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An algebraic method to solve the radial Schrödinger equation

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ABSTRACT

We propose a method of numerical integration of differential equations of the type $x^2y'' + f(x)y = 0$ by approximating its solution with solutions of equations of the type $x^2y'' + (ax^2 + bx + c)y = 0$. This approximation is performed by segmentary approximation on an interval. We apply the method to obtain approximate solutions of the radial Schrödinger equation on a given interval and test it for two different potentials. We conclude that our method gives a similar accuracy than the Taylor method of higher order.

1. Introduction and outline of the method

As we all know, many relevant fundamental laws in physics, chemistry, social sciences or economics are formulated in terms of differential equations, which are the basis to solve a great number of problems on these disciplines. And we also know that many of these important differential equations cannot be solved analytically. Therefore, many methods for obtaining numerical solutions have been developed [1].

The aim of the present article is to introduce a method for numerical integration of second order non homogeneous non autonomous ordinary differential equations of the type $x^2y''(x) + f(x)y(x) = 0$. We propose an algebraic method of integration with initial values and without singular points in the interval of integration. As usual, the method can be also used as a basis for the numerical integration of equations with boundary conditions.

One of the most interesting applications of our method is indeed the radial Schrödinger equations with potentials of different types. There are some other methods in the literature dealing with the numerical solution of the one dimensional Schrödinger equation. Among them, we should mention the so-called "piecewise perturbation method" (PPM), which is based on a perturbative decomposition of the potential [2]. In the case of the radial Schrödinger equation, previous numerical studies including PPM have been applied to a certain class of radial potentials which includes the Coulomb case [3].

In our method, described below in the second part of the present introduction, we find numerical solutions of the radial Schrödinger equation using another piecewise method based on the approximation of the original equation by another for which the solutions are well known. In our case, the radial potential could be arbitrary with no other singularity than the origin. The numerical integration is then performed on an interval of the form $[\epsilon, H]$ with $\epsilon > 0$ and H finite, so that we can compare our results with those given by the Taylor method. As particular examples of application, we have chosen the Wood–Saxon potential and the spherical oscillator.

For the numerical integration, we have used identical mesh intervals and this choice was motivated by its simplicity. Here, we have used a step size $h = 0.1$ and have checked that the use of variable step sizes does not improve the efficiency of the calculation and, in addition, requires another algorithm that increases CPU times. There are some other methods using different mesh intervals widths [4]. Our method is simple and improves the precision of the Taylor method. However, it is necessary to say that it requires more CPU times, as we have checked in the two examples studied on Sections 3.1 and 3.2.

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The quantum square well with moving boundaries: A numerical analysis

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ABSTRACT

We present some numerical discussions concerning the infinite square well in one dimension with moving boundaries. Our results show that if the speed of displacement is small, objects of physical relevance like probability density, averaged position or mean value of the energy have a smooth behavior. On the contrary, if this speed becomes large, many irregularities arise, which has a difficult qualitative explanation. These irregularities manifest themselves as sharp bumps on the probability distribution or a chaotic shape on the averaged values of position and energy. None of these patterns is the result of numerical errors and, therefore, we conclude that an unknown and very nontrivial effect is produced at high speeds of the moving wall.

1. Introduction

The resolution of the Schrödinger equation for an arbitrary time dependent Hamiltonian is a formidable task and exact solutions (even numerical solutions) can be obtained for a very limited number of cases only. In the last decade, considerable efforts have been devoted to the deceptive simpler situation posed by the one-dimensional Schrödinger equation with moving boundary conditions [1–4]. One of the approaches for solution of this system could be the replacement of the Schrödinger equation by another one with fixed boundary conditions through a change of variables. However, exact solutions have been found for a few particular number of potentials [1,4] only. The case of a particle confined in an infinite square well with one wall moving at a constant speed is one of them [5,6]. Nevertheless and up to our knowledge, no exact analytical solutions are provided in the literature for the case of an infinite square well with an arbitrary time dependent width.

