Many-body formalism for fermions: Testing the enforcement of the Pauli principle

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Enforcing the Pauli principle in many-body systems of fermions to ensure an antisymmetric wave function is typically a numerically expensive task. Numerical methods, such as coupled-cluster, correlated basis function, Monte Carlo, and traditional configuration interaction, scale with powers of N that make the determination of the energy spectrum of these systems a challenge. In a recent paper, we successfully obtained energies for large systems of fermions in the unitary regime in which we applied the Pauli principle "on paper" without obtaining an explicit wave function. This approach, an extension of the symmetry invariant perturbation method to fermions, applies the Pauli principle by imposing restrictions on the quantum numbers used to obtain the energy. As a followup to this study, we perform an explicit test of the validity of this application of the Pauli principle by comparing our energy results against the energies corresponding to explicitly antisymmetrized wave functions for an exactly solvable system of harmonically confined, harmonically interacting fermions. Our results show that our simple method of applying the Pauli principle selects from a spectrum of possible many-body energies only those energies that correspond to explicitly antisymmetrized wave functions. Our results were tested for values of N through $\approx$10 000 and for weak and strong interactions both repulsive and attractive.

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I. INTRODUCTION

The Pauli principle, a postulate of quantum mechanics introduced in 1925, and the corresponding symmetrization postulate, which restricts the permutation symmetry of indistinguishable particles, are responsible for controlling the stability of our hadronic universe, intervening in a wide range of phenomena from neutron stars to chemical bonds. Providing an effective repulsion that is dependent on particle statistics as opposed to interparticle interactions, the Pauli principle can dominate the physical interaction and control the dynamics. When this effect is dominant, systems exhibit universal behavior as found in certain nuclear interactions and in trapped Fermi superfluids at unitarity.

Enforcement of the Pauli principle, i.e., the enforcement of an antisymmetric wave function, for fermionic systems is generally responsible for much of the expense of numerical calculations. Conventional full configuration interaction can cope with at most some ten particles for an exact solution [1], and methods such as coupled cluster [2] with a computational time polynomial in N, $O(N^7)$, where N is the number of particles, are expensive. Quantum Monte Carlo (QMC) methods for fermions suffer from the so-called sign problem [3–7] resulting in an exponential growth in simulation times unless additional approximations are made. In a previous paper, we obtained accurate energies for large systems of fermions using a method that enforces the Pauli principle "on paper." [8] The current approach is an extension of the symmetry invariant perturbation method (SPT) to fermions which uses group theory coupled with the inverse dimension of space as the perturbation parameter to rearrange the numerical work required for a many-body calculation into analytic building blocks. The blocks needed through first order, most of which do not involve the two-body interaction, have been calculated and stored previously thus reducing numerical requirements to a minimum. Applicable to both weakly and strongly interacting systems, this approach allows the use of a general two-body interaction and does not scale in complexity with N resulting in minimal numerical cost for high N calculations. This method was successfully applied to the unitary regime, a testing ground for new methods for which a number of very accurate calculations are available. Our $L = 0$ energies, where L is the total angular momentum, for $N < 30$ [8] were competitive with accurate Monte Carlo energies [9,10] including some recent benchmark calculations using the auxiliary field Monte Carlo method [11]. No explicitly antisymmetrized wave functions were required to obtain these energies since the Pauli principle was enforced on paper, resulting in restrictions on the quantum numbers used in the analytic formula for the energy.

Before tackling the important, but difficult challenge of constructing the correct antisymmetrized SPT N-body analytic wave function, we have devised a simple study to test the validity of the method used to enforce the Pauli principle in our earlier work in the unitary regime [8]. The present study connects our fermion energies directly to antisymmetrized wave functions by comparing against harmonium, an exactly solvable system of harmonically confined, harmonically interacting fermions. Earlier independent studies of harmonium have constructed explicitly antisymmetrized wave functions that yield specific fermion energies for the lowest $L = 0$, closed shell states [12–14]. Our method picks the correct fermion energies (and no spurious energies) from a full spectrum of SPT energies possible for this general N-body system. The correct energies are a very small percentage of the energies possible, and are accurate for all values of N and all interaction strengths both repulsive and attractive. Although this does not constitute a general proof, it is evidence that the procedure works in this model situation which is a fully interacting many-body problem.

The SPT formalism and applications to bosonic systems with spherical confinement can be found in a series of papers which determined lowest order energies, normal mode frequencies [15,16], and the lowest order wave function [17] and density profile [18]. In a later series of papers, we extended this work for bosons to first-order wave functions and density

profiles [19,20]. We demonstrated that this method rearranges the numerical work for this many-body problem into analytic building blocks at each order giving the exact result order by order in the perturbation series [20,21]. The complexity of the rearranged problem scales with the order of the perturbation series, not with the number of particles [21]. In the following section we give a brief review of the formalism.

