New Effective Interaction for the Trapped Fermi Gas

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We apply the configuration-interaction method to calculate the spectra of two-component Fermi systems in a harmonic trap, studying the convergence of energies at the unitary interaction limit. We find that for a fixed regularization of the two-body interaction the convergence is exponential or better in the truncation parameter of the many-body space. However, the conventional regularization is found to have poor convergence in the regularization parameter, with an error that scales as a low negative power of this parameter. We propose a new regularization of the two-body interaction that produces exponential convergence for systems of three and four particles. We estimate the ground-state energy of the four-particle system to be $(5.045 \pm 0.003)\hbar\omega$.

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The study of cold trapped atomic condensates has become a rich field experimentally. By providing a strongly interacting system that is well defined, it also offers physicists an unprecedented opportunity to assess theoretical techniques that cross the boundaries of disciplines. In the unitary limit of infinite scattering length, the only dimensional scale of the problem is fixed by the harmonic trap frequency. Systematic studies have begun on small systems using fixed-node Monte Carlo [1–3] and density functional methods [4]. Remarkably, the exact wave functions and energies of the $A = 3$ system are known, calculated by solving a single transcendental equation [5]. Here we study the trapped condensate in the context of the configuration-interaction (CI) method, widely used in atomic [6], molecular [7], and nuclear [8] spectroscopy. In particular, we investigate the convergence of the condensate energies in the CI method with respect to a regularization parameter of the two-body interaction. We find that a simple regularization scheme that renormalizes the interaction produces slow convergence of the three- and four-particle spectra. We introduce a new effective interaction that gives exponential convergence.

Hamiltonian.—The cold trapped atom system is modeled by the Hamiltonian

$$H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i=1}^{A} \frac{1}{2} m\omega^2 r_i^2 + \sum_{i<j} V_0 \delta(\mathbf{r}_i - \mathbf{r}_j), \quad (1)$$

where A is the number of atoms, ω is the trap frequency, and V_0 is the interaction strength. We have two-component fermionic systems in mind, which controls the symmetry of the allowed states. The interaction is represented as a δ function (contact interaction) but as we shall see below it requires a regularization. Here we focus on an attractive contact interaction in the unitary limit.

Two-particle problem.—The two-particle system ($A = 2$) is separable in center of mass and relative coordinates $\mathbf{r} = \mathbf{r_2} - \mathbf{r_1}$. The center of mass Hamiltonian describes an harmonic oscillator with frequency ω and mass $2m$, while the relative-coordinate Hamiltonian is $H_{\rm rel} = -\frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2 + \frac{1}{2}\mu\omega^2 r^2 + V_0\delta(\mathbf{r})$ with reduced mass $\mu = m/2$. The two-particle energies are given by $E = (2\mathcal{N} + \mathcal{L} + 3/2)\hbar\omega + \varepsilon_{nl}$, where $\mathcal{N}$, $\mathcal{L}$ and n, l are the radial quantum number and angular momentum of the center of mass and relative motion, respectively. The energies ε_{nl} are the eigenvalues of $H_{\rm rel}$, and may be derived from the boundary condition at the origin imposed by the unitary limit interaction [9]. The contact interaction affects only the $l = 0$ partial waves, and shifts each s-wave oscillator energy down by one unit of $\hbar\omega$ [10]. Thus we have

$$\varepsilon_{nl} = (2n + l + 3/2 - \delta_{l,0})\hbar\omega, \qquad n = 0, 1, 2, \ldots. \quad (2)$$

Renormalized contact interaction.—In the CI method, the contact interaction in Eq. (1) must be treated explicitly. However, a δ-function interaction in three dimensions must be regularized. We shall do this by truncating the space of relative-coordinate wave functions to a q subspace of the lowest $q + 1$ oscillator $l = 0$ wave functions (see also Ref. [11]). Within the truncated space the relative-coordinate Hamiltonian can be written as

$$(H_{\rm rel})^{(q)}_{n,n'} = (2n + 3/2)\hbar\omega\delta_{n,n'} + V^{(q)}_{n,n'} \qquad (0 \le n, n' \le q), \quad (3)$$

where

$$V^{(q)}_{n,n'} = \hbar\omega\chi_q\psi_n(0)\psi_{n'}(0), \quad (4)$$

and $\psi_n(0) = \pi^{-3/4}\sqrt{(2n+1)!!/(2^n n!)}$ is the $(n, l = 0)$ oscillator wave function at $\mathbf{r} = 0$ for an oscillator of radius 1. The parameter χ_q is a dimensionless normalization constant related to V_0 by $\chi_q = (\hbar^2/\mu)^{-3/2}(\hbar\omega)^{1/2}V_0$.

