Spectral Determinant Method for Interacting N-body Systems Including Impurities

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A general expression for the Green’s function of a system of N particles (bosons/fermions) interacting by contact potentials, including impurities with Dirac-delta type potentials is derived. In one dimension for N > 2 bosons from our spectral determinant method the numerically calculated energy levels agree very well with those obtained from the exact Bethe ansatz solutions while they are an order of magnitude more accurate than those found by direct diagonalization. For N = 2 bosons the agreement is shown analytically. In the case of N = 2 interacting bosons and one impurity, the energy levels are calculated numerically from the spectral determinant of the system. The spectral determinant method is applied to an interacting fermion system including an impurity to calculate the persistent current at the presence of magnetic field.

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1. INTRODUCTION

Due to the remarkable progress in the understanding of many features of mesoscopic physics the role of electron-electron interactions has been actively studied in such systems. Two frequently studied problems are the interaction induced delocalization of two particles in disordered systems (we shall use the abbreviation TIP as it is common in the literature for two interacting particles) [1,2] and the persistent current (PC) first predicted by Büttiker et al. [3] and observed in metallic rings by Levy et al. [4] and Chandrasekhar et al. [5]. Commonly used numerical approaches to these problems are the Green’s function (GF) method [6–8], the diagonalization method [9–11], the decimation method [12], and density-matrix renormalization-group (DMRG) method [13]. The many-body systems including impurities are frequently modeled by the Anderson-Hubbard tight-binding Hamiltonian [8] given by interacting electrons (with on-site interaction), and random potentials (with random site energy) of the impurities on a lattice. In the TIP problem the GF of the full Hamiltonian is obtained from Dyson’s equation considering the interaction Hamiltonian as a perturbation. The two-particle localization length is then defined via a particular trace of the GF. In the PC problem the interplay between the interactions and impurities has generated much interest and several theoretical methods are developed (see e.g. Ref. [14] and references therein). To find the persistent current one needs to calculate the flux dependence of the ground state energy which can be obtained from the lowest pole of the GF as a possible approach. It is therefore desirable to construct the GF of the system which includes both impurities and the electron-electron interaction in order to treat the TIP and PC problems in a common framework.

In this paper we develop a formalism to determine the GF of N-particle systems in which both the potential of the impurities and the interaction between the particles are given by contact potentials, i.e. by Dirac delta functions. Unlike in the case of the Anderson tight-binding Hamiltonian, in our calculation the positions of the electrons are not restricted to lattice sites but can be continuous coordinates. In our general formalism both the impurities and the interactions are treated as perturbations where the interaction or impurity strengths are the small parameters, and the GF is obtained from Dyson’s equation. The resulting series for the GF can be expressed in terms of the GFs of the noninteracting many particle systems without impurities. If both the impurities and the interaction are given by contact potentials, the series can be given in a closed form, namely as the ratio of two determinants including only the GF of the unperturbed system. A similar (i.e. ratio of two determinants) form of the GF was found by Grosche [15] for a system containing only one electron interacting with impurities. We have used this form of the GF in Ref. [16] to investigate the diffraction of the electron by the impurities, and in Ref. [17] to study the crossover behavior of the localization problem in a waveguide with periodically placed identical point-like impurities. In this paper an extension of Grosche’s approach to treat many-body interacting systems including impurities is presented. In our formalism we consider both the spinless bosons and the spin-full fermions. The many-body wave functions are the symmetrized products of the one-particle eigenstates of the system. In our calculations the bosonic/fermionic feature of the many-body system is fully incorporated. The energy eigenvalues of many-body systems are given by the poles of the GF. It implies that the energy levels are the zeros of the determinant in the denominator of the GF. We claim that the energy levels determined through this spectral determinant are much more accurate than those found by the traditional diagonalization methods. Therefore, here we propose the method of spectral determinants (SD) as a new approach to this problem. As it is seen below the indices of the matrix elements of the determinants are continuous variables. To evaluate the necessary SD in this case, one can use any complete orthogonal set as a basis. In our examples below this will be demonstrated using one-particle eigenstates.
As an application and to test our method, we consider the one-dimensional N-body problem in which the bosonic particles interact via a Dirac delta potential. It is well known that the exact result for the energy eigenvalues can be obtained from the Bethe ansatz [18–22], so it is possible to compare our results with the exact ones. It is analytically proved that for the case of two interacting bosons the energy eigenvalues obtained from our method are identical to those found from the Bethe ansatz solutions. Moreover, in the case of three and four particles our numerical results agree very well with the Bethe ansatz solutions. Our results are compared with those obtained from direct diagonalization of the Hamiltonian, and it is demonstrated that in general our results are more than ten times more accurate. For higher energies it is shown that the direct diagonalization method is very inaccurate, which seriously limits its applicability in numerical calculations.

To see how much more effective our method is, we shall consider two nontrivial examples as a further application. We present our results for the system of two interacting bosons and one impurity, and for three interacting spin-full fermions and one impurity. In these cases no Bethe ansatz type of solution is known. Increasing the number of one-particle wave functions the energy eigenvalues converge. This way all the energy levels are calculated to four significant figures, and are taken as the exact energy levels. The errors of the energy eigenvalues found from our SD method and from the direct diagonalization of the Hamiltonian are compared using the same number of one-particle wave functions. In general, our method gives again an order of magnitude more accurate results than the diagonalization of the Hamiltonian. The accurate energy levels are necessary for calculating e.g. the persistent current which is the derivative of the ground state energy with respect to the applied magnetic flux enclosed by the system. As a demonstration we present our calculation of the persistent current for the interacting three-particle fermion system.

Since in the above mentioned TIP and PC problems the Anderson-Hubbard tight-binding Hamiltonian [8] can be regarded as a discretized version of the continuous model with Dirac delta potentials for both the interaction among the particles and with the impurities, we expect that our SD method might be applied successfully in numerical simulations. The work along this line is in progress.

The rest of the paper is organized as follows. In section II we give our most general form of the GF for interacting N-particles systems including a finite number of impurities. In section III the GF is given for spin-full case. In all these sections our results for the GF are given as the ratio of two determinants expressed in terms of the GF of the noninteracting N-particle system. In section IV our method is tested for interacting bosons for which the exact Bethe ansatz solutions are known. Our results are compared with the exact ones obtained from the Bethe ansatz solution and with those found from the numerical diagonalization of the corresponding Hamiltonian. In section V we calculate the energy levels for a system of two interacting bosons plus one impurity and compare the results with those obtained from the direct diagonalization of the Hamiltonian. In section VI the calculation of the persistent current is presented for three interacting fermions and one impurity. Our conclusions are given in section VII. In Appendix A the derivation of the GF is given for the case of two interacting particles and M impurities. In Appendix B we show that from our method the exact Bethe ansatz solution can be obtained analytically for two interacting bosons.

II. MANY-BODY BOSON SYSTEMS WITH INTERACTION AND IMPURITIES

In this section we consider the most general case, namely the system of N interacting spinless bosons plus M impurities with different strengths of potentials. To highlight the method to be applied it is useful to discuss the simple system of two noninteracting bosons with one impurity. It turns out that the full GF is a ratio of two structured determinants. However, both determinants are so called ‘continuous matrices’ i.e. their indices are continuous variables. This feature of the matrices arises from the many body character of the system.

The GF of the Hamiltonian \( H = H_0 + H_1 \) is given by

\[
G = (E - H_0 - H_1)^{-1}.
\]  

(1)

The Hamiltonian \( H_0 \) of \( N \) identical noninteracting particles can be written as

\[
H_0(x) = \sum_{i=1}^{N} h(x_i),
\]  

(2)

where the position of the \( i \)th particle is denoted by \( x_i \), and \( x = (x_1, x_2, \ldots, x_N) \). In general, the \( x_i \) are \( d \) dimensional vectors. In the examples presented below only one-dimensional systems are studied. The one-particle Hamiltonian \( h(x) \) is given by

\[
h(x) = -\nabla^2 + V(x),
\]  

(3)
where \( V(x) \) is the potential in the one-particle problem. Hereafter we shall use \( \hbar = 2m = 1 \) units, where \( m \) is the mass of the particles. We assume that both the eigenstates and the energy eigenvalues are known for the Hamiltonian \( H \) of the one-particle problem. In many applications the potential \( V(x) \) is taken to be zero inside the box and infinity at its boundaries. The other typical case is when the potential \( V(x) \) is zero inside the box and periodic boundary conditions are applied. In this paper the latter is used in our examples.