II. FORMALISM

We define dimensionally scaled quantities $\bar{E} = \kappa(D)E$ and $\bar{H} = \kappa(D)H$, where $\kappa(D)$ is a scale factor which regularizes the large-dimension limit [17]. The scaled version of the Schrödinger equation is

$$\bar{H}\Phi = \left(\frac{1}{\kappa(D)}\bar{T} + \bar{V}_{\rm eff}\right)\Phi = \bar{E}\Phi, \tag{1}$$

where barred quantities indicate variables in scaled units [$\kappa(D) = D^2/(\hbar\bar{\omega}_{\rm ho})$ for this work; see Ref. [17]]. The term $\bar{T}$ contains the derivative terms of the kinetic energy and $\bar{V}_{\rm eff}$ includes centrifugal, two-particle, and confinement potentials [17].

We assume a totally symmetric, large-dimension configuration at which the effective potential is a minimum. The N particles are arranged on a hypersphere, each particle with a radius $\bar{r}_\infty$, from the center of the confining potential. Furthermore, the angle cosines between each pair of particles take on the same value, $\overline{\gamma}_\infty$, i.e., $\lim_{D\to\infty}\bar{r}_i = \bar{r}_\infty$ $(1 \leqslant i \leqslant N)$, $\lim_{D\to\infty}\gamma_{ij} = \overline{\gamma}_\infty$ $(1 \leqslant i < j \leqslant N)$. In scaled units, the $\delta = 1/D \to 0$ $(D \to \infty)$ approximation for the energy is simply the effective potential minimum, i.e., $\bar{E}_\infty = \bar{V}_{\rm eff}(\bar{r}_\infty, \overline{\gamma}_\infty;\ \delta = 0)$.

This highly symmetric, $\delta \to 0$ structure imparts a point group structure to the system which is isomorphic to the symmetric group of N identical objects [22], S_N, allowing a largely analytic solution. The $\delta \to 0$ approximation may be systematically improved by using it as the starting point for a perturbation expansion [23]. The S_N symmetry greatly simplifies this task since the interaction terms individually have to transform as a scalar under the S_N point group.

The perturbation series for the energy has the form

$$\bar{E} = \bar{E}_\infty + \delta\sum_{j=0}^{\infty}\left(\delta^{\frac{1}{2}}\right)^j \bar{E}_j. \tag{2}$$

In practice $\bar{E}_j = 0\ \forall\ j$ odd. The $j = 0$ term is obtained from a harmonic equation and referred to as the energy at harmonic order. To obtain this harmonic correction for small values of δ, we expand about the minimum of the $\delta \to 0$ effective potential.

The harmonic-order Hamiltonian is solved using the FG matrix method [24] to obtain the normal-mode frequencies $\bar{\omega}_\mu$. The number of roots λ_μ ($\lambda_\mu = \bar{\omega}_\mu^2$) of the secular equation $N(N+1)/2$ is potentially huge; however, due to the S_N symmetry, many roots are degenerate resulting in a reduction to five distinct roots.

Since the FG matrix is invariant under S_N, it does not connect subspaces belonging to different irreducible representations of S_N [25]. Thus the normal coordinates must transform under irreducible representations of S_N. The normal coordinates are linear combinations of the internal displacement vectors $\bar{r}_i$ and γ_{ij}, which transform under reducible representations of S_N. These reduce to two 1-dimensional $[N]$ irreducible representations denoted by $\mathbf{0}^+,\mathbf{0}^-$, two $(N-1)$-dimensional $[N-1,1]$ irreducible representations denoted by $\mathbf{1}^+,\mathbf{1}^-$, and one angular $N(N-3)/2$-dimensional $[N-2,2]$ irreducible representation denoted by $\mathbf{2}$ [15].

The energy through harmonic order in δ is [15,26]

$$\overline{E} = \overline{E}_\infty + \delta\left[\sum_{\mu=\{\mathbf{0}^\pm,\mathbf{1}^\pm,\mathbf{2}\}}\left(n_\mu + \frac{1}{2}d_\mu\right)\bar{\omega}_\mu + v_o\right], \tag{3}$$

