The normal state of attractive Fermi gases from coupled-cluster theory

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We introduce coupled-cluster (CC) theory for the numerical study of the normal state of two-component, dilute Fermi gases with attractive, short-range interactions at zero temperature. We focus on CC theory with double excitations (CCD) and discuss its close relationship with—and improvement upon—the t-matrix approximation, i.e., the resummation of ladder diagrams via a random-phase approximation. We further discuss its relationship with Chevy’s variational wavefunction ansatz for the Fermi polaron and argue that CCD is its natural extension to nonzero minority species concentrations. Studying normal state energetics for a range of interaction strengths below and above unitarity, we find that CCD yields good agreement with fixed-node diffusion Monte Carlo. We find that CCD does not converge for small polarizations and large interaction strengths, which we speculatively attribute to the nascent instability to a superfluid state.

I. INTRODUCTION

Two-component Fermi gases with tunable, attractive interactions exhibit a rich phase diagram [1–4]. Experimental realizations via ultracold atoms have enabled precision studies of their quantum many-body physics, including fermionic superfluidity [5–19] and the smooth crossover from the Bardeen-Cooper-Schrieffer (BCS) limit at weak attraction to the Bose-Einstein condensate (BEC) limit at strong attraction [20–37]. An ongoing investigation concerns the fate of the paired superfluid in the presence of a spin polarization, with implications for superconductivity in solids. Specifically, at large polarizations, the superfluid is expected to exhibit an instability to a partially polarized or fully polarized normal state [38–49].

Despite the dilute nature of these systems, their precise phase boundaries and related properties can only be determined by accurate quantum many-body calculations. Near unitarity, the strength of the interaction precludes simple perturbative treatments [50, 51]. This motivates the search for affordable but accurate nonperturbative techniques, the most successful of which have been quantum Monte Carlo methods, including diffusion Monte Carlo (DMC) [40, 52–57], auxiliary field quantum Monte Carlo (AFQMC) [58–63], diagrammatic Monte Carlo [64–71], and others [72–74]. Each of these methods has its own limitations due to the fermion sign problem, e.g., necessitating the fixed-node approximation in DMC or the phaseless approximation in AFQMC for nonzero polarizations. Moreover, calculating dynamical response functions via QMC is an open challenge.

Here, we introduce coupled-cluster (CC) theory [75], which has been successfully used in nuclear physics [76, 77] and quantum chemistry [78–80], as a promising numerical technique for the simulation of Fermi gases and related systems of cold atoms. CC techniques are nonperturbative, systematically improvable, non-stochastic, and sign-problem free. Their computational cost scales polynomially with the number of particles and orbitals. In this work, we focus on CC theory with double excitations as applied to the normal state at zero temperature. This version of CC theory has a number of important physical properties that support its application to dilute Fermi gases: it is exact for interacting two-particle problems, it is exact for noninteracting ensembles of interacting two-particle problems (so-called size-consistency) [81], and it fully includes all ladder diagrams, which are known to dominate the physics of dilute systems with strong, short-range interactions [82–84].

The layout of this article is as follows. In Sec. II, we introduce the theory underlying our study, including the Hamiltonian, variational wavefunctions, CC theory, and the random-phase approximation. In Sec. III, we present our results for the energies, Tan’s contact, and phase boundaries, as functions of polarization and interaction strength. Finally, in Sec. IV, we conclude by summarizing our work and identifying many avenues for future studies.

II. THEORY

In the low-density limit where the average interparticle separation is much larger than the interaction range, the low-energy properties of Fermi gases are determined by s-wave scattering and the interaction is completely specified by the scattering length $a$. We perform our study at zero temperature in three dimensions with periodic boundary conditions in a cubic box of volume $V$ according to the Hamiltonian [85]

$$
\hat{H} = \sum_{k,\gamma} \epsilon_k \hat{c}^\dagger_{k,\gamma} \hat{c}_{k,\gamma} + \frac{g}{V} \sum_{k,q} \hat{a}^\dagger_{k,q} \hat{a}^\dagger_{k+q,\gamma} \hat{a}_{k+q,\gamma} \hat{a}_{k,\gamma},
$$