The Hamiltonian \( H_1 \) represents the effect of the impurity, and can be written as

\[
H_1(x) = \kappa \sum_{p=1}^{N} \delta(x_p - u),
\]

(4)

where the position of the impurity is denoted by \( u \), while \( \kappa \) is the strength of the Dirac delta potential. The full GF of \( H_0 + H_1 \) satisfies Dyson’s equation

\[
G = G_0 + G_0 H_1 G,
\]

(5)

where \( G_0 \) is the GF of the Hamiltonian \( H_0 \).

To proceed further, it is instructive to consider only two noninteracting particles, i.e. \( N = 2 \). The result can be easily generalized then to the case \( N > 2 \). For two noninteracting particles the GF in coordinate representation is given [23] by

\[
G_0(x_1, x_2|x_1', x_2') = \sum_n \frac{\psi_n(x_1, x_2)\psi_n^*(x_1', x_2')}{E - E_n},
\]

(6)

where \( \psi_n(x_1, x_2) \) is the \( n \)th eigenstate of the two noninteracting particles, and the corresponding eigenvalue is \( E_n \). In case of bosons the wave function is symmetric for the permutation of its variables, i.e. \( \psi_n(x_1, x_2) = \psi_n(x_2, x_1) \).

The iterative solution of Dyson’s equation results in the series

\[
G(x_1, x_2|x_1', x_2') = G_0(x_1, x_2|x_1', x_2') + \int G_0(x_1, x_2|y_1, y_2) H_1(y_1, y_2) G_0(y_1, y_2|x_1', x_2') dy_1 dy_2
\]

\[+ \int G_0(x_1, x_2|y_1, y_2) H_1(y_1, y_2) G_0(y_1, y_2|y_3, y_4) H_1(y_3, y_4) G_0(y_3, y_4|x_1', x_2') dy_1 dy_2 dy_3 dy_4 + \cdots. \]

(7)

After inserting \( H_1 \) given in Eq. (4) into Eq. (6), one can perform some of the integrals in the series due to the presence of Dirac delta potentials. Finally, making use of the fact that for bosons

\[
G(x_1, x_2|x_1', x_2') = G(x_2, x_1|x_2', x_1') = G(x_2, x_1|x_1', x_2') = G(x_1, x_2|x_1', x_2'),
\]

(8)

the series in Eq. (7) leads to

\[
G(x_1, x_2|x_1', x_2') = G_0(x_1, x_2|x_1', x_2') + 2\kappa \int G_0(x_1, x_2|y, u) G_0(y, u|x_1', x_2') dy
\]

\[+ (2\kappa)^2 \int G_0(x_1, x_2|y_1, u) G_0(y_1, u|y_2, u) G_0(y_2, u|x_1', x_2') dy_1 dy_2 + \cdots. \]

(9)

This is a Neumann series [24], known from the theory of integral equations. It can be rewritten in the more compact form

\[
G(x_1, x_2|x_1', x_2') = G_0(x_1, x_2|x_1', x_2') - \int G_0(x_1, x_2|y_1, u) K^{-1}(y_1|y_2) G_0(y_2, u|x_1', x_2') dy_1 dy_2,
\]

(10)

where the operator \( K(y_1|y_2) \) is given by

\[
K(y_1|y_2) = -\frac{1}{2\kappa} \delta(y_1 - y_2) + G_0(y_1, u|y_2, u).
\]

(11)

For calculating the inverse of \( K \) one can choose a suitable complete orthogonal set to represent the operator \( K \) as a matrix. Using the identity for hypermatrices

\[
\det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \det(d) \det(a - bd^{-1}c)
\]

(12)

3
GF can be given similarly as a ratio of two determinants

\[ G(x_1, x_2 | x'_1, x'_2) = \frac{\det \begin{bmatrix} G_0(x_1, x_2 | x'_1, x'_2) & G_0(x_1, x_2 | y_2, u) \\ G_0(y_1, u | x'_1, x'_2) & K(y_1 | y_2) \end{bmatrix}}{\det K(y_1 | y_2)}, \]  

(13)

where the matrix in the numerator is discrete in its first row and column, but the rest is indexed by the continuous variables \( y_1, y_2 \). The ‘continuous matrix’ \( K \) can be given in matrix representation. Examples for treating this type of matrices will be given in Secs. \([\text{V}]\) and \([\text{VIII}]\). Rewriting equation (10) in the form given by Eq. (13) is formal since in the numerator of Eq. (13) the dimension of the 1,1 matrix element of the determinant is unity. However, later it turns out that in the more general case in which more than two particles are included as well as many impurities, the GF can be given similarly as a ratio of two determinants.

Turning to the more general case of \( N > 2 \), the necessary steps to obtain the full GF are similar to those made in case of \( N = 2 \). The crucial point is to make use of the identity of the bosonic GF

\[ G(x|x') = G(Px|Py'), \]  

(14)

where \( Px \) is an arbitrary permutation of the set \((x_1, x_2, ..., x_N)\). One then finds

\[ G(x|x') = \frac{\det \begin{bmatrix} G_0(x|x') & G_0(x|y', y) \\ G_0(y, y' | x') & K(y | y') \end{bmatrix}}{\det K(y | y')}, \]  

(15)

where

\[ K(y | y') = -\frac{1}{N\kappa} \delta^{(N-1)}(y - y') + G_0(u, y | u, y'), \]  

(16)

and \( y = (y_1, y_2, ..., y_{N-1}) \). The structure of the GF is similar to that given in Eq. (13) except that now the matrix \( K \) depends on some multidimensional variables. The indices of the ‘matrix’ \( K \) in Eq. (14) are ‘continuous’ variables. The appearance of this kind of infinite-sized matrix is a consequence of the many-body feature of the Hamiltonian.

We now turn to the case of interacting bosons. The previously presented method is suitable to handle the more complicated systems in which the interactions between particles are also taken into account. The derivation of the full GF of the two interacting bosons with many impurities is very similar to that shown before for the case of noninteracting particles, and the details are given in Appendix [\text{I}].

In the most general case the Hamiltonian \( H_0 \) of the noninteracting N-particle system without impurities is given by Eq. (3). The rest of the total Hamiltonian of the system with \( M \) impurities and Dirac delta interactions with \( N \) particles is

\[ H_1(x) = \sum_{i=1}^{M} \kappa_i \sum_{p=1}^{N} \delta(x_p - u_i) + \lambda \sum_{p,q=1}^{N} \delta(x_p - x_q), \]  

(17)

where \( x_p \) are the positions of the bosons \( p = 1, \ldots, N \), \( u_i \) and \( \kappa_i \) is the position and the strength of the impurity \( i = 1, \ldots, M \), and \( \lambda \) is the strength of the interactions between particles. For simplifying the notations we shall use the vector \( \mathbf{x} = (x_1, x_2, ..., x_N) \).

To find the full GF, a similar procedure given in Appendix [\text{I}] can also be carried out in this case, and the final result is

\[ G(x|x') = \frac{\det \begin{bmatrix} G_0(x|x') & G_0(x|y', y) \\ G_0(y, y' | x') & K(y | y') \end{bmatrix}}{\det K(y | y')}, \]  

(18)
where
\[
K_i(y|y') = -\frac{1}{N\kappa} \delta^{(N-1)}(y - y') + G_0(u_i, y|u'_i, y'),
\]
\[
L(y_1, \bar{y}|y'_1, \bar{y}') = -\frac{2}{N(N-1)} \delta(y_1 - y'_1) \delta^{(N-2)}(\bar{y} - \bar{y}') + G_0(y_1, y_1; \bar{y}|y'_1, \bar{y}', \bar{y}').
\]
The variables \(y = (y_1, y_2, y_3, \ldots, y_N)\) and \(\bar{y} = (y_3, y_4, \ldots, y_N)\) (and the corresponding primed ones) appearing in the operators \(L\) and \(K_i\) are \((N - 1)\)-component and \((N - 2)\)-component vectors, respectively.

At first sight the final form of the Green’s function seems to be very complicated but the matrices have a simple structure. The GF is again expressed as the ratio of two determinants. The variables of the full GF appear only in the numerator the remaining matrix is the same as that in the denominator. The matrix in the denominator has an obvious structure, too: the 1,1 element of the matrix, i.e. the first row and first column of the matrix in the numerator the remaining matrix is the same as that in the denominator. The matrix in the denominator contains the operator \(K\) of two noninteracting particles. The interacting part of the Hamiltonian \(H_0\) of the noninteracting, impurity free system. Then, it is ensured that the Green function of system of the interacting particles with impurities is also symmetrized according the nature of the particles. As we shall see below, the truncation introduce less error in the energy levels compared to that obtained by direct diagonalization than the lack of this symmetrization.