We determine the normalization constant χ_q by requiring the ground-state energy of the truncated Hamiltonian to equal the exact value for the unitary limit contact interaction, $\varepsilon_{00} = \hbar\omega/2$. The separable form of (4) permits an

algebraic diagonalization of the Hamiltonian. Each eigenvalue ε of (3) satisfies the dispersion formula

$$\chi_q^{-1} = -\sum_{n=0}^{q} \frac{\psi_n^2(0)}{(2n+3/2) - \varepsilon/\hbar\omega}. \tag{5}$$

Requiring $\varepsilon = \varepsilon_{00} = \hbar\omega/2$ in (5), we obtain a closed expression for the normalization constant

$$\chi_q = -\pi^{3/2}\left(\sum_{n=0}^{q} \frac{(2n-1)!!}{2^n n!}\right)^{-1}. \tag{6}$$

We note that the sum in (6) diverges as $q^{1/2}$ for large q [12]. Thus, the strength of the δ function goes to zero as $q \to \infty$, showing the need for a renormalization procedure. A similar relation between the strength of the interaction and the cutoff can be derived for a plane-wave basis. In that case the relation is $V_0 = -\pi^2\hbar^2/\mu\Lambda$ where Λ is a momentum cutoff [13]. This value of V_0 agrees with the asymptotic expression of Eq. (6) [12] once we equate the corresponding cutoff energies as $\hbar^2\Lambda^2/2\mu = (2q+3/2)\hbar\omega$.

The excited states of the q-truncated Hamiltonian (3) have energies $\varepsilon_{n0}^{(q)}$ that differ from the exact unitary limit spectrum (2). Using the dispersion relation (5), we find that the error in the energy $\delta\varepsilon_{n0}^{(q)} = \varepsilon_{n0}^{(q)} - \varepsilon_{n0}$ goes to zero at large q, but only at a rather slow rate, $\delta\varepsilon_{n0}^{(q)} \sim q^{-1/2}$. We present evidence below that this slow convergence is also present in the q-renormalized energies for the $A = 3$ and $A = 4$ systems. This makes it problematic to extrapolate the q series to estimate the true $q \to \infty$ energies.

A new effective interaction.—We have considerably more freedom to construct the q-space interaction than we have exploited so far. The only requirement on the q-space Hamiltonian is that it converge to the unitary limit for $q \to \infty$. For example, in effective field theory one may introduce derivatives of the contact interaction to fit certain properties of the two-particle Hamiltonian. Here we propose the following prescription to improve the q-space interaction: simply require that the relative-coordinate Hamiltonian reproduce all $q+1$ s-wave eigenvalues of Eq. (2). We can do this and still keep the separable form for the interaction,

$$V_{n,n'}^{\mathrm{eff}(q)} = -\hbar\omega f_n f_{n'}. \tag{7}$$

A motivation for preserving the separable form is given in the discussion below. There are $q+1$ independent variables f_n in the interaction (7) and the same number of eigenvalue equations having the form of Eq. (5) with f_n replacing $\sqrt{|\chi_q|}\psi_n(0)$. Using the conditions that all $q+1$ lowest $l = 0$ unitary limit eigenvalues (2) ($0 \le n \le q$) are reproduced, we find the following $q+1$ equations for f_n:

$$\sum_{n=0}^{q} \frac{f_n^2}{2(n-r)+1} = 1 \qquad (r = 0, \ldots, q). \tag{8}$$

Equations (8) determine a unique solution for f_n^2 ($n = 0, \ldots, q$) [14]. We choose the sign of the real numbers f_n to coincide with the sign of $\psi_n(0)$. Using the convention that the harmonic oscillator wave functions be positive at the origin, the unique solution for f_n is

$$f_n = \sqrt{\frac{(2n+1)!!}{(2n)!!}\frac{[2(q-n)-1]!!}{[2(q-n)]!!}}. \tag{9}$$

The interaction defined by (7) and (9) is different from the renormalized contact interaction for any q. Both interactions give eigenfunctions that converge to the correct $q \to \infty$ limit, but the convergence rates differ. The individual components of the eigenfunctions converge with an error proportional to $\sim q^{-1}$ for the proposed interaction, with a proportionality constant depending on the component. In comparison, the eigenvector components of the renormalized contact interaction converge to the same unitary limit eigenvector components but at a slower rate of $\sim q^{-1/2}$.