The purpose of the present paper is to discuss some aspects of the latter model, i.e., the quantum infinite square well with moving boundaries. From the physical point of view, the motivation for this study is double. On the one hand, it is perhaps the simplest nontrivial model of a potential with moving boundaries, which in addition it is very easily exactly solvable in the case of fixed walls. In addition, there is a reason that makes this model quite interesting, which is its relevance in the study of both classical as well as quantum chaotic systems. The story of this potential may be traced back to the so-called "Fermi accelerator". As early as 1949, Fermi suggested for the first time [7] that cosmic ray particles may be accelerated and gain enormous quantities of energy by interacting with moving galactic magnetic fields. After this, Ulam [8] in a seminal work modeled the situation as a classical particle confined in an infinite square potential with a moving wall. Later on, his model became quite known in the field of chaos as his numerical results present a diversity of behaviors from regular to chaotic [9,10]. In this way, several works were devoted to study the quantum problem for different motions of the wall.

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The origin of the hidden supersymmetry

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ABSTRACT

The hidden supersymmetry and related tri-supersymmetric structure of the free particle system, the Dirac delta potential problem and the Aharonov–Bohm effect (planar, bound state, and tubule models) are explained by a special nonlocal unitary transformation, which for the usual $N = 2$ supercharges has a nature of Foldy–Wouthuysen transformation. We show that in general case, the bosonized supersymmetry of nonlocal, parity even systems emerges in the same construction, and explain the origin of the unusual $N = 2$ supersymmetry of electron in three-dimensional parity even magnetic field. The observation extends to include the hidden superconformal symmetry.

1. Introduction

Some quantum systems possess a hidden symmetry associated with nontrivial integrals of motion, which reflect their peculiar properties. A hidden supersymmetry [1] was revealed recently in a class of quantum mechanical systems with a local Hamiltonian. The list of such systems includes the Dirac delta potential problem [2], the Aharonov–Bohm effect (bound state [2] and planar [3] models), the finite-gap periodic quantum systems, and their infinite period limit in the form of reflectionless systems [4,5]. All the listed systems possess a degeneration in the energy spectrum associated with a (twisted) parity symmetry. The hidden supersymmetry of the first two systems is characterized by the linear in the momentum supercharge operators; in the last two families, the hidden supersymmetry is related to the higher derivative nontrivial operator of the Lax pair of the associated nonlinear integrable system. A usual $N = 2$ superextension of all these systems is accompanied by a rich tri-supersymmetric structure rooted in the hidden supersymmetry [6–8].

A natural question arises whether the hidden and usual supersymmetry are somehow related.

In this Letter we show how the hidden supersymmetry and the associated tri-supersymmetric structure originate from the usual $N = 2$ supersymmetry and the (twisted) parity symmetry. The observation is illustrated by the models of the Dirac delta potential problem and the Aharonov–Bohm (AB) effect. We also discuss the nature of the earlier revealed *bosonized* supersymmetry of nonlocal spinless quantum systems with parity even potentials [1], that appears in the same construction, and explain the origin of the unusual $N = 2$ supersymmetry of electron in three-dimensional parity-even magnetic field [9,10]. Finally, we indicate that the observation extends to include the hidden superconformal symmetry [3,11].

2. One-dimensional case: special unitary transformation

Consider an $N = 2$ supersymmetric one-dimensional quantum mechanical system [12,10,13]. It is described by the Hamiltonian

$$H = P^2 + W^2 + \sigma_3 W', \tag{2.1}$$

and supercharges

$$Q_1 = \sigma_1 P + \sigma_2 W, \qquad Q_2 = i\sigma_3 Q_1 = -\sigma_2 P + \sigma_1 W, \tag{2.2}$$

where $P = -i\frac{d}{dx}$, $W = W(x)$ is a superpotential, $W' = dW/dx$, $2m = 1$ and $\hbar = 1$. The H and Q_a, $a = 1, 2$, generate the $N = 2$ supersymmetry,

$$\{Q_a, Q_b\} = 2\delta_{ab} H, \qquad [Q_a, H] = 0, \tag{2.3}$$

for which the integral $\Gamma = \sigma_3$ plays a role of the grading operator, $[\Gamma, H] = \{\Gamma, Q_a\} = 0$.