III. SPIN-FULL FERMIONS WITH INTERACTION AND IMPURITIES

In this section our spectral determinant method is generalized to an interacting many-body systems in which the particles can be bosons or fermions with spins. The Green function can be derived in a way similar to the spinless bosons discussed in the previous sections. Note that for spinless fermions with the Dirac-delta interaction potential the energy levels are the same as in the case of noninteracting fermions.

The GF now depends on the spin indices and for noninteracting particles GF is
\[
G_0(x|x', E)_{s|s'} = \sum_n \frac{\psi_n(x)\psi^*_n(x')}{E - E_n},
\]
where \(s = (s_1, s_2, \ldots, s_N)\) is a compact notation of the spins of the \(N\) particles. The interacting part of the Hamiltonian again consist of two terms:
\[
H_1(x)_{s|s'} = \sum_{i=1}^M \kappa_i \sum_{p=1}^N \delta(x_p - u_i)\delta_{s, s'} + \lambda \sum_{p < q}^N \delta(x_p - x_q)\delta_{s, s'},
\]
where all the terms are diagonal in the spin indices. Here \(u_i\) and \(\kappa_i\) are positions and the strength of the impurity \(i = 1, \ldots, M\), and \(\lambda\) is the strength of the interactions between particles.

Following the method developed in the previous sections we find that the GF for the system of interacting particles (fermion or bosons) with spins and impurities is given by
\[ G(x|x') = \frac{\det}{\det} \begin{bmatrix} G_0(x|x') & G_0(y_1, y_1, y_1') & G_0(x|y_1, y') \\ G_0(y_1, y_1, y_1') & L(y_1, y, y') & G_0(y_1, y_1, y_1') \\ G_0(u_i, y|x') & K_{i,j}(y'y') & K_{i,j}(y'y') \end{bmatrix}, \quad (23) \]

where

\[ K_{i,j}(y'y') = -\frac{1}{N\kappa_i} \delta_{i,j} \delta^{(N-1)}(y - y') \delta_s^N + G_0(u_i, y|y_j, y') \]

and

\[ L(y_1, y|y_1, y') = -\frac{2}{N(N-1)\lambda} \delta(y_1 - y_1') \delta^{(N-2)}(y - y') \delta_s^N + G_0(y_1, y_1, y_1'|y_1, y') \]

Here the same notations are used for \( y = (y_1, y_3, y_4, ..., y_N) \) and \( \bar{y} = (y_3, y_4, ..., y_N) \) as in Eq. (18). The \( s, \bar{s} \) denote the \( N \) spin indices.

**IV. THE TEST OF THE SPECTRAL DETERMINANT METHOD FOR BOSONS**

In this section we apply our formalism in one dimension using periodic boundary conditions to two, three, and four interacting spinless bosons without including impurities, as well as two bosons with one impurity. The energy eigenvalues of these many-body systems can be found from the zeros of a SD derived from GF formalism. In these systems one can calculate the exact energy levels from the well known Bethe ansatz [18] solutions. Thus, our results can be compared with the exact ones. Using one-particle wave functions one can build up the symmetrized many-body wave functions, and in this truncated basis the Hamiltonian of the system can be diagonalized numerically. We use the same number of one-particle wave functions in the SD method as in the diagonalization of the Hamiltonian. If the number of one-particle wave functions used in the SD method is \( p \), then for \( N > 2 \) interacting particles one needs to find the zeros of a SD of size \( p^{N-1} \). On the other hand, in the diagonalization of the Hamiltonian using the same \( p \) one-particle wave functions the size of the matrix that should be diagonalized is \( \binom{p+N-1}{N} \).

It is interesting to mention that for two interacting particles the energy levels are exactly the same as those obtained from the Bethe ansatz solutions. The details of the derivation is given in Appendix B. In sections V.A and V.B the derivation of the equations for the energy eigenvalues and the numerical results are presented for three and four interacting particles. The comparison of the SD method with direct diagonalization shows that the SD method leads to an order of magnitude improvement in the accuracy even in the worst case.

**A. Three interacting bosons in one dimension**

Now the method developed in section II is applied for \( N = 3 \) interacting particles in a one-dimensional box with periodic boundary conditions. To determine the Green’s function \( G_0 \) for the case of three particles, it is again convenient to use the one-particle wave functions and the corresponding eigenvalues given by Eqs. (31) and (32). Hereafter we shall use the length unit \( a = 1 \) for the size of the box. Then the Green’s function \( G_0 \) is given by

\[ G_0(x_1, x_2, x_3|x_1', x_2', x_3') = \sum_{\{n_1 n_2 n_3\}} \frac{\psi_{n_1 n_2 n_3}(x_1, x_2, x_3) \psi^*_{n_1 n_2 n_3}(x_1', x_2', x_3')}{E - E_{n_1} - E_{n_2} - E_{n_3}}, \quad (26) \]

where the \( \psi_{n_1 n_2 n_3}(x_1, x_2, x_3) \) are the eigenfunctions of the system of three noninteracting particles, and \( n_1, n_2, n_3 = 0, \pm 1, \pm 2, \ldots \). For bosons these wavefunctions can be built up from the one-particle wave functions given by Eq. (33). Finally, the GF can be simplified as

\[ G_0(x_1, x_2, x_3|x_1', x_2', x_3') = \frac{1}{3!} \sum_{n_1 n_2 n_3} \sum_{P \in S_3} \frac{\psi_{n_1}(x_1) \psi_{n_2}(x_2) \psi_{n_3}(x_3) \psi^*_{n_{P(1)}}(x_1') \psi^*_{n_{P(2)}}(x_2') \psi^*_{n_{P(3)}}(x_3')}{E - E_{n_1} - E_{n_2} - E_{n_3}}, \quad (27) \]

where \( S_3 \) denotes the permutation group of the numbers 1, 2, 3, and \( P \) is an element of the group, while \( P(i) \) is the number in the \( i \)th place in permutation \( P \).
The energy levels of the system are the poles of the GF given by Eq. (18). From the form of the GF we can see that obtaining the poles is equivalent to finding the solutions of the equation \( \det L = 0 \) for \( E \), where \( L \) is given by Eq. (28), i.e.:

\[
\det L(y, x|y', x') = \det \left( -\frac{1}{3\lambda} \delta(y - y') \delta(x - x') + G_0(y, x|y', x'; E) \right) = 0,
\]

where \( \lambda \) is the strength of the interaction between bosons. Using Eqs. (B10) and (B17) the second term in \( \det L \) becomes

\[
G_0(y, x|y', x') = \frac{1}{3} \sum_{m_1m_2m_3} e^{2\pi i [(n_1+n_2)(y-y')+n_3(x-x')]} + 2e^{2\pi i [n_1(y-x') + n_2(x-y') + n_3(y-y')]}
\]

\[
E - E_{m_1} - E_{m_2} - E_{m_3}.
\]

The determinant of the operator \( L \) in Eq. (28) can be rewritten as a determinant of an infinite sized matrix using any convenient basis (which is not necessarily that of symmetrized wave functions). In our calculation we chose

\[
\varphi_{kl}(y, x) = e^{2\pi i (ky + lx)}.
\]

Thus, the operator \( L \) in this basis can be given by

\[
L(kl|k'l') = \int \varphi_{kl}(y, x) L(y, x|y', x') \varphi_{k'l'}(y', x') \ dy \ dx \ dy' \ dx'.
\]

After some tedious but straightforward algebra one can find that

\[
L(kl|k'l') = -\frac{1}{3\lambda} \delta_{k,k'} \delta_{l,l'} + \frac{1}{3} \left( \frac{2 \delta_{k+l,k'+l'}}{E - E_{l'} - E_{l} - E_{k'}} + \sum_n \frac{\delta_{k,k'} \delta_{l,l'}}{E - E_{k-n} - E_{n} - E_{l}} \right).
\]

The sum in this equation has a similar structure to Eq. (B10), therefore using the identities given in Eq. (B11) the summation can be carried out yielding

\[
L(k, l|k', l') = \begin{cases} 
\delta_{k,k'} \delta_{l,l'} \left( -\frac{1}{3\lambda} + \frac{1}{12\pi^2} \cot \frac{\pi z}{2} \right) + A(E; k, l|k', l'), & \text{for } k \text{ even}, \\
-\delta_{k,k'} \delta_{l,l'} \left( \frac{1}{3\lambda} + \frac{1}{12\pi^2} \tan \frac{\pi z}{2} \right) + A(E; k, l|k', l'), & \text{for } k \text{ odd},
\end{cases}
\]

where

\[
A(E; k, l|k', l') = \frac{2}{3} \frac{\delta_{k+l,k'+l'}}{E - 4\pi^2 [(l^2 + l'^2 + (k - l')^2]}
\]

\[
z = \sqrt{\frac{E}{2\pi^2} - 2l^2 - k^2}.
\]

One can see that choosing an appropriate basis it is possible to express all the matrix elements of the operator \( L \) in a closed form. We now solve Eq. (28) numerically to find the energy levels from our method and compare them with the Bethe ansatz solutions determined in Eqs. (B14) and (B15).