CI method and truncation of many-particle space.—In the CI approach, one uses a single-particle basis in the laboratory frame and constructs a many-particle basis of Slater determinants for A fermions. In our problem, a natural choice for the single-particle basis is the eigenstates of the three-dimensional harmonic oscillator. These states are labeled by orbital quantum numbers $a = (n_a, l_a)$, the orbital magnetic quantum number m_a, and an additional two-valued quantum number (e.g., spin) to distinguish the two species of fermions.

A way to truncate the many-particle space must be specified. There are a number of truncation schemes in the literature; here we will define a truncated single-particle orbital basis and construct the A-particle wave function allowing all possible antisymmetrized product states. In particular, we shall use all single-particle states in the oscillator shells $N = 0, \ldots, N_{\max}$ with $N = 2n_a + l_a$. There will be two limiting processes necessary to calculate the many-particle energies. The first is $N_{\max} \to \infty$ at fixed q. Then, with converged q-regulated energies we estimate the $q \to \infty$ limit.

Two technical aspects of our calculations should be mentioned. The two-particle matrix elements of the interaction in the oscillator basis are conveniently calculated using the Talmi-Moshinsky brackets to transform to relative and center of mass coordinates [15]. The many-particle Hamiltonian is diagonalized using the shell model codes OXBASH [16] and NUSHELL [17]. Unlike the nuclear shell model, our orbitals are characterized by integer angular momentum values. The two fermion species are distinguished in the same way as neutrons and protons are distinguished in the nuclear application.

$A = 3$ system.—We now show results for the $A = 3$ system. Its ground state is a negative-parity state with orbital angular momentum $L = 1$ and energy $4.272\,724\,3\ldots\hbar\omega$ [5,18]. In our CI convergence studies we computed the ground-state energies $E_{N_{\max}}^{(q)}$ for $q = 1, 2, 3, 4$ and $N_{\max} = q, \ldots, 7$.

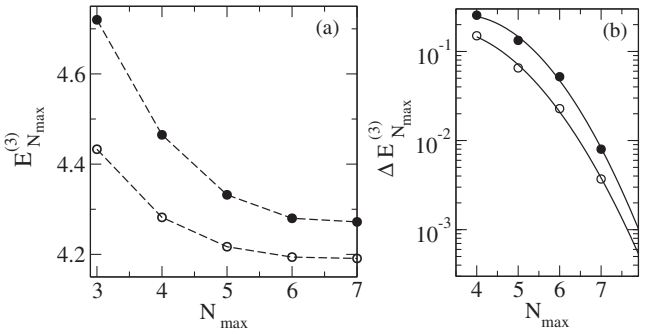

FIG. 1. Convergence in $N_{\max}$ for the $A = 3$ ground-state energy. (a) $E^{(q)}_{N_{\max}}$ versus $N_{\max}$ for $q = 3$. Open circles correspond to the renormalized contact interaction and solid circles to the interaction defined by (7) and (9). (b) $\Delta E^{(3)}_{N_{\max}}$ versus $N_{\max}$ in a logarithmic scale. All energies are in units of $\hbar\omega$.

