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Many-body formalism for fermions: The partition function

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The partition function, a fundamental tenet in statistical thermodynamics, contains in principle all thermodynamic information about a system. It encapsulates both microscopic information through the quantum energy levels and statistical information from the partitioning of the particles among the available energy levels. For identical particles, this statistical accounting is complicated by the symmetry requirements of the allowed quantum states. In particular, for Fermi systems, the enforcement of the Pauli principle is typically a numerically demanding task, responsible for much of the cost of the calculations. The interplay of these three elements—the structure of the many-body spectrum, the statistical partitioning of the N particles among the available levels, and the enforcement of the Pauli principle—drives the behavior of mesoscopic and macroscopic Fermi systems. In this paper, we develop an approach for the determination of the partition function, a numerically difficult task, for systems of strongly interacting identical fermions and apply it to a model system of harmonically confined, harmonically interacting fermions. This approach uses a recently introduced many-body method that is an extension of the symmetry-invariant perturbation method (SPT) originally developed for bosons. It uses group theory and graphical techniques to avoid the heavy computational demands of conventional many-body methods which typically scale exponentially with the number of particles. The SPT application of the Pauli principle is trivial to implement since it is done "on paper" by imposing restrictions on the normal-mode quantum numbers at first order in the perturbation. The method is applied through first order and represents an extension of the SPT method to excited states. Our method of determining the partition function and various thermodynamic quantities is accurate and efficient and has the potential to yield interesting insight into the role played by the Pauli principle and the influence of large degeneracies on the emergence of the thermodynamic behavior of large-N systems.

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I. INTRODUCTION

A fundamental challenge in many branches of physics is understanding the emergence of properties of macroscopic systems. These large systems not only depend on microscopic information but are believed to be subject to powerful and general principles of organization. The emergence of thermodynamic properties at large particle number depends on collective organizational phenomena that are insensitive to the details of the microscopic interactions. Such collective states of matter exhibit what is called universal behavior that becomes exact in a macroscopic system but typically is inexact or even nonexistent in a small ensemble.

Recently universal behavior for controlled systems has been measured in a number of laboratories. Stabilized by the Pauli exclusion principle, strongly interacting ultracold Fermi gases exhibit signatures of the unitary regime including a superfluid phase transition [1–3], a large pairing gap [4–6], a high ratio of transition temperature T_c to Fermi energy E_F [1–3], and low viscosity [7–9]. Various thermodynamics quantities have been measured including the compressibility, the chemical potential, the entropy, the density, the pressure, and the heat capacity [1,2,5,10–14]. Theoretically this strongly interacting regime has been shown to obey a set of universal relations that connect the physics of few-body systems to many-body systems [15–18]. Universal behavior is also seen in a variety of other systems of current interest including the quark-gluon plasmas of the early universe, high-temperature superconductivity, and nuclear matter including neutron stars. Knowledge of the thermodynamics of the unitary gas thus has consequences for understanding the equation of state in these other interesting regimes.

Determining thermodynamic quantities theoretically requires the calculation of the partition function, i.e., access to the full energy spectrum and the corresponding degeneracies for the many-body states for which the correct symmetry has been imposed. For systems at higher temperatures that are weakly interacting, one can model the system using a continuum approximation such as the Fermi-Dirac distribution function or use a virial expansion approach [19–24].

In this study, we develop an approach to determine the partition function that is applicable to the ultracold, strongly interacting, controlled fermion systems currently of interest in the laboratory. The canonical partition function Z, a natural choice for systems with a constant particle number, is given by

$$Z = \sum_{j=0}^{\infty} g_j \exp(-E_j/T), \tag{1}$$

where the E_j are the many-body energy levels that correspond to wave functions with the appropriate symmetry, g_j is the degeneracy of the jth many-body state, and T is the temperature measured in energy units with the Boltzmann constant $k_B = 1$.