In numerical calculations we have to truncate the matrix \( L(k, l|k', l') \). To form the basis \( \varphi_{kl}(x, y) \) given in (30) we chose \( 2m+1 \) one-particle states \( \psi_k(x) \) \( (k = 0, \pm 1, \pm 2, \cdots, \pm m) \) as given in Eq. (B14). Therefore, we have \((2m+1)^2 \) different basis functions \( \varphi_{kl}(x, y) \) with \( k, l = 0, \pm 1, \pm 2, \cdots, \pm m \). Thus, the infinite sized matrix \( L(k, l|k', l') \) is truncated to a \((2m+1)^2 \times (2m+1)^2 \) matrix.

The logarithm of the absolute value of \( \det L(k, l|k', l') \) is plotted as a function of the energy \( E \) in Fig. 1. In this plot \( 2m+1 = 7 \) one-particle wave functions were used. The zeros of \( \det L(k, l|k', l') \) (i.e., in the plot at the energy values where the logarithm of \( \det L(k, l|k', l') \) goes to \(-\infty\)) give the energy levels of the system. One can see from the figure that these energy values agree very well with those found from the Bethe ansatz solution. Note that the \( \det L(k, l|k', l') \) has poles at the energy levels of the noninteracting system. This can be seen clearly from the figure.
FIG. 1. The logarithm of the absolute value of $\det L(k, l|k', l')$ as a function of $E$ for $N = 3$ interacting particles (solid line). The strength of the interactions is $\lambda = 4.0$. The number of one-particle wave functions was $2m + 1 = 7$. Including the interactions, the energy levels, i.e. the position of the zeros obtained from the Bethe ansatz solution are shown by dashed vertical lines. For clarity, we indicate the energy levels of noninteracting particles with dotted vertical lines ($E_k = 4\pi^2 k^2$, where $k = 0, 1, 2, \cdots$).

In Fig. 2 the relative errors of the first six energy levels obtained from Bethe ansatz solutions and our SD method using $2m + 1$ one-particle wave functions are plotted as a function of $m$. One can see that the relative errors decrease with increasing $m$. It implies that including only a few number of one-particle wave functions in our SD method is enough to get a very satisfactory agreements with the exact energy levels obtained by Bethe ansatz solutions.

FIG. 2. The relative errors (in percentage) of the energy levels found (the different energy levels are indicated by different symbols) from the SD method using $2m + 1$ one-particle wave functions as a function of $m$ for the first six energy levels. The strength of the interactions is $\lambda = 4.0$.

In Fig. 3 we plotted the relative errors of the energy levels found from the SD method for the first 100 energy levels.
Diagonalization of the Hamiltonian can be performed by using the same one-particle wave functions as in the SD method. In Table I we have listed the first few energy levels obtained from Bethe ansatz solutions, diagonalization of the Hamiltonian of the system and the SD method. It can be seen from Table I that the relative errors of the energy levels obtained from the SD method are an order of magnitude smaller than those of the diagonalization of the Hamiltonian.

One can see that the errors of the first 50 energy levels are less than 0.01%, in spite of the fact that only 9 one-particle wave functions were used. It is surprising that only a relatively small number of one-particle wave functions needs to be used for obtaining a rather accurate result. The accuracy breaks down after the first 50 energy levels. This is the point where the unperturbed energy levels corresponding to the calculated levels start missing in case of 9 one-particle base functions.

Table I: The energy levels from Bethe ansatz, diagonalization of the Hamiltonian and the SD method. In the diagonalization method we used the same one-particle wave functions as in the SD method. The percentage errors are indicated in brackets. The strength of the interactions is $\lambda = 4.0$.

<table>
<thead>
<tr>
<th>$E$</th>
<th>$m = 2$</th>
<th>$m = 3$</th>
<th>$m = 4$</th>
<th>$m = 2$</th>
<th>$m = 3$</th>
<th>$m = 4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.3284947</td>
<td>10.7066 (3.7)</td>
<td>10.5994 (2.6)</td>
<td>10.5403 (2.05)</td>
<td>10.3264 (0.02)</td>
<td>10.3277 (0.008)</td>
<td>10.3281 (0.004)</td>
</tr>
<tr>
<td>57.1227798</td>
<td>57.9505 (1.4)</td>
<td>57.6827 (1.0)</td>
<td>57.5488 (0.75)</td>
<td>57.1508 (0.05)</td>
<td>57.1196 (0.006)</td>
<td>57.1508 (0.049)</td>
</tr>
<tr>
<td>96.6011996</td>
<td>97.4767 (0.9)</td>
<td>97.1866 (0.6)</td>
<td>97.0426 (0.46)</td>
<td>96.5507 (0.05)</td>
<td>96.6507 (0.051)</td>
<td>96.6507 (0.051)</td>
</tr>
<tr>
<td>101.131830</td>
<td>102.8964 (1.7)</td>
<td>102.7003 (1.6)</td>
<td>102.5885 (1.44)</td>
<td>101.1061 (0.03)</td>
<td>101.1231 (0.008)</td>
<td>101.1277 (0.004)</td>
</tr>
<tr>
<td>128.7637540</td>
<td>129.3888 (0.5)</td>
<td>129.1411 (0.3)</td>
<td>129.0332 (0.21)</td>
<td>128.7006 (0.05)</td>
<td>128.7584 (0.004)</td>
<td>128.7756 (0.009)</td>
</tr>
<tr>
<td>137.2597820</td>
<td>137.7723 (0.4)</td>
<td>137.4139 (0.1)</td>
<td>137.2811 (0.02)</td>
<td>137.2505 (0.01)</td>
<td>137.3005 (0.030)</td>
<td>137.2630 (0.002)</td>
</tr>
<tr>
<td>176.7382020</td>
<td>177.5799 (0.5)</td>
<td>177.0631 (0.2)</td>
<td>176.8474 (0.06)</td>
<td>176.6504 (0.05)</td>
<td>176.7394 (0.007)</td>
<td>176.7340 (0.002)</td>
</tr>
<tr>
<td>219.5666420</td>
<td>221.0227 (1.1)</td>
<td>221.1095 (0.7)</td>
<td>221.2000 (0.33)</td>
<td>212.7003 (3.13)</td>
<td>219.5003 (0.030)</td>
<td>219.6003 (0.015)</td>
</tr>
<tr>
<td>220.2550290</td>
<td>222.4741 (1.0)</td>
<td>221.8307 (0.7)</td>
<td>221.6792 (0.65)</td>
<td>220.1503 (0.05)</td>
<td>220.2378 (0.008)</td>
<td>220.3003 (0.021)</td>
</tr>
<tr>
<td>254.5148790</td>
<td>256.0261 (0.6)</td>
<td>255.0061 (0.2)</td>
<td>254.8096 (0.12)</td>
<td>252.7502 (0.69)</td>
<td>254.4002 (0.045)</td>
<td>254.5502 (0.014)</td>
</tr>
</tbody>
</table>
B. Four interacting bosons in one dimension

In this subsection the equation for the energy levels is derived for \( N = 4 \) interacting particles in a one-dimensional box with periodic boundary conditions. The necessary steps to find this equation are similar to those in the previous subsection. In fact, the SD method can be generalized straightforwardly to any number of interacting particles, although the algebra becomes more complicated for \( N > 4 \). The energy levels for \( N = 4 \) particles are the zeros of the determinant of operator \( L \) given in Eq. (20).

The first few energy levels obtained from solving are listed in Table II. The strength of the interactions is \( \lambda = 4.0 \).

For the sake of comparison the exact energy levels obtained from the Bethe ansatz solution and the results found from the direct diagonalization of the Hamiltonian are also listed in the table. Both in the SD method and in the diagonalization method the same \( 2m + 1 \) one-particle wave functions were used. The percentage errors with respect to the exact Bethe ansatz solutions are indicated in brackets.

From the table one can see that the relative errors using the SD method are more than an order of magnitude smaller than those obtained from direct diagonalization. In particular, using a rather small number of one-particle wave functions, \( 2m + 1 = 9 \), the ground state energy is much more accurate (0.01\%) compared to those obtained from the diagonalization method.