Assume that the superpotential is an odd function, $W(-x) = -W(x)$. Then the Hamiltonian is the even operator. The reflection

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Self-isospectrality, mirror symmetry, and exotic nonlinear supersymmetry

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We study supersymmetry of a *self-isospectral* one-gap Pöschl-Teller system in the light of a mirror symmetry that is based on spatial and shift reflections. The revealed exotic, partially broken, nonlinear supersymmetry admits seven alternatives for a grading operator. One of its local, first order supercharges may be identified as a Hamiltonian of an associated one-gap, nonperiodic Bogoliubov-de Gennes system. The latter possesses a nonlinear supersymmetric structure, in which any of the three nonlocal generators of a Clifford algebra may be chosen as the grading operator. We find that the supersymmetry generators for both systems are the Darboux-dressed integrals of a free spin-1/2 particle in the Schrödinger picture, or of a free massive Dirac particle. Nonlocal Foldy-Wouthuysen transformations are shown to be involved in the supersymmetric structure.

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I. INTRODUCTION

A $\mathbb{Z}_2$ grading structure lies in the basis of supersymmetry. In the early years of supersymmetric quantum mechanics [1,2], Gendenshtein and Krive observed [3] that in some systems the $\mathbb{Z}_2$ grading may be provided by a reflection operator. The origin of such a hidden supersymmetric structure [4–6] was explained recently in [7] by means of a Foldy-Wouthuysen transformation for the case of a *linear* supersymmetry that is based on the *first order* Darboux transformations [8] and is described by the Lie superalgebraic relations.

Braden and Macfarlane [9], and in a more broad context Dunne and Feinberg [10] revealed that a linear $N = 2$ supersymmetric extension of the *periodic* finite-gap quantum systems may produce completely isospectral systems characterized by the same, but a shifted potential. The name *self-isospectrality* was coined by the latter authors for such a phenomenon, which was studied later by Fernandez *et al.* [11] as *Darboux displacements*, see also [12].

The both periodic and nonperiodic finite-gap quantum systems, being related to nonlinear integrable systems [13], find many important applications in diverse areas of physics, ranging from condensed matter physics, QCD and cosmology, to the string theory [14–25].

A higher order generalization of the Darboux transformations, known as the Darboux-Crum transformations [8], gives rise to a higher derivative generalization of supersymmetric quantum mechanics [26], characterized by nonlinear superalgebraic relations [5,27–29].

Soon after the discovery of the self-isospectrality, it was found that in some periodic finite-gap systems this phenomenon may be associated with not a linear, but nonlinear supersymmetry [30]. Later on, hidden nonlinear supersymmetry [5] was revealed in unextended finite-gap periodic finite-gap systems [31]. It was also established that self-isospectral n-gap periodic systems with a half-period shift are described by a special nonlinear supersymmetric structure that includes a hidden supersymmetry of the order $2n + 1$, whose local generator, being a Lax operator, factorizes into the Darboux intertwining operators of the explicit nonlinear, of order $2k$, $k \geq 1$, and linear or nonlinear, of order $2(n - k) + 1$, supersymmetries [32].

There is an essential difference between supersymmetries of the periodic and nonperiodic *self-isospectral* finite-gap systems. In the former case, linear $N = 2$ supersymmetry generators, as a part of a broader structure, may annihilate two states of zero energy, while they cannot have zero modes in the nonperiodic case. A little attention was given, however, to the study of the self-isospectrality phenomenon in the nonperiodic finite-gap systems.

In the present paper, we investigate the interplay of the self-isospectrality, reflections, Darboux transformations, and nonlinear and hidden supersymmetries for nonperiodic finite-gap quantum systems. This is done here for the simplest case of a one-gap, self-isospectral reflectionless Pöschl-Teller (PT) system, and an associated one-gap Bogoliubov-de Gennes (BdG) system that is described by a first order Hamiltonian.[1] We reveal a rich supersymmetric structure, related to several admissible choices of the grading operator (seven for PT and three for BdG) in these related systems. Our analysis is based on a mirror symmetry that includes a free particle as an essential element. We find that all the nontrivial integrals are a Darboux-dressed

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[1]The BdG system [33] appears in many physical problems, including, particularly, superconductivity theory, fractional fermion number, the Peierls effect, and the crystalline condensates in the chiral Gross-Neveu and Nambu-Jona Lasinio models, see [14–19,34–36].