where $\epsilon_k = k^2/(2m)$, $\hat{a}^\dagger_{k,\gamma}$ ($\hat{a}_{k,\gamma}$) annihilates (creates) a fermion with spin $\sigma$ and wavevector $k$, and we restrict our study to the case of equal masses $m$ (and set $\hbar = 1$). We discretize space into unit cells of volume $b^3$ and sample the Brillouin zone using a uniform mesh of $N_k$ $k$-points, where $N_k = V/b^3$. The two-body interaction strength $g < 0$ is chosen to have the scattering length $a$ on the lattice,

$$
g^{-1} = m \int_{BZ} \frac{d^3k}{(2\pi)^3} \frac{1}{2\epsilon_k} = \frac{m}{4\pi a} - \frac{mK}{4\pi b^3}. \tag{2}
$$

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where $\mathcal{K} = 2.442749$ for the quadratic dispersion used here [86–89]. Continuum results are obtained in the limit $N_k \to \infty$ with the particle number fixed.

We consider a partially polarized Fermi gas containing $N_\uparrow$ majority particles and $N_\downarrow$ minority particles in the box of volume $V$. In the above limits, the properties of the Fermi gas are universal and defined only by the dimensionless interaction strength $1/k_{F\sigma}^2$ [2, 50], where $k_{F\sigma}$ is the Fermi wavevector of the majority particles. On the basis of the behavior at low minority spin concentrations $x = N_\downarrow/N_\uparrow$, the ground-state energy of the normal state has been parameterized by the form $[40, 52, 90]$

$$E = \frac{3}{5} N_\uparrow \varepsilon_F \left(1 - Ax + \frac{m}{m^*} x^{5/3} + F x^2 \right),$$

where $\varepsilon_F$ is the Fermi energy of the majority particles and the parameters $A$, $m^*$, and $F$ depend on the interaction strength $1/k_{F\sigma}^2$. Specifically, $A$ and $m^*$ are the polaron binding energy and effective mass, respectively, while $F$ quantifies the interactions between polaron quasiparticles.

Using a single determinant corresponding to a filled Fermi sea $|0\rangle$ yields the energy

$$E_0 = \langle 0 | \hat{H} | 0 \rangle = \frac{3}{5} N_\uparrow \varepsilon_F \left(1 + x^{5/3} \right) + \frac{g}{\sqrt{V}} N_\uparrow N_\downarrow,$$

which is the sum of the non-interacting energy and the mean-field interaction energy; the latter vanishes in the continuum limit of strong interactions. For example, at unitarity, Chevy’s ansatz gives a polaron energy of $E_p \approx -0.6066 \varepsilon_F$, which is extremely close to the diagrammatic Monte Carlo energy of $E_p \approx -0.6157 \varepsilon_F$ [66, 71]. Configuration interaction calculations are systematically improvable by considering additional particle-hole excitations, as was done in Ref. 96. In quantum chemistry, such calculations would be described as configuration interaction with double, triple, quadruple, etc. excitations (CIDT, CIDTQ, etc.).

In principle, such variational wavefunctions can be straightforwardly applied to partially polarized Fermi gases with nonzero minority spin concentrations $x$, as studied here. However, as is well-known in the quantum chemistry community, such variational wavefunctions lack the important property of size-extensivity, $E(N) \propto N$, or the closely related property of size-consistency, which can be traced to the inclusion of unlinked diagrams in a diagrammatic expansion of their total energies [79, 80, 97, 98]. Therefore, energies obtained from truncated CI expansions are expected to deteriorate for systems with increasing numbers of particles. Unfortunately, this behavior makes it inappropriate to extend Chevy’s simple but successful wavefunction ansatz to partially polarized Fermi gases, which we demonstrate numerically in this work (vide infra).