Obtaining this information for strongly interacting systems presents a challenge theoretically due to the exponential scaling of complexity as a function of particle number N. The brute force approach to determining the information needed, i.e., energy levels and degeneracies, is deceptively straightforward. The diagonalization of the full N-particle Hamiltonian with the Pauli principle enforced through

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appropriate antisymmetrization of the wave function yields the N-particle energy levels and their degeneracies. The diagonalization implicitly performs the partitioning of the energy among the different particles to yield the correct total energies, and the multiplicity of each many-body energy gives the degeneracy for this term in the partition function.

This approach, while conceptually straightforward, is numerically intractable for almost all systems. The ground-state energy alone requires computer resources that limit exact solutions using traditional full configuration interaction to about ten particles [25]. Accurate partition functions can require thousands if not many millions of energy levels depending on, among other things, the temperature. To date, determining the full energy spectrum of systems with four or more particles remains a challenge [26].

Interestingly, even determining the partition function for model systems with a completely known spectrum such as the confined ideal gas presents a nontrivial problem. This fact directs attention away from the usually challenging task of obtaining a many-body spectrum to focus on the difficulty of determining the degeneracies of the many-body states and enforcing the correct symmetry on those states. Both of these tasks are typically numerically demanding particularly for identical fermions which must obey the Pauli principle.

Previous studies on confined ideal gases readily reveal the challenge of determining an accurate partition function even with the complete spectrum at hand [27–32]. Exact recursion relations for the partition function can be formulated for a confined ideal gas of N identical particles with either Fermi-Dirac or Bose-Einstein statistics [27,28]. In fact the partition function of any system whose energies can be written as a sum of one-particle energies such as harmonium, a harmonically confined, harmonically interacting system, can be written recursively [27,33,34]. The resulting recursion relations are typically feasible only for $N \leqslant 10$. For fermions these recursion relations suffer from a "sign" problem due to enforcing the Pauli exclusion principle.

Other attempts to obtain the partition function of the ideal gas use large-N approximations including a Thomas-Fermi approximation [30] and the Fermi-Dirac distribution function [31,32].

Studies for interacting Fermi gases in harmonic traps have used the Hartree-Fock approximation [35], a path-integral approach which extracts out the partition function from a generating function [33,34], a method that determines the degeneracy of each energy level recursively and then performs an explicit summation [36], and a virial expansion method that uses results for two and three particles to get the two lowest orders [24].

In this paper, we present a conceptually different approach to the determination of the partition function. Although, in the present study, we apply it to a model problem, this approach is, in principle, applicable to systems with realistic interactions and has the potential to yield new insight into the influence of the Pauli principle and the degeneracies on the emergence of macroscopic behavior. It uses a recently introduced extension of a symmetry-invariant perturbation method (SPT) to fermion systems [37,38] which was originally developed for bosons [39–46]. This method uses the symmetry of high dimensions to bring the powerful methods of group theory and graphical techniques to bear on the many-body problem of identical particles. Specifically, we are able to rearrange the numerical work, which typically scales exponentially with the number of particles, into analytic building blocks that allow a formulation that does not scale with particle number N. These analytic building blocks have been calculated and stored previously, minimizing the work needed for new calculations. Results for all N at the same level of approximation, i.e., through first order in the perturbation, can be obtained simultaneously. The Pauli principle is applied "on paper," resulting in trivial numerical demands compared to conventional methods that explicitly enforce the antisymmetry of the many-body wave function. This method was recently successfully applied to the unitary regime where ground-state energies comparable in accuracy to benchmark Monte Carlo results for $N \leqslant 30$ were obtained in a few seconds of computer time [37]. We also performed an explicit test of our method of enforcing the Pauli principle using an exactly solvable model system of harmonically confined, harmonically interacting fermions [38].

In this method, first-order results for the full energy spectrum are readily accessible in the form of five normal-mode energies. The first-order spectrum is thus harmonic and fully known even for nonmodel problems with realistic interactions. The Pauli principle can be applied very simply through a trivial normal-mode quantum number assignment for each term in the infinite sum of states without ever obtaining the actual wave function. The degeneracy of each energy level is a natural result of doing a straightforward partitioning of the number of energy quanta among all N particles into different normal-mode assignments according to the Pauli principle and collecting the statistics.

In the following section we give a brief review of the formalism emphasizing the enforcement of the Pauli principle and the determination of the full spectrum of excited states at first order in the perturbation. This constitutes an extension of the SPT formalism to excited states.