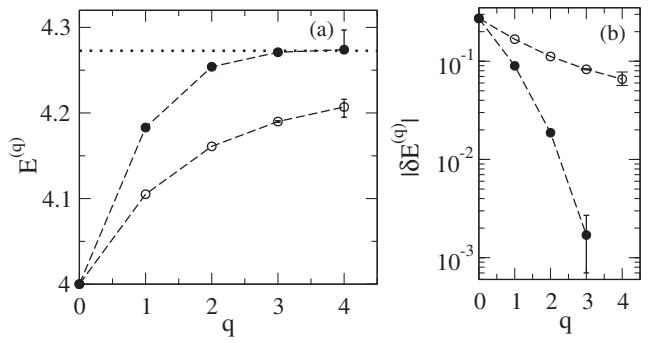

FIG. 2. Convergence of the q-regulated energies for the $A = 3$ ground state. (a) $E^{(q)}$ versus q for both interactions (symbols and units as in Fig. 1). The dotted line is the exact ground-state energy. (b) The error $|\delta E^{(q)}|$ in a logarithmic scale.

For a fixed q, we find that $E^{(q)}_{N_{\max}}$ converge exponentially or better in $N_{\max}$ for both interactions. This is demonstrated in Fig. 1. Figure 1(a) shows $E^{(q)}_{N_{\max}}$ versus $N_{\max}$ for $q = 3$. The energies for both the renormalized contact interaction (open circles) and the new interaction (solid circles) are monotonically decreasing, as they must when the space gets larger. We find [see Fig. 1(b)] that the energy differences $\Delta E^{(q)}_{N_{\max}} \equiv E^{(q)}_{N_{\max}-1} - E^{(q)}_{N_{\max}}$ decrease rapidly on a logarithmic scale. In fact, the decrease is steeper than linear on that scale, suggesting that the convergence might be faster than exponential. The solid lines are quadratic fits to $\log(\Delta E^{(q)}_{N_{\max}})$, used to extrapolate to a value of $E^{(q)} \equiv E^{(q)}_{\infty}$. We observe the decrease rate of $\Delta E^{(q)}_{N_{\max}}$ to be monotonically increasing with $N_{\max}$, so a conservative lower bound in $E^{(q)}$ is obtained using a fixed-rate extrapolation above $N_{\max} = 7$ with an average rate determined by the points $N_{\max} = 5, 6, 7$. An upper bound for $E^{(q)}$ is given by $E^{(q)}_7$.

Figure 2(a) shows the converged or extrapolated energies $E^{(q)}$ versus q. These energies are monotonically increasing in q. For the new interaction (solid circles), we observe a fast convergence to the exact value (dotted line). Figure 2(b) shows the deviation $|\delta E^{(q)}| \equiv |E^{(q)} - E^{(\infty)}|$ from the exact result in a logarithmic scale. The concavity of the curve for the renormalized contact interaction (open circles) indicates the convergence in q is slower than exponential. We find this convergence to be consistent with a low negative power law $\sim q^{-\alpha}$ where $\alpha \sim 0.5$–1.5 (for the excited $A = 2$ system it can be shown analytically that $\alpha = 1/2$). However, for the new interaction (solid circles) the convergence is at least exponential.

This exponential convergence allows for an accurate estimate of $E^{(\infty)}$. We calculated successive energy differences $\Delta E^{(q)} \equiv E^{(q-1)} - E^{(q)}$ and determined an average rate of decrease λ of $|\Delta E^{(q)}|$ for q below a given q'. Assuming a fixed rate λ for $q > q'$, the extrapolated energy is $[\lambda E^{(q')} - E^{(q'-1)}]/(\lambda - 1)$. We can take this value to be an upper bound for $E^{(\infty)}$, since the rate of decrease of $|\Delta E^{(q)}|$ seems to be a monotonically nondecreasing function of q. Using $q' = 3$ and an average decrease rate of 3.28 (determined from $\Delta E^{(q)}$ at $q = 1, 2, 3$), we find $E^{(\infty)} = (4.274 \pm 0.004)\hbar\omega$, an accuracy of 0.1%.

For the $L^{\pi} = 0^{+}$ first excited state at $E^{(\infty)} = 4.6662\ldots\hbar\omega$ [5,18] we find $E^{(\infty)} = (4.646 \pm 0.025)\hbar\omega$, an accuracy better than 0.6% [see Fig. 3(a)].