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Eigenfunction Expansions and Transformation Theory

Manuel Gadella · Fernando Gómez-Cubillo

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Abstract Generalized eigenfunctions may be regarded as vectors of a basis in a particular direct integral of Hilbert spaces or as elements of the antidual space $\Phi^\times$ in a convenient Gelfand triplet $\Phi \subseteq \mathcal{H} \subseteq \Phi^\times$. This work presents a fit treatment for computational purposes of transformations formulas relating different generalized bases of eigenfunctions in both frameworks direct integrals and Gelfand triplets. Transformation formulas look like usual in Physics literature, as limits of integral functionals but with well defined kernels. Several approaches are feasible. Vitali approach is used.

Keywords Eigenfunction expansion · Spectral measure · Direct integral of Hilbert spaces · Gelfand triplet · Rigged Hilbert space · Dirac transformation theory · Vitali system

Mathematics Subject Classification (2000) 47A70 · 47N50

1 Introduction

Eigenfunction expansions appear in the most varied domains as for example in the basis of Dirac formulation of Quantum Mechanics [23], where each complete set of commuting observables (csco) $A_1, A_2, \ldots, A_n$ is supposed to have a generalized basis of kets $|\lambda_1, \lambda_2, \ldots, \lambda_n\rangle$ satisfying the following properties:

1. The kets $|\lambda_1, \lambda_2, \ldots, \lambda_n\rangle$ are generalized eigenvectors of the observables $A_1, A_2, \ldots, A_n$, i.e.,

$$A_j|\lambda_1, \lambda_2, \ldots, \lambda_n\rangle = \lambda_j|\lambda_1, \lambda_2, \ldots, \lambda_n\rangle \quad (j = 1, 2, \ldots, n),$$

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ORIGINAL PAPER

Exchange energy for two closed shells generated by a bare Coulomb potential energy $-Ze^2/r$ in the limit of large Z, in two dimensions

M. L. Glasser · N. H. March · L. M. Nieto

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Abstract Two-dimensional (2D) inhomogeneous electron assemblies are becoming increasingly important in Condensed Matter and associated technologies. Here, therefore, we contribute to the Density Functional Theory of such 2D electronic systems by calculating, analytically, (i) the idempotent Dirac density matrix $\gamma(\mathbf{r}, \mathbf{r}')$ generated by two closed shells for the bare Coulomb potential $-Ze^2/r$ and (ii) the exchange energy density $\varepsilon_x(\mathbf{r})$. Some progress is also possible concerning the exchange potential $V_x(r)$, one non-local approximation being the Slater potential $2\varepsilon_x(r)/n(r)$, with $n(r)$ the ground state electron density. However, to complete the theory of $V_x(r)$, the functional derivative of the single-particle kinetic energy per unit area $\delta t(s)/\delta n(r)$ is still required.

Keywords Exchange · Nuclear cusp condition · Slater potential

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A new proof of the higher-order superintegrability of a noncentral oscillator with inversely quadratic nonlinearities

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The superintegrability of a rational harmonic oscillator (noncentral harmonic oscillator with rational ratio of frequencies) with nonlinear "centrifugal" terms is studied. In the first part, the system is directly studied in the Euclidean plane; the existence of higher-order superintegrability (integrals of motion of higher order than 2 in the momenta) is proved by introducing a deformation in the quadratic complex equation of the linear system. The constants of motion of the nonlinear system are explicitly obtained. In the second part, the inverse problem is analyzed in the general case of n degrees of freedom; starting with a general Hamiltonian H and introducing appropriate conditions for obtaining superintegrability, the particular "centrifugal" nonlinearities are obtained. © *2010 American Institute of Physics.* [doi:10.1063/1.3374665]