II. THE SPT FORMALISM

The SPT method uses a dimensionally scaled version of the Schrödinger equation:

$$\bar{H}\Phi = \left(\frac{1}{\kappa(D)}\bar{T} + \bar{V}_{\rm eff}\right)\Phi = \bar{E}\Phi, \tag{2}$$

where $\kappa(D)$ is a scale factor which regularizes the large-dimension limit [42] and the barred quantities indicate variables in scaled units ($\kappa(D) = D^2/(\hbar\bar{\omega}_{\rm ho})$ for this work; see Ref. [42]). The term $\bar{T}$ contains the derivative terms of the kinetic energy and $\bar{V}_{\rm eff}$ includes centrifugal, two-particle, and confinement potentials [42].

At large dimension, a totally symmetric configuration of the N particles is chosen. Each particle has the same radius, $\bar{r}_\infty$, from the center of the confining potential, and the same angle cosine, $\overline{\gamma}_\infty$, with every other particle. This highly symmetric, $\delta = 1/D \to 0$ $(D \to \infty)$ structure imparts a point group structure to the system which is isomorphic to the symmetric group of N identical objects [47], 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 [41] whose terms individually have to transform as a scalar under the S_N point group.

The perturbation series for the energy has the form

$$\bar{E} = \bar{E}_\infty + \delta \sum_{j=0}^{\infty} (\delta^{\frac{1}{2}})^j \bar{E}_j, \tag{3}$$

where $\bar{E}_j = 0 \; \forall \; j$ odd. The $j = 0$ term is obtained from a harmonic equation and referred to as the first-order energy. 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 [48] to obtain the normal-mode frequencies $\bar{\omega}_\mu$. The $N(N+1)/2$ roots, $\bar{\omega}_\mu^2$, of the secular equation are highly degenerate due to the S_N symmetry, resulting in a reduction to five distinct roots irrespective of the number of particles.

Since the FG matrix is invariant under S_N, its normal coordinates must transform under irreducible representations of S_N [49]. 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 one-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 $\mathbf{2}$ [39].

The energy through first order in δ is [39]

$$\overline{E} = \overline{E}_\infty + \delta \left[\sum_{\mu = \{\mathbf{0}^\pm, \mathbf{1}^\pm, \mathbf{2}\}} \left(n_\mu + \frac{1}{2} d_\mu \right) \bar{\omega}_\mu + v_o \right], \tag{4}$$

where n_μ is the total number of quanta in the normal mode with the 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. [39] and see Ref. [15] in Ref. [42]); and v_o is a constant. The $\mathbf{2}$ normal modes are phonon, i.e., compressional modes; $\mathbf{1}^+$ has single-particle angular behavior while $\mathbf{1}^-$ shows single-particle radial behavior. The $\mathbf{0}^+$ mode describes center-of-mass motion, and the $\mathbf{0}^-$ mode is a symmetric breathing motion.

This energy expression gives the full spectrum of excited states through the assignment of the normal-mode quantum numbers that enforce the Pauli principle.

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 $[V_{\text{conf}}(r_i) = \frac{1}{2} m \omega_{\text{ho}}^2 {r_i}^2]$ for which the restrictions imposed by antisymmetry are known. These two series of states can be related in the double limit $D \to \infty$, $\omega_{\text{ho}} \to \infty$, where both representations are valid. Two conditions result [38]:

$$2n_{\mathbf{0}^-} + 2n_{\mathbf{1}^-} = \sum_{i=1}^{N} 2\nu_i, \quad 2n_{\mathbf{0}^+} + 2n_{\mathbf{1}^+} + 2n_{\mathbf{2}} = \sum_{i=1}^{N} l_i, \tag{5}$$

where the radial and orbital angular momentum quantum numbers of the three-dimensional harmonic oscillator, ν_i and l_i, respectively, satisfy $n_i = 2\nu_i + l_i$, with n_i, the energy level quanta of the ith particle, defined by

$$E = \sum_{i=1}^{N} \left[n_i + \frac{3}{2} \right] \hbar\omega_{\text{ho}} = \sum_{i=1}^{N} \left[(2\nu_i + l_i) + \frac{3}{2} \right] \hbar\omega_{\text{ho}}. \tag{6}$$

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 harmonic oscillator configurations. As particles are added to the system at the $\omega_{\text{ho}} \to \infty$ limit, additional harmonic oscillator quanta, ν_i and l_i, i.e., additional subshells, are, of course, needed to satisfy the Pauli principle. Equivalently, this corresponds to additional normal-mode quanta that must accompany each new particle to maintain antisymmetry.