Note that to find the energy levels with the above indicated errors only the determinant of a \( 9 \times 9 \) matrix had to be calculated. This suggests that in numerical calculations the SD method is much more efficient than the conventional diagonalization method. Comparing the two methods one realizes that although in our method more algebra is needed than in the diagonalization methods, less numerical effort is required to obtain the values of the energy levels accurately. It is important to note that the expression for determining the energy eigenvalues becomes more complicated with increasing the number of interacting particles but the necessary steps are quite straightforward and a quite simple algorithm can be given.

<table>
<thead>
<tr>
<th>Bethe ansatz</th>
<th>Diagonalization</th>
<th>Spectral determinant method</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E )</td>
<td>( m = 2 )</td>
<td>( m = 3 )</td>
</tr>
<tr>
<td>20.8016</td>
<td>21.34 (2.6)</td>
<td>21.22 (2.01)</td>
</tr>
<tr>
<td>70.8207</td>
<td>71.74 (1.3)</td>
<td>71.51 (0.97)</td>
</tr>
<tr>
<td>113.7688</td>
<td>114.83 (0.9)</td>
<td>114.56 (0.69)</td>
</tr>
<tr>
<td>118.4289</td>
<td>119.59 (1.0)</td>
<td>119.31 (0.74)</td>
</tr>
<tr>
<td>149.7776</td>
<td>150.78 (0.7)</td>
<td>150.51 (0.49)</td>
</tr>
<tr>
<td>158.5862</td>
<td>159.78 (0.8)</td>
<td>159.49 (0.57)</td>
</tr>
<tr>
<td>178.7153</td>
<td>179.47 (0.4)</td>
<td>179.25 (0.30)</td>
</tr>
<tr>
<td>191.2125</td>
<td>192.43 (0.6)</td>
<td>192.08 (0.46)</td>
</tr>
<tr>
<td>195.3592</td>
<td>196.46 (0.6)</td>
<td>196.20 (0.43)</td>
</tr>
<tr>
<td>237.5430</td>
<td>239.00 (0.6)</td>
<td>238.59 (0.44)</td>
</tr>
<tr>
<td>238.2730</td>
<td>239.68 (0.6)</td>
<td>239.31 (0.43)</td>
</tr>
<tr>
<td>276.3426</td>
<td>277.84 (0.5)</td>
<td>277.40 (0.38)</td>
</tr>
<tr>
<td>277.9374</td>
<td>279.30 (0.5)</td>
<td>278.97 (0.37)</td>
</tr>
<tr>
<td>281.8038</td>
<td>283.42 (0.6)</td>
<td>282.94 (0.40)</td>
</tr>
</tbody>
</table>

TABLE II. The exact energy levels obtained from the Bethe ansatz and our numerical results using \( 2m + 1 \) one-particle wave functions. In the diagonalization method we used the same one-particle wave functions as in the SD method. The relative errors in percentage are indicated in brackets. The strength of the interactions is \( \lambda = 4.0 \).
V. TWO INTERACTING BOSONS WITH ONE IMPURITY IN ONE DIMENSION

As a further illustration of the SD method, in this subsection we consider a system including two particles and an impurity in a one-dimensional box with periodic boundary conditions. In this case no exact results, such as Bethe ansatz solutions, are known for the energy levels. The Hamiltonian of the system is $H = H_0 + H_1$, where $H_0$ is given by Eq. (8). The interaction Hamiltonian of the system can be written as

$$H_1(x_1, x_2) = \lambda \delta(x_1 - x_2) + \kappa [\delta(x_1 - u) + \delta(x_2 - u)],$$

where the strength of the interaction between the two particles and the strength of the potential for the impurity are denoted by $\lambda$ and $\kappa$, respectively. The impurity is located at $u$. The GF of the system is given by Eq. (18) with $M = 1$. The energy levels of the system are the roots of the denominator in (15), which in our case, can be written as

$$\det \begin{bmatrix} L(y, y'; E) & G_0(y, y|y', u; E) \\ G_0(y, u|y', y; E) & K(y, y'; E) \end{bmatrix} = 0,$$

where

$$L(y, y') = -\frac{1}{\lambda} \delta(y - y') + G_0(y, y|y', y'),$$

$$K(y, y') = -\frac{1}{2\kappa} \delta(y - y') + G_0(y, u|y', u).$$

The Green’s function $G_0(x_1, x_2|x_1', x_2')$ of the Hamiltonian $H_0$ can be written as

$$G_0(x_1, x_2|x_1', x_2') = \frac{1}{2\pi} \sum_{n_1 n_2} \sum_{P \in S_2} \psi_{n_1}(x_1) \psi_{n_2}(x_2) \frac{\psi^{*}_{n_{P_1}}(x'_1) \psi^{*}_{n_{P_2}}(x'_2)}{E - E_{n_1} - E_{n_2}}$$

$$= \frac{1}{2} \left( \sum_{n,m} \psi_n(x_1) \psi_m(x_2) \frac{\psi^*_{n}(x'_1) \psi^{*}_{m}(x'_2)}{E - E_n - E_m} + \sum_{n,m} \psi_n(x_1) \psi_m(x_2) \frac{\psi^*_{n}(x'_1) \psi^{*}_{m}(x'_2)}{E - E_n - E_m} \right),$$

where $\psi_n(x)$ and $E_n$ are given by Eqs. (31) and (32), respectively (with $\alpha = 1$). In Eq. (36) the four matrix elements contain the two-particle Green’s function $G_0(x_1, x_2|x_1', x_2')$ with different arguments. The four matrix elements are operators but for numerical calculations we need to represent them by matrices. This can be done by using a set of orthogonal wave functions:

$$\varphi_k(y) = e^{2\pi i k(y-u)},$$

where the extra phase $e^{-2\pi i u}$ is introduced for the sake of convenience. Then, in this basis, the Green’s function $G_0$ appearing in the matrix elements 1, 1, 1, 2, 2, and 2, 2 of Eq. (36) becomes

$$G^{(11)}_0(k|l) = \delta_{k,l} \sum_n \frac{1}{E - E_n - E_{k-n}},$$

$$G^{(12)}_0(k|l) = \frac{1}{E - E_l - E_{k-l}},$$

$$G^{(21)}_0(k|l) = \frac{1}{E - E_k - E_{l-k}} = G^{(12)}_0(l|k),$$

$$G^{(22)}_0(k, l) = \frac{1}{2} \left( \frac{1}{E - E_k - E_l} + \delta_{k,l} \sum_n \frac{1}{E - E_k - E_n} \right).$$

The sum over $n$ in $G^{(11)}_0(k|l)$ can be carried out by using the identities Eq. (31), while the summation in $G^{(22)}_0(k|l)$ can be performed using the identity (25)

$$\sum_{n=\infty}^{\infty} \frac{1}{z^2 - n^2} = \frac{\pi \cot \pi z}{z}.\quad (42)$$

Finally, the matrix representation of Eq. (36) becomes
where the four elements of the hypermatrix are

\[
\begin{align*}
M'_{k,l}^{(11)} &= \delta_{k,l} \left( -\frac{1}{\lambda} + S_k \right), \\
M'_{k,l}^{(12)} &= \frac{1}{E - 4\pi^2 [l^2 + (k - l)^2]}, \\
M'_{k,l}^{(21)} &= M'_{k,l}^{(12)}, \\
M'_{k,l}^{(22)} &= \delta_{k,l} \left( -\frac{1}{2\kappa} + \frac{1}{4\pi^2} \cot \pi z_2 \right) + \frac{1}{E - 4\pi^2 (k^2 + l^2)},
\end{align*}
\]

with

\[
S_k = \begin{cases} 
\frac{1}{4\pi z_1} \cot \left( \frac{\pi}{2} z_1 \right) & \text{for } k \text{ even,} \\
\frac{1}{4\pi z_2} \tan \left( \frac{\pi}{2} z_1 \right) & \text{for } k \text{ odd,}
\end{cases}
\]

\[
z_1 = \sqrt{\frac{E}{2\pi^2} - k^2} \quad \text{and} \quad z_2 = \sqrt{\frac{E}{4\pi^2} - k^2}.
\]

Note that to calculate numerically the determinant in Eq. (43) it is useful to apply an equivalent form of the general matrix identity for hypermatrices given in Eq. (12)

\[
\det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \det(a) \det(d - ca^{-1}b)
\]

which holds for arbitrary square matrices \(a\) and \(d\), with \(\det a \neq 0\). Then, the dimensions of the minors are half of the original one. Since the matrix \(L^{-1}\) is diagonal, it is easy to calculate its inverse.

The first few energy levels obtained from solving Eq. (43) numerically are listed in Table III. The strength of the interactions and the strength of potential for the impurity are \(\lambda = 3.0\) and \(\kappa = 2.0\), respectively.