where n_μ is the total number of quanta in the normal modes with the same frequency $\bar{\omega}_\mu$; μ is a label which runs over $\mathbf{0}^+$, $\mathbf{0}^-$, $\mathbf{1}^+$, $\mathbf{1}^-$, and $\mathbf{2}$, regardless of the number of particles in the system (see Ref. [15]), and v_o is a constant. The multiplicities of the five roots are $d_{\mathbf{0}^+} = 1$, $d_{\mathbf{0}^-} = 1$, $d_{\mathbf{1}^+} = N-1$, $d_{\mathbf{1}^-} = N-1$, and $d_{\mathbf{2}} = N(N-3)/2$. An analysis of the character of the normal modes reveals that the $\mathbf{2}$ normal modes are phonon, i.e., compressional modes; the $\mathbf{1}^\pm$ modes show single-particle character, $\mathbf{1}^+$ has single-particle angular behavior while $\mathbf{1}^-$ shows single-particle radial behavior. The $\mathbf{0}^+$ mode describes center-of-mass motion and $\mathbf{0}^-$ mode is a symmetric breathing motion.

III. ENFORCING THE PAULI PRINCIPLE

To study quantum systems of fermions, we must enforce the Pauli principle, thus requiring the N-body wave function to be antisymmetric. This is enforced by placing certain restrictions on the occupancies of the normal modes, i.e., on the values of the normal mode quantum numbers n_μ, $\mu = \mathbf{0}^\pm,\mathbf{1}^\pm,\mathbf{2}$ in Eq. (3) [26]. The possible assignments are found by relating the normal mode states $|n_{\mathbf{0}^+},n_{\mathbf{0}^-},n_{\mathbf{1}^+},n_{\mathbf{1}^-},n_{\mathbf{2}}\rangle$ to the states of the confining potential, a spherically symmetric three-dimensional harmonic oscillator, $V_{\rm conf}(r_i) = \frac{1}{2}m\omega_{\rm ho}^2 {r_i}^2$, for which the restrictions imposed by antisymmetry are known. These two series of states can be related in the double limit $D \to \infty$, $\omega_{\rm ho} \to \infty$ where both representations are valid.

For large D, the normal mode description given by Eq. (3) is exact. Applying the large $\omega_{\rm ho}$ limit results in

$$E = N\frac{D}{2}\hbar\omega_{\rm ho} + (2n_{\mathbf{0}^+} + 2n_{\mathbf{0}^-} + 2n_{\mathbf{1}^+} + 2n_{\mathbf{1}^-} + 2n_{\mathbf{2}})\hbar\omega_{\rm ho}. \tag{4}$$

Now consider $\omega_{\rm ho} \to \infty$ first and then $D \to \infty$. The harmonic oscillator levels are exact:

$$\begin{aligned} E &= \sum_{i=1}^{N}\left[n_i + \frac{D}{2}\right]\hbar\omega_{\rm ho} = \sum_{i=1}^{N}\left[(2v_i + l_i) + \frac{D}{2}\right]\hbar\omega_{\rm ho} \\ &= N\frac{D}{2}\hbar\omega_{\rm ho} + \sum_{i=1}^{N}(2v_i + l_i)\hbar\omega_{\rm ho}, \end{aligned} \tag{5}$$

where $n_i = 2v_i + l_i$, v_i is a radial, and l_i is an orbital angular momentum quantum number. Equating these two expressions which are equal in the double limit, the quantum numbers in the two representations can now be related to show the restrictions on normal mode states imposed by antisymmetry. Because of

the separation of radial and angular motions, two conditions result:

$$2n_{\mathbf{0}^-} + 2n_{\mathbf{1}^-} = \sum_{i=1}^{N} 2\nu_i,$$
$$2n_{\mathbf{0}^+} + 2n_{\mathbf{1}^+} + 2n_{\mathbf{2}} = \sum_{i=1}^{N} l_i. \quad (6)$$

These equations determine a set of possible normal mode states $|n_{\mathbf{0}^+},n_{\mathbf{0}^-},n_{\mathbf{1}^+},n_{\mathbf{1}^-},n_{\mathbf{2}}\rangle$ that are consistent with an antisymmetric wave function from the known set of permissible $L = 0$ harmonic oscillator configurations. As particles are added to the system at the $\omega_{\rm ho} \to \infty$ limit, additional harmonic oscillator quanta, ν_i and l_i, are, of course, needed to satisfy the Pauli principle. Equivalently, this corresponds to additional vibrational, i.e., normal mode quanta, that must accompany each new particle to maintain antisymmetry.