III. APPLICATION: HARMONIUM

We studied the model system of harmonically confined, harmonically interacting, spin-polarized identical fermions. This model not only constitutes a fully interacting many-body system but is also a realistic model for various physical systems such as quantum dots in a magnetic field and trapped fermions with the interaction parameters adjusted to reproduce properties of real systems [36], an approach also used in nuclear and condensed matter physics for many years [50,51]. This system has been the subject of many accurate studies allowing comparison of the current work with more than one method, for both attractive and repulsive interactions, and against benchmark accuracy. The Hamiltonian for harmonium is

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

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 normal-mode frequencies are $\bar{\omega}_{0^+} = 2$, $\bar{\omega}_{0^-} = 2\lambda$, $\bar{\omega}_{1^+} = 2\lambda$, $\bar{\omega}_{1^-} = 1 + \lambda$, and $\bar{\omega}_2 = 2\lambda$, where

$$\lambda = \sqrt{1 + N\lambda_p^2}, \tag{8}$$

and $\lambda_p = \frac{\omega_p}{\omega_t}$ is a measure of the relative strength of the interaction versus the confinement. For a repulsive interaction ω_p^2 and λ_p^2 are brought in with a negative sign, so $0 < \lambda < 1$, while an attractive interaction corresponds to positive ω_p^2 and λ_p^2 so $\lambda > 1$.

The SPT energies are obtained using Eq. (4) with the normal-mode quanta n_μ determined from Eqs. (5) to ensure antisymmetry. We choose quanta that correspond to the lowest values of the normal-mode frequencies to yield the lowest energy for each excited state. For repulsive interaction, i.e., $0 < \lambda < 1$, this results in occupation in $n_{\mathbf{0}^-}$ and $n_{\mathbf{2}}$ which have the lowest radial and angular frequencies, respectively, while if $\lambda > 1$, i.e., an attractive interaction, the occupation becomes $n_{\mathbf{1}^-}$ and $n_{\mathbf{0}^+}$ which then have the lowest radial and angular frequencies. The conditions are, for repulsive interaction,

$$2n_{\mathbf{0}^-} = \sum_{i=1}^{N} 2\nu_i, \quad 2n_{\mathbf{2}} = \sum_{i=1}^{N} l_i, \tag{9}$$

and for attractive interaction,

$$2n_{\mathbf{1}^-} = \sum_{i=1}^{N} 2\nu_i, \quad 2n_{\mathbf{0}^+} = \sum_{i=1}^{N} l_i. \tag{10}$$

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.

