potential is infinite on the negative semiaxis. These models often come from a Hamiltonian with a spherically symmetric potential, when restricted to $\ell = 0$. On the other hand, Hamiltonians with singular potentials has been recently the object of study [4–7]. Combining both fields of research, the authors of a recent paper [8] study the resonances produced by a one-dimensional Hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0(x) + \gamma\delta(x-a), \quad \gamma > 0,\ a > 0, \tag{1}$$

with

$$V_0(x) := \begin{cases} \infty & \text{if } x \leqslant 0, \\ 0 & \text{if } x > 0. \end{cases} \tag{2}$$

In this model, the existence of an infinite number of resonances is shown. The study [8] is made by using the Krein formula that relates Green functions for potentials that are extensions of the same symmetric operator with identical deficiency indices [5]. Complex poles of the Green function are often associated to resonances. However, although the Krein formula gives precise results, it is not quite familiar to physicists. Instead, a calculation of resonances based in the idea of *purely outgoing boundary conditions* is more familiar to physicists and the eventual complexity in the equations giving the resonances is facilitated by the use of packages like Mathematica.

Resonances of physical systems can be of different types, depending on the character of the poles of the associated S matrix. Usually, the interest is centered around its simple poles, but not exclusively. Indeed, the search for systems with resonances from multiple poles of the S matrix has been initiated by Mondragón and coworkers [9]. These poles lead to degenerate resonances, for which the exponential decay on time is multiplied by a polynomial on time [3,9]. It is shown in [9] that if we replace in (1) the term $\gamma\delta(x-a)$ by $\gamma_1\delta(x-a)+\gamma_2\delta(x-b)$, with $\gamma_{1,2} > 0$, $b > a$, and these constants are suitably chosen, a double pole arise in the analytic continuation of the S matrix. This justifies the interest for the theoretical search of degenerated resonances. We show that in the

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Bound states and scattering coefficients of the $-a\delta(x)+b\delta'(x)$ potential

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ABSTRACT

We show that a one-dimensional Schrödinger equation in which the potential is a delta well plus a δ' interaction at the same point has a bound state, and we obtain the energy of this bound state in terms of the parameters. In addition, the expression of the reflection and transmission coefficients is also fully determined.

The goal of the present communication is to analyze the one-dimensional quantum Hamiltonian

$$H=\frac{p^2}{2m}-a\delta(x)+b\delta'(x),\quad a>0,\ b\in\mathbb{R}, \tag{1}$$

showing that (i) it has a unique bound state, whose energy will be given in terms of a and b, and (ii) its reflection and transmission coefficients can be also determined explicitly for any (positive) energy.

This model is very well known when $b=0$, a case that appears as a nice toy model in many textbooks [1]. Indeed, it is known that for $b=0$, the Hamiltonian in (1) is self-adjoint in a domain D of continuous functions $\psi(x)$ such that $\psi'(0+)-\psi'(0-)=ma\psi(0)$, where $\psi'(0+)$ and $\psi'(0-)$ are respectively the right and left limits of $\psi'(x)$ at the origin [2,3], and in this case it can be easily checked that H has a bound state of energy $E=-\frac{1}{2}ma^2$, with $\hbar=1$. In addition, the Dirac delta potential has been also used together with background potentials, for example in [4] combined with a constant electric field to illustrate a model for resonances.

Nevertheless, to our knowledge, the general case considered in Eq. (1) does not seem to have been treated before in the literature. As we will see, its solution is not complicated at all but it has many interesting features which deserves a careful attention. Actually, there is some controversy on the meaning of the $\delta'(x)$ potential [5], as different regularizations produce different reflection and transmission coefficients [6–8]. In our treatment for $V(x)=-a\delta(x)+b\delta'(x)$, and hence for the particular case $a=0$, $b=1$, we have followed the general approach proposed by Kurasov and coworkers [3,9,10]. This has the clear advantage that the definitions for the singular potentials depend on matching conditions at the origin and not on the choice of a particular regularization.

First of all, let us remark that the domain of self adjointness of H in (1) has been well established in [3]. This is the subspace of functions $\psi(x)$ satisfying the following matching conditions at the origin[1]:

$$\begin{pmatrix}\psi(0+)\\ \psi'(0+)\end{pmatrix}=\begin{pmatrix}\frac{1+mb}{1-mb} & 0\\ \frac{-2am}{1-m^2b^2} & \frac{1-mb}{1+mb}\end{pmatrix}\begin{pmatrix}\psi(0-)\\ \psi'(0-)\end{pmatrix}, \tag{2}$$

where $\psi(0+)$, $\psi(0-)$, $\psi'(0+)$ and $\psi'(0-)$ are the right and left limits at the origin of the function $\psi(x)$ and its first derivative, respectively. Therefore, possible bound states of H in (1) must fulfill these matching conditions at the origin.