I. INTRODUCTION

A superintegrable system is a system that is integrable (in the sense of Liouville–Arnold) and that, in addition to this, possesses more constants of motion than degrees of freedom. At this point, we must note that the maximum number N of functionally independent constants of motion for a system in a d-dimensional manifold is $N=d-1$. Thus, if a Lagrangian (or Hamiltonian) system has n degrees of freedom, then, as the phase space is $2n$ dimensional, we have that the maximum number of independent constants of motion is $N=2n-1$. There are three well known examples of this very particular class of systems, namely, the Kepler problem, the isotropic harmonic oscillator, and the nonisotropic oscillator with commensurable frequencies. The two-dimensional harmonic oscillator is a system trivially integrable since it can be considered as a kind of "direct sum" of two systems with one degree of freedom. If the oscillator is isotropic, then it has the angular momentum as an additional integral of motion. If the oscillator is nonisotropic, the angular momentum is not preserved as the potential is not central; nevertheless, when the quotient of the two frequencies is a rational number, then the system has another additional integral. Concerning the three-dimensional Kepler problem, it possesses not only the energy and the angular momentum as constants of motion but also the Runge–Lenz vector; only five out of these seven integrals are functionally independent since in this case the number of degrees of freedom is $n=3$. In these three cases it is well known that all the orbits became closed for the case of bounded motions. This high degree of regularity (the existence of periodic motions) is a consequence of the superintegrable character.

Fris *et al.*[1] studied the two-dimensional Euclidean systems, which admit separability in two different coordinate systems and obtained four families of potentials V_r, $r=a,b,c,d$, possessing

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TOPICAL REVIEW

n-ary algebras: a review with applications

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Abstract

This paper reviews the properties and applications of certain *n*-ary generalizations of Lie algebras in a self-contained and unified way. These generalizations are algebraic structures in which the two-entry Lie bracket has been replaced by a bracket with *n* entries. Each type of *n*-ary bracket satisfies a specific *characteristic identity* which plays the role of the Jacobi identity for Lie algebras. Particular attention will be paid to *generalized Lie algebras*, which are defined by even multibrackets obtained by antisymmetrizing the associative products of its *n* components and that satisfy the *generalized Jacobi identity*, and to *Filippov (or n-Lie) algebras*, which are defined by fully antisymmetric *n*-brackets that satisfy the *Filippov identity*. 3-Lie algebras have surfaced recently in multi-brane theory in the context of the Bagger–Lambert–Gustavsson model. As a result, Filippov algebras will be discussed at length, including the cohomology complexes that govern their central extensions and their deformations (it turns out that Whitehead's lemma extends to all semisimple *n*-Lie algebras). When the skewsymmetry of the Lie or *n*-Lie algebra bracket is relaxed, one is led to a more general type of *n*-algebras, the *n*-Leibniz algebras. These will be discussed as well, since they underlie the cohomological properties of *n*-Lie algebras. The standard Poisson structure may also be extended to the *n*-ary case. We shall review here the even *generalized Poisson structures*, whose generalized Jacobi identity reproduces the pattern of the generalized Lie algebras, and the *Nambu–Poisson structures*, which satisfy the Filippov identity and determine Filippov algebras. Finally, the recent work of Bagger–Lambert and Gustavsson on superconformal Chern–Simons theory will be briefly discussed. Emphasis will be made on the appearance of the 3-Lie algebra structure and on why the A_4 model may be formulated in terms of an ordinary Lie algebra, and on its Nambu bracket generalization.

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On the local virial theorems for linear and isotropic harmonic oscillator potentials in *d* dimensions

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Abstract

For the system of noninteracting fermions in a one-body potential $V(\vec{r})$, the local virial theorems (LVT) are relations, at a given point $\vec{r}$ in space, between this potential, kinetic energy and particle densities. It was recently shown (Brack *et al* 2010 *J. Phys. A: Math. Theor.* **43** 255204) that for *d*-dimensional linear and also for isotropic harmonic oscillator potentials these LVTs are exactly satisfied. We present alternative and simple proofs of these theorems, by consideration of the canonical or Bloch density matrix and its relation to the kinetic energy density. The explicit analytical forms of the Bloch density matrix are used for the above-mentioned potentials to achieve the proofs. For the case of linear potential, we obtain a more general result for the so-called semilocal virial theorem, and for the harmonic oscillator potential case we derive a new relationship between the diagonal part of the canonical bloch density and the kinetic energy density.