IV. PARTITIONING THE ENERGY AND COLLECTING STATISTICS: DEGENERACIES

Obtaining the degeneracies of a many-body state is a nontrivial task. Various ways to obtain this include the straightforward diagonalization of the many-body Hamiltonian, recursive methods, and using a high-N approximation such as the Fermi-Dirac distribution. The present method offers a conceptually different approach. The sum over levels in the partition function is a sum over the many-body energy levels of the three-dimensional harmonically confined, harmonically interacting system with the N particles distributed among the available energy levels so the total energy is correct. The degeneracies of this interacting system do not depend on the strength of the two-body interaction; i.e., the number of states that belong to a degenerate level is constant and does not change with a continuous variation of the interaction. This means that the correct degeneracy of the many-body energy levels of the *interacting* system can be obtained from the degeneracy of the many-body energy levels of the *noninteracting* three-dimensional harmonic oscillator at the double limit $D \to \infty$, $\omega_{\text{ho}} \to \infty$ where both representations are valid. For each partition into particular levels with energy quantum numbers $n_i, i = 1, \ldots, N$, there are sublevels labeled with the radial and orbital angular momentum quantum numbers of the three-dimensional harmonic oscillator, ν_i and l_i, respectively, satisfying $n_i = 2\nu_i + l_i$, and having a defined sublevel degeneracy of $2l_i + 1$. The many-body degeneracy for *each* partition of the energy into specific n_i, $i = 1, \ldots, N$, so that $E = \sum_{i=1}^{N} [n_i + \frac{3}{2}]\hbar\omega_{\text{ho}}$ can be calculated by determining the number of ways the particles filling in a sublevel, ν_i, l_i, can be arranged, i.e., using the binomial coefficient for p particles in $m = 2l_i + 1$ states, i.e., $\binom{m}{p} = \frac{m!}{(m-p)!p!}$. These sublevel degeneracies are multiplied by other sublevel degeneracies for this partition, resulting in the degeneracy for this partition. Given a total many-body energy, there can be many different partitions (in the same way that change for a dollar can be made in many different ways given a fixed number of pennies, nickels, dimes, and quarters) whose degeneracies must be added together to determine the total many-body degeneracy for this energy. The sum in the expression for the partition function sums over all many-body energy levels, each of which must be partitioned among all N particles as described above and the statistics collected into the correct many-body degeneracy.

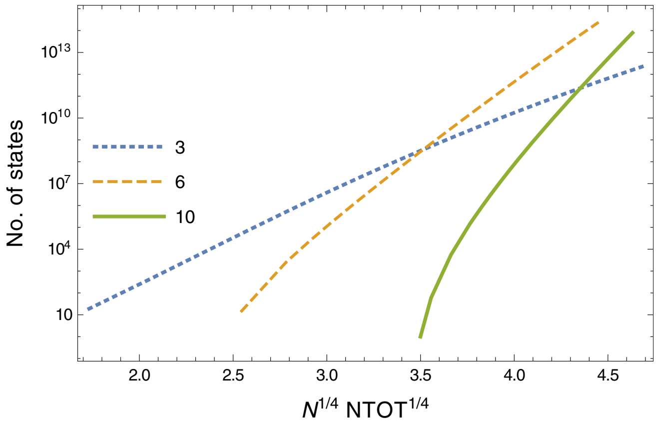

FIG. 1. Number of states as a function of N_{tot} excitation quanta for 3, 6, and 10 fermions for the harmonically trapped harmonically interacting gas.

Each partition identifies particular radial and orbital angular momentum quantum numbers, ν_i and l_i, for each level occupied, and these quantum numbers are then summed as in Eqs. (5) in order to make the assignments to the normal-mode quantum numbers that enforce the Pauli principle using Eqs. (9) and (10) which are used in Eq. (4) to obtain the corresponding many-body energy of the *interacting* system that has the correct symmetry satisfying the Pauli principle needed in this term in the partition function.

Figure 1 shows the sharp increase in the degeneracy even for modest increases of the number of quanta and/or the number of particles. This rapid increase of the degenerate states to many powers of ten as the energy of the many-body state increases competes with the decay of the Boltzmann factor to determine the impact of each term in the partition function.

V. RESULTS

We determined the following thermodynamic quantities: the free energy F, the energy E, the entropy S, and the heat capacity C_V,

$$F = -T \ln Z = E - TS, \quad E = T^2 \frac{\partial \ln Z}{\partial T}, \quad C_V = \frac{\partial E}{\partial T}, \tag{11}$$

for both attractive and repulsive interactions and compared our SPT results to values in the literature. As discussed above [see Eqs. (9) and (10)], we chose normal-mode quantum numbers that enforced the Pauli principle by choosing the quantum numbers that minimized the energy. We checked that this choice also maximized the entropy and minimized the free energy.

Figure 2 shows our SPT results for the free energy for a system with repulsive interactions compared to a method that used a combination of the path-integral method and a symmetrized density matrix formulation with the partition function itself extracted from a generating function [34].