IV. APPLICATION: HARMONIUM

The Schrödinger equation for harmonium is

$$H = \frac{1}{2}\left(\sum_{i=1}^{N}\left[-\frac{\partial^2}{\partial \boldsymbol{r}_i^2} + \omega_t^2 \boldsymbol{r}_i^2\right] + \sum_{i=1}^{N-1}\sum_{j>i}^{N} \omega_p^2 \boldsymbol{r}_{ij}^2\right). \quad (7)$$

The exact lowest $L = 0$ antisymmetric eigenstate and corresponding energy have been determined in earlier studies [12–14]. We list some of these energies for several values of N up to ≈10 000 in Table I for two attractive potentials with $\lambda_p = 10^{-6}$ and $\lambda_p = 100$ where $\lambda_p = \frac{\omega_p}{\omega_t}$ is a measure of the interaction strength versus the confinement.

We obtain the SPT energies using the full formalism, defining symmetry coordinates from the internal displacement coordinates and using the FG method to solve for the five normal coordinates and their frequencies. The SPT energies are then obtained using Eq. (3) with the normal mode quanta n_μ determined from Eq. (6) to ensure antisymmetry. We choose quanta that correspond to the lowest values of the normal mode frequencies to yield the lowest $L = 0$ closed shell energy for each N. This results in occupation in $n_{\mathbf{1}^-}$ and $n_{\mathbf{2}}$ which have the lowest radial and angular frequencies, respectively:

$$2n_{\mathbf{1}^-} = \sum_{i=1}^{N} 2\nu_i, \quad 2n_{\mathbf{2}} = \sum_{i=1}^{N} l_i. \quad (8)$$

Note that the center-of-mass quanta $n_{\mathbf{0}^+}$ will always be zero for the ground state since there exists a lower angular frequency to occupy, ω_2. This result has also been derived independently for harmonium [13].

SPT actually yields the exact energies for this problem since at this order the Hamiltonian has been transformed into normal coordinates and yields the normal mode energies for the system. This normal mode spectrum includes energies that do not correspond to systems which obey the Pauli principle. Our method of enforcing the Pauli principle chooses only those energies that correspond to explicitly antisymmetrized wave functions, which are a small percentage of the full spectrum. The accuracy achieved is greater than or equal to the number of digits shown in Table I and is excellent for all energies, particle numbers, and interaction strengths, and for both attractive and repulsive cases. The fact that this method obtains the exact harmonium energies at harmonic order, although useful for making definitive identifications in regimes where energies are close together, is of course completely irrelevant to the actual enforcement of the Pauli principle which is simply a restriction placed on the normal mode quantum numbers at the double limit where one has access to knowledge about the Pauli principle.

TABLE I. Energies for closed shells in units of $\hbar\omega_t$ for a weakly attractive interaction ($\lambda_p^2 = 10^{-6}$) and a strongly attractive interaction ($\lambda_p^2 = 100$), from the exact solution [12] $E_{\rm ex}$ and using SPT, $E_{\rm SPT}$, with Eq. (3) after the correct quanta are determined from Eq. (6). Noninteracting energies are shown in column two.

N	$E_{\rm nonint}$	$E_{\rm ex} = E_{\rm SPT}(\lambda_p^2 = 10^{-6})$	$E_{\rm ex} = E_{\rm SPT}(\lambda_p^2 = 100)$
8	18.0	18.00006	4.684820×10^{2}
42	161.0	161.0033	1.033951×10^{4}
112	588.0	588.0328	6.207359×10^{4}
572	5148.0	5149.471	1.230876×10^{6}
1632	20808.0	20824.97	8.405441×10^{6}
3542	58443.9	58546.40	3.478133×10^{7}
10912	261888.0	263312.9	2.735681×10^{8}

V. CONCLUSIONS

The Pauli principle and symmetrization postulate have long been known to play critical roles in the stability of our universe. Particle statistics can also be powerful driving forces in the emergence of collective states of matter such as Bose-Einstein condensates. More recently particle statistics have been proposed as a mechanism for performing quantum information tasks [27]. In this paper we have performed an explicit test of our simple method of enforcing the Pauli principle using the SPT method that avoids the heavy numerical demands of constructing an explicitly antisymmetrized wave function. The correct selection from the many-body spectrum of harmonium of the fermion energies that are known to correspond to antisymmetric states and the absence of any spurious energies is strong evidence that this method of enforcing the Pauli principle on paper is valid. To date, the challenging task of obtaining the wave function using the SPT method has been achieved only for boson systems. Constructing the correct antisymmetrized SPT analytic wave function for large N systems of fermions remains an important goal for the full development of this formalism. However, the ability to obtain fermion energies, frequencies, and multiplicities for large N systems without the considerable numerical expense of explicitly antisymmetrizing the many-body wave function, and the success of this approach in obtaining energies competitive with Monte Carlo [8] in the unitary regime and other successful applications within conventional dimensional perturbation theory to fermion systems, including atoms, molecules, and quantum dots [26,28–30], suggest that this approach will offer interesting opportunities for the study of other systems of fermions.

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