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1. Introduction

The local virial theorems are relations, at a given point $\vec{r}$ in space, between particle density, potential energy and kinetic energy density. In their early work March and Young [2] derived the so-called differential virial theorem, which is a version of the local virial theorem, when the particle motion is restricted along, say the x axis and move in a potential $V(x)$. Due to the current considerable experimental activity in the area of confined cold atoms and since most experimental setups use harmonic traps [3], this theorem has been generalized for the specific case of isotropic harmonic oscillator potential in two and three dimensions [4]. In the *d* dimension the proof is given in [5].

In a recent work Brack *et al* [1] presented a study on the particle and kinetic energy densities for a system of N noninteracting fermions in an arbitrary one-body potential $V(\vec{r})$.

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Correlated fermionic densities for many harmonically trapped particles interacting with repulsive forces

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Fermion densities

ABSTRACT

This study is motivated by the very recent work on correlation energy as approximated by the Thomas–Fermi (TF) semiclassical limit [B.R. Landry, et al., Phys. Rev. Lett. 103 (2009) 066401]. In contrast, and motivated by the Hohenberg–Kohn theorem, our work is focussed primarily on the correlated TF ground-state density. We invoke directly the Holas et al. result that for two-fermion systems with harmonic trapping, the fermion–fermion interaction u simply adds to the trapping potential. We conclude this report with some results on correlation kinetic energy for two-fermion systems.

This Letter is motivated by the recent contribution of Landry et al. [1] proposing a correlated Thomas–Fermi (TF) method to approximate ground-state energies of many-electron systems.

Since, of course, modern DFT [2] builds on the formally exact theorem of Hohenberg and Kohn [3] that the ground-state energy E is given by

$$E = E[n] \tag{1}$$

where n is the ground-state density, it is a natural consequence of [1] to raise the question of a correlated TF ground-state density n. In the illustrative examples in [1], Landry et al. refer to one-dimensional (1D) models and we shall therefore first consider 1D problems. Going back to early work of Lawes and March [4], the ground-state density $n(x)$ of 1D harmonically trapped independent fermions has been widely studied theoretically, motivation being provided by the experiments of DeMarco and Jin [5] on magnetically trapped ultracold fermion vapors, where, by varying the magnetic field, one can simulate such systems from 1D to 3D.

We therefore follow closely the presentation of March and Nieto [6] on 1D harmonically trapped fermions, modeled to occupy the first 50 levels of the trapping potential

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2. \tag{2}$$

Below we take units such that $k = m\omega^2 = 1$ for the non-interacting limit. Fig. 3 of [6] gives the exact ground-state density $n(x)$ of this model for 50 singly occupied levels, the result being presented as Fig. 1 of the present Letter compared with the TF limit

$$n_{TF}(x) = \frac{2^{1/2}}{\pi}\left[N - \frac{1}{2}x^2\right]^{1/2}. \tag{3}$$

With $N = 50$, the classically forbidden region defined from (3) by $x_c^2 = 2N = 100$ is clearly discernable already in the exact fermion density shown also, with the TF result (3), in Fig. 1(c).

We now turn to 'switch on' interactions for the uncorrelated density in (3) to yield a correlated TF (CTF) density $n_{CTF}(x)$. This can be done exactly using the recent study by Zaluska-Kotur et al. [7] for the special case where repulsive interactions themselves have harmonic form. The modification that fully quantum-mechanical results lead to in the semi-classical limit of TF theory is to change (3) to read, for the harmonic correlated case

$$n_{CTF}(x) = \frac{2^{1/2}}{\pi}\left[N\omega - \frac{1}{2}\omega^2x^2\right]^{1/2} \tag{4}$$

where $\omega^2 < 1$ due to the repulsive harmonic interactions.

For the parameters chosen for the interacting N-body system in [7], ω is taken to be 0.5 and 0.9. For these cases the density $n_{CTF}(x)$ calculated from (4) is shown in Fig. 1(a)–(b) in comparison with the quantal density of March and Nieto [6]. At $\omega = 0.5$, there is seen to be a dramatic increase in the size of the classically allowed region in which $n_{CTF}(x) \neq 0$, from the non-interacting limits.

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