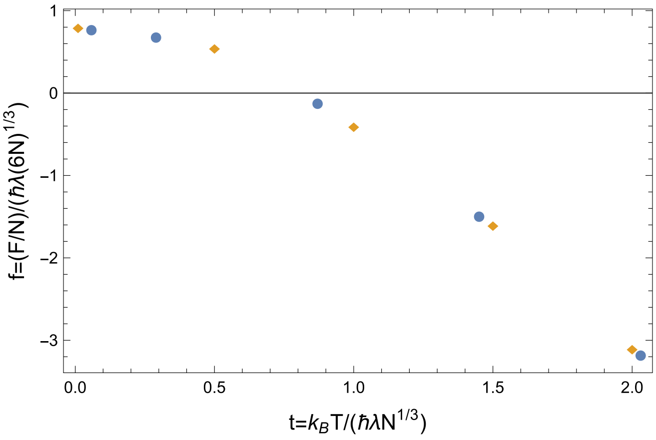

FIG. 2. Scaled free energy per particle, $f = (F/N)/(\hbar\lambda(6N)^{1/3})$, for a repulsive interaction with $\lambda = 0.8$ and 10 particles. Our SPT results (solid circles) are compared to a path-integral method (solid diamonds) [34] as a function of scaled temperature $t = k_BT/(\hbar\lambda N^{1/3})$.

Our approach, which does an explicit summation, included energies corresponding to energy quanta up through 120 in order to converge the results at $t = 2.0$ in scaled units of $k_BT/(\hbar\lambda N^{1/3})$. Our results, shown here for $N = 10$ particles and $\lambda = 0.8$, show excellent agreement with the scaled results of Ref. [34].

In Fig. 3 we compare our SPT results using an attractive interaction with $\lambda = 1.5$ and $N = 10$ to a recursive method introduced by Armstrong and co-workers, which they applied mostly to two-dimensional systems [36]. To compare to our three-dimensional results, we extended their work to three dimensions with the results shown in the plot. The agreement is quite good. (The agreement is particularly close at the first three temperatures so we have used slightly different temperatures for the two methods to spread out the symbols on the graph.)

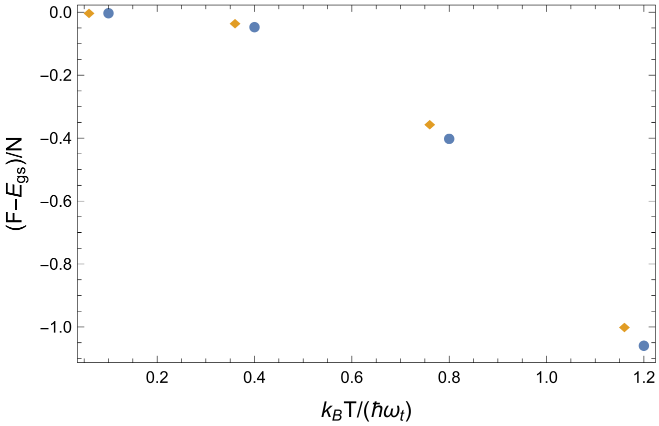

FIG. 3. Free energy of the harmonically trapped, harmonically interacting gas for an attractive interaction with $\lambda = 1.5$ and 10 particles. Our SPT results (solid circles) are compared to a recursive method (solid diamonds) [36] as a function of temperature. The ground-state energy, E_{gs}, is subtracted and the energies and temperature are in units of $\hbar\omega_t$.

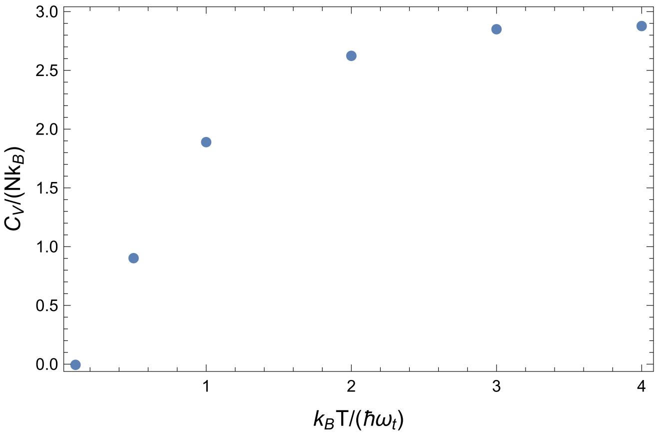

FIG. 4. Heat capacity SPT results for the harmonically trapped harmonically interacting gas for an attractive interaction with $\lambda = 1.5$ for 6 particles show convergence to the high-temperature limit of $3Nk_B$ from the equipartition theorem.