One of the most successful size-extensive theories of quantum many-body systems is coupled-cluster theory, which can be truncated after any number of particle-hole excitations, analogous to the variational CI wavefunctions discussed above. For example, the (right-hand) wavefunction used in coupled-cluster theory with double excitations (CCD) is $|\Psi_0\rangle = e^{T_2}|0\rangle$, where

$$\hat{T}_2 = \sum_{k_i,k_i,q} t_{k_i,k_i,q} \hat{A}_{k_i,k_i,q}^\dagger \hat{A}_{k_i,k_i,q}^\dagger$$

The amplitudes $t_{k_i,k_i,q}$ are determined to satisfy the nonlinear CCD equations

$$0 = \langle 0 | \hat{A}_{k_i,k_i,q} e^{-\hat{T}_2} \hat{H} e^{\hat{T}_2} | 0 \rangle$$

from which the energy is evaluated as

$$E = \langle 0 | e^{-\hat{T}_2} \hat{H} e^{\hat{T}_2} | 0 \rangle = E_0 + \frac{g}{\sqrt{V}} \sum_{k_i,k_i,q} t_{k_i,k_i,q}.$$  

For the uniform systems studied here, the memory cost of CCD is $O(N_\uparrow N_\downarrow N_k)$ and the computational cost of iteratively solving Eqs. (8) is $O(N_\uparrow N_\downarrow N_k^2)$.

The CCD energy (9) is nonvariational because $\hat{T}_2^\dagger \neq -\hat{T}_2$. Rather, CCD is an infinite order perturbation theory. To lowest order in $g$, the $t$-amplitudes are given by

$$t_{k_i,k_i,q} = \frac{g}{\sqrt{V}} (\varepsilon_{k_i+q} + \varepsilon_{k_i-q} - \varepsilon_{k_i} - \varepsilon_{k_i})^{-1},$$

which, together with Eq. (9), just gives the second-order perturbation theory energy. This perturbative energy expression
FIG. 1. Energetics of the normal state of attractive Fermi gases over a range of spin polarizations and interaction strengths. (a)-(d) Total energy (scaled by the non-interacting energy of the spin-up particles) as a function of the concentration of minority spin-down particles at respective interaction strengths of 1/k_F a = –0.5, 0, 0.2, 0.4. Our continuum predictions from CID (crosses), CCD (circles), and ppRPA (plusses) are compared with FN-DMC results (squares) from Ref. 40. As a guide, solid black lines give the total energy in the absence of two-body interactions. The green shaded region indicates the range of one-parameter fits for the interaction parameter F using Eq. 3, as detailed in the text. (e) Comparison between F calculated for CCD and FN-DMC results, compared to the analytic result of Ref. 90. Error bars indicate two standard deviations of the F parameter fit.

was used to provide a picture of interacting Fermi polarons in Ref. 90.

The full CCD energy contains all ring diagrams, ladder diagrams, and mixtures of rings and ladders—all with their exchange counterparts, resulting in a properly fermionic theory [84]. Ladder diagrams are known to be important at low densities and such a restricted theory is equivalent to a non-self-consistent t-matrix approximation, also known as the particle-particle random-phase approximation (ppRPA) [82, 83, 99–101]. This ppRPA energy can be obtained as an approximation to CCD, by only including a subset of the terms in Eqs. (8). Such t-matrix or ppRPA approaches have been extensively used in the study of dilute Fermi gases [102–109], but their quantitative accuracy is largely confined to the regime of very weak attractions. In the next section, we show that the richer diagrammatic content of CCD leads to results with significantly greater quantitative accuracy.

III. RESULTS

A. Ground-State Energy

We have applied CCD, CID, and ppRPA to the Hamiltonian (1) for several values of x = N↓/N↑. To avoid breaking spatial symmetries in the Fermi sea determinant, we limit our calculations to closed shell configurations with N↑ = 1, 7, 19, 27, 33. To obtain continuum predictions, we performed calculations using two different mesh sizes Nk and extrapolated the energies to Nk → ∞, assuming N_k^{-1/3} convergence [89, 110]. For CID, we used N_k = 8^3, 10^3; while for CCD and ppRPA, we used N_k = 10^3, 12^3.