$A = 4$ system.—We also studied the $L = 0$ ground state of the $A = 4$ system with two particles of each species. The results for $E^{(q)}$, using a cutoff of $N_{\max} = 7$, are shown in Fig. 3(b). The $q = 4$ energy is not sufficiently converged to be useful. The straight line in the inset is a fit to $\log(\Delta E^{(q)})$ using $q = 1, 2, 3$ and provides an average decrease rate for determining a lower bound. Using $E^{(3)}_7$ as an upper bound, we estimate $E^{(\infty)} = (5.051 \pm 0.024)\hbar\omega$. This result is consistent with fixed-node Monte Carlo estimates of $(5.1 \pm 0.1)\hbar\omega$ [1] and $(5.069 \pm 0.009)\hbar\omega$ [2].

Increasing the cutoff to $N_{\max} = 9$, we find $E^{(4)} = (5.047 + 0.001 - 0.003)\hbar\omega$. Following a similar method

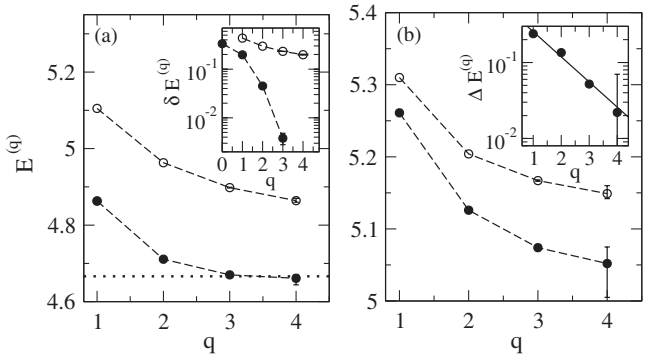

FIG. 3. (a) $E^{(q)}$ versus q for the lowest $L = 0$ excited state of the $A = 3$ system. The inset shows $\delta E^{(q)}$ versus q in a logarithmic scale. Symbols and units as in Fig. 2. (b) $E^{(q)}$ versus q for the $L = 0$ ground state of the $A = 4$ system. The inset shows $\Delta E^{(q)}$ versus q for the new interaction in a logarithmic scale. The solid line is a linear fit to $q = 1, 2, 3$.

as above but using $q = 1, 2, 3, 4$ we now find $E^{(\infty)} = (5.045 \pm 0.003)\hbar\omega$, an order of magnitude improvement in accuracy compared with our estimate above and with the result $(5.03 \pm 0.02)\hbar\omega$ of Ref. [3].

Discussion.—There are a number of methodologies in current use to construct effective interactions for many-particle systems; among them, effective field theory (EFT) and the unitary-transformation method have a connection to the interactions discussed here. In EFT, the interaction is parametrized by contact terms (leading order) and their derivatives. Our procedure to construct the q-renormalized contact interaction can thus be considered as leading-order EFT. Its poor convergence suggests that EFT treatments will require derivative terms to accurately model trapped fermion systems (see also Ref. [11]).

Our improved interaction has some connection with Suzuki's unitary regularization [19], a method widely used in nuclear physics [20–22]. In Suzuki's approach, an effective interaction is determined by a unitary transformation of the Hamiltonian that decouples a subspace from its complementary subspace. In practice, the transformation is performed on the two-particle Hamiltonian, giving a transformed Hamiltonian that is block diagonal. This block diagonal structure guarantees that the energy eigenvalues are reproduced in the truncated subspace. Our effective interaction also reproduces the exact two-particle spectrum in a truncated subspace but has the advantage of being simple, i.e., separable.

The unitary transformation of the two-particle Hamiltonian cannot be carried out independently for all possible pairings in the many-body Hamiltonian. When this transformation is applied to the many-particle system, it generates higher-order many-body interactions that are usually simply neglected. Rather than attempting to compute these higher-order terms, we have studied the convergence in the large q limit, where our effective interaction coincides with the contact interaction. By studying the convergence, one can assess the usefulness of many of the specific details of the different methodologies. For example, there are other choices of the many-particle space truncation that might be more efficient. Nonunitary transformations might give faster convergence. The no-core-shell-model methodology [23] is an example where a particular choice was made.

Our method can be applied for interaction strengths away from unitarity, at the slight cost of inverting a $(q + 1)$-dimensional matrix. It may also be interesting to apply the method to uniform systems, using the separability of the interaction in a plane-wave basis. Fock space auxiliary-field Monte Carlo methods can be used with the new interaction to extract the thermodynamic properties of the trapped condensate for a large number of particles.

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