<table>
<thead>
<tr>
<th>'Exact' (E) (4 digits)</th>
<th>Diagonalization</th>
<th>Spectral determinant method</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E)</td>
<td>(m = 2)</td>
<td>(m = 3)</td>
</tr>
<tr>
<td>6.1175</td>
<td>6.3153 (3.2)</td>
<td>6.2583 (2.3)</td>
</tr>
<tr>
<td>46.8629</td>
<td>47.1405 (0.6)</td>
<td>47.0458 (0.4)</td>
</tr>
<tr>
<td>50.4776</td>
<td>50.8832 (0.8)</td>
<td>50.7582 (0.6)</td>
</tr>
<tr>
<td>82.9012</td>
<td>83.0716 (0.2)</td>
<td>82.9998 (0.1)</td>
</tr>
<tr>
<td>85.5893</td>
<td>85.8157 (0.3)</td>
<td>85.7852 (0.2)</td>
</tr>
<tr>
<td>91.2389</td>
<td>91.7645 (0.6)</td>
<td>91.5606 (0.4)</td>
</tr>
<tr>
<td>165.5271</td>
<td>165.9033 (0.2)</td>
<td>165.7284 (0.1)</td>
</tr>
<tr>
<td>169.3990</td>
<td>170.0690 (0.4)</td>
<td>169.7556 (0.2)</td>
</tr>
<tr>
<td>203.1501</td>
<td>203.5057 (0.2)</td>
<td>203.3933 (0.1)</td>
</tr>
<tr>
<td>206.9552</td>
<td>207.5140 (0.3)</td>
<td>207.2107 (0.1)</td>
</tr>
<tr>
<td>207.1812</td>
<td>207.5666 (0.2)</td>
<td>207.4673 (0.1)</td>
</tr>
<tr>
<td>210.9868</td>
<td>211.9115 (0.4)</td>
<td>211.4817 (0.2)</td>
</tr>
</tbody>
</table>

TABLE III. The ‘exact’ energy levels (results to four significant figures using 61 one-particle wave functions) and our numerical results obtained from Eq. (13) using \(2m + 1\) one-particle wave functions. In the diagonalization method we used the same one-particle wave functions as in the SD method. The percentage errors are indicated in brackets. The strength of the interactions and the strength of potential for the impurity are \(\lambda = 3.0\) and \(\kappa = 2.0\), respectively.

No Bethe ansatz type solution is known when the system includes impurity. The ‘exact’ energy eigenvalues are calculated by increasing the number of one-particle wave functions until all the energy levels listed in the first column of the table are converged to four significant figures. To reach this convergence, 61 one-particle wave functions were used. Then the errors of the energy eigenvalues found from the SD method and from the direct diagonalization of the Hamiltonian are compared using the same number of one-particle wave functions. As it is seen from Table III, our method usually gives again an order of magnitude more accurate results than the diagonalization of the Hamiltonian.
VI. THREE INTERACTING FERMIONS WITH ONE IMPURITY IN ONE DIMENSION AND CALCULATION OF THE PERSISTENT CURRENT

In this section our SD method is applied for a more complicated problem. We consider the one dimensional ring including \( N = 3 \) interacting 1/2 spin-fermions. The external magnetic field is applied along the axis perpendicular to the plane of the ring. In addition, a single impurity is also included in an arbitrary position. The persistent current is the derivative of the ground state with respect to the flux of the magnetic field inside the ring \([55] \):

\[
I = -e \frac{dE(\Phi)}{d\Phi},
\]

where \( E(\Phi) \) is the energy of the ground state of the system with flux \( \Phi \) through the ring. The ground state energy is the smallest poles of the GF for fermion systems given by Eq. \([23] \) in section \([11] \).

The GF is constructed from the one-particle wavefunctions:

\[
\psi_{n,\sigma}(x) = e^{2\pi i (n+\Phi) x} \sigma_s,
\]

where \( \sigma = |\uparrow>, |\downarrow> \), \( s = 1, 2 \) denoting the spinor index of the spin state \( \sigma \) and \( \Phi \) is the magnetic flux in units of flux quantum \( h/e \). The corresponding eigenvalues of the free one-electron Hamiltonian are \( E_n = 4\pi^2(n + \Phi)^2 \) with \( n = 0, \pm 1, \pm 2, \cdots \).

The unperturbed GF appearing in Eq. \([23] \) can be constructed from the above given one-particle wave functions. For fermions the symmetrized form is:

\[
G_0 = \frac{1}{3!} \sum_{p,q,r} (-1)^p \psi_{n_1,\sigma_1}(x_1) \psi_{n_2,\sigma_2}(x_2) \psi_{n_3,\sigma_3}(x_3) \delta_{\sigma_1\sigma_2\sigma_3} \sigma_s \sigma_s \psi_{n_1,\sigma_1}^* \psi_{n_2,\sigma_2}^* \psi_{n_3,\sigma_3}^* \delta_{\sigma_1\sigma_2\sigma_3} \sigma_s \delta_{E_n_1 - E_n_2 - E_n_3},
\]

where the \( S_3 \) denotes the permutation group as given after Eq. \([27] \). The denominator of the GF in \([23] \) can be transformed into a matrix form by using the non-symmetrized product of the one-particle wave functions as it was done in the case of bosons. The determinant of this matrix takes the following 2 by 2 hypermatrix form:

\[
\det \begin{bmatrix}
M^{(11)} & M^{(12)} \\
M^{(21)} & M^{(22)}
\end{bmatrix},
\]

where the \( p = (k,l,s_1,s_2,s_3) \), \( q = (k',l',s'_1,s'_2,s'_3) \) matrix element of the matrices \( M \) is given by

\[
M^{(11)}_{pq} = -\frac{1}{3!} \delta_{k,k'} \delta_{l,l'} \delta_{s_1,s'_1} \delta_{s_2,s'_2} \delta_{s_3,s'_3} + \frac{1}{6} \sum_{P \in S_3} \sum \frac{\delta_{n_1+n_2,k} \delta_{n_3,l} \delta_{n_{P(1)},n_{P(2)},k} \delta_{n_{P(3)},l'}}{E - E_{n_1} - E_{n_2} - E_{n_3}} \delta_{s_{P(1)},s'_1} \delta_{s_{P(2)},s'_2} \delta_{s_{P(3)},s'_3},
\]

\[
M^{(12)}_{pq} = \frac{1}{6} \sum_{P \in S_3} \sum \frac{\delta_{n_1+n_2,k} \delta_{n_3,l} \delta_{n_{P(1)},n_{P(2)},k'} \delta_{n_{P(3)},l'}}{E - E_{n_1} - E_{n_2} - E_{n_3}} \delta_{s_{P(1)},s'_1} \delta_{s_{P(2)},s'_2} \delta_{s_{P(3)},s'_3},
\]

\[
M^{(21)}_{pq} = \frac{1}{6} \sum_{P \in S_3} \sum \frac{\delta_{n_2,n_3,k} \delta_{n_{P(1)}} \delta_{n_{P(2)},k'} \delta_{n_{P(3)},l'}}{E - E_{n_1} - E_{n_2} - E_{n_3}} \delta_{s_{P(1)},s'_1} \delta_{s_{P(2)},s'_2} \delta_{s_{P(3)},s'_3},
\]

\[
M^{(22)}_{pq} = -\frac{1}{3!} \delta_{k,k'} \delta_{l,l'} \delta_{s_1,s'_1} \delta_{s_2,s'_2} \delta_{s_3,s'_3} + \frac{1}{6} \sum_{P \in S_3} \sum \frac{\delta_{n_2,n_3,k} \delta_{n_{P(1)}} \delta_{n_{P(2)},k'} \delta_{n_{P(3)},l'}}{E - E_{n_1} - E_{n_2} - E_{n_3}} \delta_{s_{P(1)},s'_1} \delta_{s_{P(2)},s'_2} \delta_{s_{P(3)},s'_3}.
\]

Since these matrices are infinite dimensional ones we truncate them by restricting \( k, l \) between \(-m \) and \( m \), where \( 2m+1 \) is the number of one-particle wave functions given by \([19] \). Because of the spin indices each \( (k,l),(k',l') \) elements of the matrices \( M \) still correspond to 8 by 8 matrices. Therefore in Eq. \([23] \) the hypermatrix is a \( 2 \cdot 8 \cdot (2m+1)^2 \) dimensional matrix. Grouping these elements by the total \( S_2 \) of the three fermions we may reduce the dimension of the matrix into a \((2+3) \cdot (2m+1)^2 \) dimensional one. This dimensional reduction is possible because we omit the energy independent factors in the matrix elements.