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[1] For the sake of mathematical rigor, it must be said that the wave functions $\psi(x)$ must belong to the Sobolev space $W_2^2(\mathbb{R}/\{0\})$ of continuous functions (except for a finite jump at the origin) from $\mathbb{R}$ into $\mathbb{C}$ such that: (i) any $f\in W_2^2(\mathbb{R}/\{0\})$ admits a first continuous derivative (except at the origin), (ii) the second derivative exists almost everywhere, and (iii) both $f\in W_2^2(\mathbb{R}/\{0\})$ and its second derivative are a.e. square integrable, so that

$$\int_{-\infty}^{\infty}\left\{\left|f(x)\right|^2+\left|f''(x)\right|^2\right\}dx<\infty.$$

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Bloch equation for the canonical density matrix in terms of its diagonal element: The Slater sum

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ABSTRACT

In early work, March and Murray (MM) solved the Bloch equation for the canonical density matrix generated by a given potential $V(\mathbf{r})$ using perturbation theory to all orders in V, the unperturbed problem being that of free homogeneous electrons. Here, we avoid perturbation theory by using, but now in one dimension, the MM differential equation for the so-called Slater sum $S(x,\beta)$ for given $V(x)$, to write the Bloch equation for $C(x,x',\beta)$ in terms of its diagonal element $C(x,x',\beta)|_{x'=x} = S(x,\beta)$, where $\beta = (k_B T)^{-1}$. In the language of the Feynman propagator, $\beta \to it$ where t is the time, and this propagator is then characterized solely by its diagonal element in one dimension. The connection with ground-state density functional theory is finally emphasized.

1. Introduction

In an early study, March and Murray (MM) [1,2] used the Bloch equation for the canonical density matrix $C(\mathbf{r},\mathbf{r}',\beta)$ generated by a given one-body potential $V(\mathbf{r})$ to generate C to all orders in powers of V, the unperturbed wave functions being plane waves. MM also solved the one-dimensional analogue $C(x,x',\beta)$ to obtain its diagonal element $S(x,\beta)$ defined by

$$S(x,\beta) = C(x,x',\beta)|_{x'=x}, \tag{1}$$

where

$$C(x,x',\beta) = \sum_i \psi_i^*(x)\psi_i(x')\exp(-\beta\epsilon_i). \tag{2}$$

Here, $\psi_i(x)$ and ϵ_i are wave functions and corresponding eigenvalues generated by the given $V(x)$ potential inserted in the Schrödinger equation. In Eq. (2) $\beta = (k_B T)^{-1}$.

The 'kinetic energy per unit length' $t_L(x,\beta)$ is defined from the canonical density matrix $C(x,x',\beta)$ as

$$t_L(x,\beta) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}C(x,x',\beta)\bigg|_{x'=x}. \tag{3}$$

As summarized by March and Howard [3], following [1], the Slater sum $S(x,\beta)$ itself satisfies the following differential equation into which the input is the chosen potential $V(x)$:

$$\frac{\hbar^2}{8m}\frac{\partial^3 S(x,\beta)}{\partial x^3} = \frac{\partial^2 S(x,\beta)}{\partial x \partial \beta} + V(x)\frac{\partial S(x,\beta)}{\partial x} + \frac{1}{2}\frac{dV(x)}{dx}S(x,\beta). \tag{4}$$

We shall utilize Eq. (4) below as a first-order linear differential equation for $V(x)$, given the Slater sum $S(x,\beta)$ as an input.

To complete the introduction, we note that the Bloch equation for $C(\mathbf{r},\mathbf{r}',\beta)$ reads [4]

$$H_{\mathbf{r}}C(\mathbf{r},\mathbf{r}',\beta) = -\frac{\partial C(\mathbf{r},\mathbf{r}',\beta)}{\partial \beta}, \tag{5}$$

where the Hamiltonian $H_{\mathbf{r}}$ is given by

$$H_{\mathbf{r}} = -\frac{\hbar^2}{2m}\nabla_{\mathbf{r}}^2 + V(\mathbf{r}). \tag{6}$$

Below, our considerations are restricted to the one-dimensional analogue of Eq. (6) with potential $V(x)$ appearing in Eq. (4).

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