The Fermi polaron problem is defined by the choice N↓ = 1 and N↑ → ∞, i.e., x → 0. For this problem, with all values of N↑ and N↓, we find that CCD and CID give numerically identical results, which are therefore identical to those of Chevy’s ansatz [85, 95] in the appropriate limits. Despite their different physical content, CID and CCD are equivalent for the polaron problem: neither include triple excitations involving one spin-down and two spin-up particles, which are responsible for the majority of the energy difference between Chevy’s ansatz and diagrammatic Monte Carlo results [96]. At polarizations away from the polaron limit, the equivalence between CID and CCD no longer holds, which will be the main focus of our work.

In Figs. 1(a)-(d), we show the total energies as a function of x for four values of the interaction strength, 1/k_F a = –0.5, 0, 0.2, 0.4, where 1/k_F a = 0 corresponds to unitarity. For the latter three values of the interaction strength, we also compared to fixed-node DMC from Ref. 40. Although the CCD procedure does not always converge at large g or x (see below), our CCD results agree very well with DMC results.
spin fermions are close together [2, 111]. In the universal limits of the Fermi gas, $C$ can be determined via several different approaches via relations derived by Tan and subsequently expanded upon by others [111–117]. For example, the contact density determines the tail of the momentum distribution via $n(k) \sim C/k^4$, and it can also be understood as the conjugate variable to the interaction strength and thus calculated by the derivative of the ground-state energy [41, 111, 118, 119],

$$C \frac{k^4_{\text{F}}} = -(5\pi)^{-1} \frac{\partial \left( \frac{E}{\frac{1}{2} N_\uparrow \epsilon_{\text{F}}} \right)}{\partial \left( 1/k_{\text{F}} a \right)}$$  \hspace{1cm} (11)

We calculated the derivative by fitting our data to the functional form $E = A - B/C^{1/k_{\text{F}} a}$. In Fig. 2, we show our results for the dimensionless contact density as a function of the interaction parameter $1/k_{\text{F}} a$ at a representative set of minority spin concentrations $x$. We compare CCD to FN-DMC, with the latter being calculated from the parametrization in Ref. 42 based off of the FN-DMC data from Ref. 40. We find overall good agreement between the two methods, with CCD predicting a slightly smaller contact at large interaction strengths. For reference, we also include, at each minority spin concentration, the contact density in the BEC ($1/k_{\text{F}} a \to +\infty$) limit to leading order in $k_{\text{F}} a$ [41, 111, 118].

C. Phase Boundary

As can be seen in Figs. 1(a)-(d), we cannot obtain CCD results beyond a critical interaction-dependent concentration $x_c(1/k_{\text{F}} a)$. In practice, this occurs when the iterative method used to solve Eq. (8) does not converge. This behavior suggests (but does not guarantee) that Eq. (8) has no solution. Similar to the use of the Thouless criterion for the vertex function [102, 120, 121] or to the presence of multiple solutions in other nonlinear numerical techniques, we can use this behavior to speculatively identify a phase boundary for the partially polarized normal state. In Fig. 3, we plot the critical polarization, $P_c = (1 - x_c)/(1 + x_c)$, below which the CCD iteration...
IV. CONCLUSION

To summarize, we have introduced coupled-cluster theory as a promising computational method for the study of dilute Fermi gases. We have established the performance of coupled-cluster theory with double excitations (CCD) for the normal state of polarized three-dimensional gases at a range of interaction strengths.

Our promising findings motivate a large number of future studies enabled by the power and generality of the CC framework. In particular, CC theory can be systematically improved by increasing the number of excitations considered. It can be used to calculate one- and two-particle Green’s functions directly on the real frequency axis [122–129], as done recently for the uniform electron gas with long-range, repulsive Coulomb interactions [130, 131]. This straightforward access to dynamical response functions should be contrasted with that of most QMC methods, which require analytic continuation. CC methods can also be applied to nonuniform systems, precluding the local density approximation for trapped gases, as well as at nonzero temperature [132–137] and in non-equilibrium settings [138–140]. Lastly and perhaps most importantly, CC theory can be formulated with respect to a BCS reference wavefunction, as opposed to the normal Fermi sea wavefunction used here, allowing a more accurate study of pairing and superfluidity [141–146]. Work along all of these lines is currently in progress.

V. DATA AVAILABILITY STATEMENT

The data that support the findings of this study are openly available at https://github.com/jamescallahan7/jmc-js_tcb_2022.

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