The above given matrix elements still contain summations which can be evaluated by using the following identity \([23] \):

\[
\sum \delta_{s_{P(1)},s'_1} \delta_{s_{P(2)},s'_2} \delta_{s_{P(3)},s'_3} = \frac{1}{3!} \delta_{s_{P(1)},s_{P(2)},s_{P(3)}}.
\]

13
\[ \sum_{n=-\infty}^{\infty} \frac{1}{(n+\Phi)^2 - z^2} = \frac{\pi}{2z} \left( \cot \pi(\Phi - z) - \cot \pi(\Phi + z) \right). \]  

In Fig. 4 the persistent currents obtained by our SD method as a function of flux in units of flux quantum \( h/e \) are shown for different impurity strengths \( \kappa \). In this calculation \( 2m + 1 = 5 \) one-particle wave functions are used.

FIG. 4. The persistent current calculated by the SD method is plotted (in arbitrary units) as a function of the flux (in units of \( \Phi_0 = h/e \)) for fixed interaction strength \( \lambda = 2 \) and different impurity strength \( \kappa \). We used \( 2m + 1 = 5 \) one-particle wave functions.

One can see that the persistent current suppresses with increasing the strength of the impurity. Our purpose in this paper is to demonstrate how our SD method can be applied to different problems such as the calculation of the persistent current. A more complete analysis of the persistent current problem is beyond the scope of this paper. The work along this line is in progress.

VII. CONCLUSIONS

In this paper the Green’s functions of many-body systems were calculated when the interactions between the particles are Dirac-delta type contact potentials, and when the system contains impurities described by contact potentials. The Hamiltonian of the system is taken as a sum of two parts, the first of which contains only the sum of the one-particle Hamiltonians, while the second contains the rest, namely the interactions between the particles and the potentials of the impurities. Using the Dyson equation for the Green’s function the iterative solution for the Green’s function can be formally given as the ratio of two determinants. However, in this formal expression the matrix elements of the determinants are ‘indexed’ by continuous variables. To handle these determinants one can use any complete orthogonal set of wave functions and the corresponding operators in the determinants can be given in the usual matrix representation. This makes the numerical calculation of the Green’s function possible.

After presenting the general formalism for deriving the Green’s function, several examples were discussed in order to show the relevant steps in the algebra as well as to test the method. Only the energy eigenvalues were calculated for different systems. However, in our method the full Green’s function is given, therefore, in principle, it can be used for calculating other types of physical quantities. The energy levels can be found by determining the poles of the Green’s function. Since the Green’s function of the system is given by the ratio of two determinants, one only needs to calculate the zeros of the spectral determinant (in the denominator of the Green’s function) to obtain the energy eigenvalues of the system.

For testing our method, we used a one-dimensional model of bosons interacting via Dirac-delta interactions. In this case the energy eigenvalues can be calculated exactly from the well known Bethe ansatz solution. In the case of two interacting bosons it was shown algebraically that the SD method yields exactly the same energy levels as those obtained from the Bethe ansatz solution. For the case of three and four interacting bosons an equation for determining the energy levels was derived and then it was solved numerically. The results obtained from our method are in very good agreement with those obtained from the Bethe ansatz solution. A comparison of our method with
the direct diagonalization of the Hamiltonian was also presented. The same number of one-particle wave functions was used in the latter method as in the SD approach. It was demonstrated that our method gives, in general, ten times smaller relative errors than the diagonalization method. The energy of the ground state of the system can be obtained with even better accuracy in spite of the fact that only a few one-particle wave functions were used (typically 9; the relative errors were then less than 0.01%). As a nontrivial example we calculated the energy levels of a system including two interacting bosons and one impurity. Both the interactions and the potential of the impurity were of Dirac-delta type. Applying our general method, we derived an equation for the energy levels of the system. Since no Bethe ansatz type of solution is known in this case, by increasing the number of one-particle wave functions we calculated the energies by making the result convergent to 4 significant figures. Taking these energy levels as the exact ones, we compared our method with direct diagonalization. A much better accuracy was found in the SD method (e.g. for the ground state with 9 one-particle wave functions the relative error was about 0.003%, while it was 2.6% with the diagonalization method).

Our method was also applied to spin-full fermion systems. A better accuracy was achieved in calculating the ground state energy comparing the diagonalization method. Therefore our method is expected to be suited for numerical calculations for the persistent current. We demonstrated the applicability of our SD method for the case of three interacting fermions and one impurity, and calculated the persistent current. We defer a thorough study of the persistent current in a later publication.

In summary, we developed a spectral determinant method with which much more accurate values of the energy levels can be obtained numerically than with the usual direct diagonalization method. In our formalism the full Green’s function is available, thus it might be used in the TIP and persistent current problem mentioned in the introduction.

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APPENDIX A: TWO INTERACTING PARTICLES WITH M IMPURITIES

In this section an expression for the GF is derived for the case of two interacting particles and M impurities. The interaction Hamiltonian \( H_1 \) is given by

\[
H_1 = \sum_{i=1}^{M} \kappa_i (\delta(x_1 - u_i) + \delta(x_2 - u_i)) + \lambda \delta(x_1 - x_2),
\]

(A1)

where \( u_i \) is the location of the \( i \)th impurity, of strength \( \kappa_i \) and \( \lambda \) is the strength of the interaction between the particles. As in the case of a single impurity, the first-order correction (in \( H_1 \)) of the iterative solution of the Dyson equation is

\[
G^{(1)} = \int G_0(x_1, x_2|y_1, y_2) H_1(y_1, y_2) G_0(y_1, y_2|x'_1, x'_2) \, dy_1 dy_2.
\]

(A2)

Inserting \( H_1 \) into the above expression the integrals can be performed exactly for Dirac delta potentials. Collecting the identical terms arising from permutational symmetry, the first order correction of the GF is

\[
G^{(1)} = \int \sum_{i=1}^{M} 2 \kappa_i G_0(x_1, x_2|y, u_i) G_0(y, u_i|x'_1, x'_2) + \lambda G_0(x_1, x_2|y, y) G_0(y, y|x'_1, x'_2) \, dy.
\]

(A3)

Similarly, the second order correction takes the form

\[
G^{(2)} = \int G_0(x_1, x_2|y_1, y_2) H_1(y_1, y_2) G_0(y_1, y_2|y'_1, y'_2) H_1(y'_1, y'_2) G_0(y'_1, y'_2|x'_1, x'_2) \, dy_1 dy_2 dy'_1 dy'_2.
\]

(A4)

Higher order corrections can be easily found. In a way similar to the case of \( G^{(1)} \) we have
Using Eqs. (A7), (A8), and the matrix identity in Eq. (12), the GF can be rewritten as the ratio of two determinants:

$$G^{(2)} = \int \sum_{i,j=1}^{M} 2\kappa_i G_0(x_1, x_2|y, u_i) 2\kappa_j G_0(y, u_i|y', u_j) G_0(y', u_j|x_1', x_2') \, dydy'$$

$$+ \int \sum_{i=1}^{M} 2\kappa_i G_0(x_1, x_2|y, u_i) \lambda G_0(y, u_i|y', y') G_0(y', y'|x_1', x_2') \, dydy'$$

$$+ \int \sum_{j=1}^{M} \lambda G_0(x_1, x_2|y, y) 2\kappa_j G_0(y, y|y', u_j) G_0(y', u_j|x_1', x_2') \, dydy'$$

$$+ \int \lambda G_0(x_1, x_2|y, y) G_0(y, y|y', y') G_0(y', y'|x_1', x_2') \, dydy'.$$

It can be shown that the GF including the higher order corrections is

$$G = G_0 + \int \sum_{\alpha=1}^{M+1} A_\alpha(y) B_\alpha(y) \, dy + \int \sum_{\alpha,\beta=1}^{M+1} A_\alpha(y) C_{\alpha\beta}(y, y') B_\beta(y') \, dydy' + \ldots$$

$$= G_0 + \int \sum_{n=0}^{\infty} \sum_{\alpha,\beta=1}^{M+1} A_\alpha(y) \left( C_{\alpha\beta}(y, y') \right)^n B_\beta(y') \, dydy',$$

where

$$A_\alpha(y) = \left( \frac{2\kappa_i G_0(x_1, x_2|y, u_i)}{\lambda G_0(x_1, x_2|y, y)} \right), \quad B_\beta(y') = \left( \frac{G_0(y', u_j|x_1', x_2')}{G_0(y'|x_1', x_2')} \right),$$

are \((M+1)\)-component vectors \((i = 1, \ldots, M)\) and

$$C_{\alpha\beta}(y, y') = \left( \begin{array}{c} 2\kappa_j G_0(y, u_i|y', u_j) \\ 2\kappa_j G_0(y, y|y', y') \\ \lambda G_0(y, u_i|y', y') \end{array} \right),$$

is an \((M+1) \times (M+1)\) matrix. This is a Neumann series which can be summed:

$$G = G_0 + \int \sum_{\alpha,\beta=1}^{M+1} A_\alpha(y) \left( \delta(y - y') \delta_{\alpha\beta} - C_{\alpha\beta}(y, y') \right)^{-1} B_\beta(y') \, dydy'.$$