The studies we used for comparison with our SPT results use quite different approaches to enforce the Pauli principle and to determine the degeneracies. The path-integral method obtained the partition function directly after using a permutation matrix to enforce antisymmetry [34]. The recursive method determined the number of degenerate states of the correct symmetry recursively for each total number of particles and total quanta, then performed an explicit summation [36]. Our method agrees very well with both of these studies for all the thermodynamic quantities tested, for different particle numbers, for repulsive and attractive interactions, and for low temperatures where we expect quantum statistical effects to be important as well as for higher temperatures where we confirmed the correct thermodynamic limits.

In Fig. 4, we show the results for the SPT heat capacities for six particles in units of Nk_B. Our SPT method correctly gives the high-temperature behavior of $3Nk_B = \frac{3}{2}Nk_B + \frac{3}{2}Nk_B$ as predicted by the equipartition theorem.

VI. CONCLUSIONS

In a general sense, the partition function for an ensemble of N particles tells us the number of thermally accessible states at the temperature of interest. This number depends of course on the temperature, but, more interesting, it depends on the structure of the spectrum of energy levels of the appropriate symmetry and the degeneracies, the number of ways the total energy of a many-body state can be partitioned among the N particles. The Pauli principle is known to have a profound effect on the energy levels as well as the quantum statistics particularly at low temperature.

This study of the partition function has tested the SPT method in several ways. It constitutes an extension of the SPT method to excited states. As previously stated, the entire spectrum of excited states *at first order* is accessible once the normal-mode frequencies are determined even for real systems with arbitrary interactions. For harmonium, the first-order energies are actually the exact energies of the system since the normal-mode coordinates yield an exact solution for harmonium. The spectrum is determined by the application of the Pauli principle, which picks out the correct normal-mode quantum numbers to choose states that correspond to antisymmetric wave functions. This study also constitutes a successful test of the simple enforcement of the Pauli principle for excited states, yielding thermodynamic quantities in excellent agreement with independent results. (Choosing normal-mode quantum numbers not corresponding to the dictates of the Pauli principle gave erroneous results for thermodynamic quantities.) The validity of our method of determining the degeneracies for each many-body energy as described in Sec. IV also is confirmed by the excellent agreement of multiple thermodynamic quantities with the results of independent studies in the literature. Neither of the methods used for comparison offers a direct check on the degeneracies themselves.

The method presented in this paper does an explicit summation of the partition function. Converging the results for the particle numbers and the temperatures used in this paper for comparison to the literature was tractable on a desktop computer with a few hours of time. The increase in resources needed as the particle number and/or the temperature increases is severe but does not appear to be exponential. This is to be expected since we are not obtaining the explicitly antisymmetrized wave functions for each state in a degenerate level. However, we are obtaining the normal-mode quantum numbers that uniquely specify each state within a degenerate level. This is valuable information that is typically not obtained in other approaches that seek to avoid determining the wave function. Knowing the normal-mode quantum numbers and the corresponding degeneracies that are relevant as N increases has the potential to yield interesting insight into the emergence of the collective organizational phenomena that are characteristic of mesoscopic and macroscopic behavior when this method is applied to real systems.

In this paper we have developed an approach for the determination of the partition function for confined, interacting identical fermions using our simple SPT method of enforcing the Pauli principle which is trivial to implement. Our first application has been for harmonically confined, harmonically interacting fermions, a system interesting in its own right as a model for various physical systems. We expect the application to real, strongly interacting systems of fermions will be more challenging, but the ability to obtain both the full spectrum of energies through first order and the many-body degeneracies needed to determine the partition function without the considerable numerical expense of obtaining explicitly antisymmetrized many-body wave functions suggests that this approach will offer interesting opportunities for the study of the thermodynamic behavior of real systems of fermions.

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