Using Eqs. (A7), (A8), and the matrix identity in Eq. (12), the GF can be rewritten as the ratio of two determinants:

$$G(x_1, x_2|x_1', x_2') = \frac{\det \begin{bmatrix} G_0(x_1, x_2|x_1', x_2') & G_0(x_1, x_2|y', y') & G_0(x_1, x_2|u_1, y') & \cdots & G_0(x_1, x_2|u_M, y') \\ G_0(y, y|x_1', x_2') & L(y|y') & G_0(y, y|u_1, y') & \cdots & G_0(y, y|u_M, y') \\ G_0(u_1, y|x_1', x_2') & G_0(u_1, y|y', y') & K_1(y|y') & \cdots & G_0(u_1, y|u_M, y') \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G_0(u_M, y|x_1', x_2') & G_0(u_M, y|y', y') & G_0(u_M, y|u_1, y') & \cdots & K_M(y|y') \end{bmatrix}}{\det \begin{bmatrix} L(y|y') & G_0(y, y|u_1, y') & \cdots & G_0(y, y|u_M, y') \\ G_0(u_1, y|y', y') & K_1(y|y') & \cdots & G_0(u_1, y|u_M, y') \\ \vdots & \vdots & \ddots & \vdots \\ G_0(u_M, y|y', y') & G_0(u_M, y|u_1, y') & \cdots & K_M(y|y') \end{bmatrix}}.$$  

\(K_i(y|y') = -\frac{1}{2\kappa_i} \delta(y - y') + G_0(u_i, y|u_i', y'),\)  

and  

\(L(y|y) = -\frac{1}{\lambda} \delta(y - y') + G_0(y, y|y', y').\)
APPENDIX B: TWO INTERACTING BOSONS IN ONE DIMENSION

In this subsection an equation for the energy levels of a system with two interacting electrons in one dimension with periodic boundary conditions is derived. It turns out that this equation is the same as that obtained from the Bethe ansatz solution. Thus, the two methods lead to the same energy levels in this case.

Consider a one dimensional box of length $a$, with periodic boundary conditions. The one-particle Hamiltonian is given by Eq. (3), the potential $V(x)$ is zero. Using periodic boundary conditions the one-particle eigenfunctions of this Hamiltonian are given by

$$\psi_k(x) = \frac{1}{\sqrt{a}} e^{2\pi i k x/a},$$  \hspace{1cm} (B1)

and the eigenvalues are

$$E_k = \frac{4\pi^2 k^2}{a^2},$$ \hspace{1cm} (B2)

where $k = 0, \pm 1, \pm 2, \cdots$. From these wave functions one can construct the bosonic two-particle wave functions which may be written as

$$\psi_{n,m}(x,y) = \left\{ \begin{array}{ll}
\frac{\psi_n(x)\psi_m(y)+\psi_m(x)\psi_n(y)}{\sqrt{2}}, & \text{for } n > m, \\
\frac{\psi_n(x)\psi_m(y)}{\sqrt{2}}, & \text{for } n = m.
\end{array} \right.$$ \hspace{1cm} (B3)

For two interacting particles the GF and the operator $L(y_1, y_2)$ are given in Eqs. (18) and (20), respectively. Using Eqs. (B1) and (B3) the unperturbed two-particle GF and the operator $L(y_1, y_2)$ can be expressed in terms of the one particle eigenfunctions given in Eq. (B1):

$$G_0(x, x'|y, y') = \frac{1}{2} \sum_{n,m} \frac{\psi_n(x)\psi_m(x')\psi_n^*(y)\psi_m^*(y')}{E - E_n - E_m} + \frac{\psi_n(x)\psi_m(x')\psi_n^*(y)\psi_m^*(y')}{E - E_n - E_m},$$ \hspace{1cm} (B4)

$$L(y_1, y_2) = -\frac{1}{\lambda} \delta(y_1 - y_2) + \sum_{n,m} \frac{\psi_n(y_1)^*\psi_m(y_1)\psi_n^*(y_2)\psi_m^*(y_2)}{E - E_n - E_m},$$ \hspace{1cm} (B5)

where the strength of the interaction between the two particles is $\lambda$, and $E_n$ is given in Eq. (B2).

The poles of the Green’s function given in Eq. (B4) are the energy eigenvalues of the system. The equation determining the poles of GF is

$$\det L(y_1 | y_2) = 0,$$ \hspace{1cm} (B6)

where the operator $L(y_1 | y_2)$ is given by Eq. (B3). To evaluate the determinant it is convenient to use the basis given by Eq. (B1). The matrix element $L_{kl}$ of the operator $L(y_1 | y_2)$ is then

$$L_{kl} = \int_0^a \psi_k^*(y_1) L(y_1, y_2) \psi_l(y_2) \ dy_1 \ dy_2 = \delta_{k,l} \left( -\frac{1}{\lambda} + \frac{1}{a} \sum_{n} \frac{1}{E - E_n - E_{k-n}} \right),$$ \hspace{1cm} (B7)

where we have used the integral

$$\int_0^a \psi_k^*(x) \psi_n(x) \ \psi_m(x) \ dx = \frac{1}{\sqrt{a}} \delta_{n+m-k,0}.$$ \hspace{1cm} (B8)

Since the matrix $L_{kl}$ is diagonal, its determinant is

$$\det L_{kl} = \prod_{k=-\infty}^{+\infty} \left( -\frac{1}{\lambda} + \frac{1}{a} \sum_{n=-\infty}^{+\infty} \frac{1}{E - E_n - E_{k-n}} \right).$$ \hspace{1cm} (B9)

Thus, Eq. (B6) is equivalent to

$$\frac{a}{\lambda} = \sum_{n=-\infty}^{+\infty} \frac{1}{E - \frac{4\pi^2}{a^2} (n^2 + (k-n)^2)}.$$ \hspace{1cm} (B10)
where \( k = 0, \pm 1, \pm 2, \ldots \). Using the following identities

\[
\sum_{n=-\infty}^{+\infty} \frac{1}{z^2 - (2n)^2} = \frac{\pi}{2z} \cot \frac{\pi}{2z},
\]
\[
\sum_{n=-\infty}^{+\infty} \frac{1}{z^2 - (2n+1)^2} = -\frac{\pi}{2z} \tan \frac{\pi}{2z}.
\]

(B11)

the right hand side of Eq. (B10) can be written as

\[
2 \sqrt{2E - 4\pi^2 k^2 / a^2} = \cot \frac{a}{4} \sqrt{2E - 4\pi^2 k^2 / a^2} \text{ for } k \text{ even,} \tag{B12}
\]
\[
2 \sqrt{2E - 4\pi^2 k^2 / a^2} = -\tan \frac{a}{4} \sqrt{2E - 4\pi^2 k^2 / a^2} \text{ for } k \text{ odd.} \tag{B13}
\]

This result is equivalent to the Bethe ansatz solution \([19,22]\) for a one-dimensional Bose gas with Dirac delta interactions. According to the Bethe ansatz solution, the energy eigenvalues \( E \) of the \( N \) interacting particles can be determined from the solution for \( k_j \) of the following \( N \) equations:

\[
(-1)^{N-1} e^{-ik_ja} = \exp \left( i \sum_{s=1}^{N} -2 \arctan \frac{k_s - k_j}{\lambda / 2} \right), \tag{B14}
\]

where \( j = 1, 2, \ldots, N \) and

\[
E = \sum_{j=1}^{N} k_j^2. \tag{B15}
\]

For two particles, the two equations for \( k_1 \) and \( k_2 \) can be rewritten as

\[
e^{-iPa} = 1, \tag{B16}
\]
\[
e^{ia\sqrt{2E - P^2}} = \exp \left( -4i \arctan \frac{\sqrt{2E - P^2}}{\lambda / 2} \right), \tag{B17}
\]

where \( P = k_1 + k_2 \) is the total momentum of the particles. From the first equation we have \( P = 2\pi n/a \), where \( n \) is an integer, and the second equation may be written as \( \sqrt{2E - P^2} + 2\pi n_1 = -4 \arctan \frac{\sqrt{2E - P^2}}{\lambda / 2} \), where \( n_1 \) is another integer. Taking the tangent of this equation we find the same forms as given in Eqs. (B12)-(B13) for even and odd \( n_1 \), respectively.