Normal state of attractive Fermi gases from coupled-cluster theory

James M. Callahan,[1] John Sous,[2,*] and Timothy C. Berkelbach[1,3,†]
[1]*Department of Chemistry, Columbia University, New York, New York 10027, USA*
[2]*Department of Physics, Columbia University, New York, New York 10027, USA*
[3]*Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA*

(Received 21 June 2022; accepted 25 August 2022; published 6 September 2022)

We apply coupled-cluster (CC) theory to numerically study 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 wave-function 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.

DOI: 10.1103/PhysRevA.106.033303

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 apply coupled-cluster (CC) theory [75], which has been successfully used in nuclear physics [76,77] and quantum chemistry [78–80]. We argue that CC theory is a promising numerical technique for the simulation of Fermi gases and related systems of cold atoms as was previously shown by Grining and co-workers [81,82] in one dimension. CC techniques are nonperturbative, systematically improvable, nonstochastic, and sign-problem free. Their computational cost scales polynomially with the number of particles and orbitals. In this paper, 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) [83], and it fully includes all ladder diagrams, which are known to dominate the physics of dilute systems with strong short-range interactions [84–86].

The layout of this article is as follows. In Sec. II, we introduce the theory underlying our study, including the Hamiltonian, variational wave functions, 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 paper 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

*Present address: Department of Physics, Stanford University, Stanford, CA 93405.
†tim.berkelbach@gmail.com

in three dimensions with periodic boundary conditions in a cubic box of volume V according to the Hamiltonian [87],

$$\hat{H} = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} \hat{a}^\dagger_{\boldsymbol{k},\sigma} \hat{a}_{\boldsymbol{k},\sigma} + \frac{g}{V} \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} \hat{a}^\dagger_{\boldsymbol{k},\uparrow} \hat{a}^\dagger_{\boldsymbol{k}',\downarrow} \hat{a}_{\boldsymbol{k}'+\boldsymbol{q},\downarrow} \hat{a}_{\boldsymbol{k}-\boldsymbol{q},\uparrow}, \quad (1)$$

where $\varepsilon_{\boldsymbol{k}} = k^2/(2m)$, $\hat{a}_{\boldsymbol{k},\sigma}$ ($\hat{a}^\dagger_{\boldsymbol{k},\sigma}$) annihilates (creates) a fermion with spin σ and wave-vector $\boldsymbol{k}$, and we restrict our paper 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,

$$g^{-1} = \frac{m}{4\pi a} - \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} \frac{1}{2\varepsilon_{\boldsymbol{k}}} = \frac{m}{4\pi a} - \frac{m\mathcal{K}}{4\pi b}, \quad (2)$$

where $\mathcal{K} = 2.442\,749$ for the quadratic dispersion used here [88–91]. 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 $1/k_{\mathrm{F}\uparrow}a$ [2,50], where $k_{\mathrm{F}\uparrow}$ is the Fermi wave vector 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 parametrized by the form [40,52,92]

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

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

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

$$E_0 = \langle 0|\hat{H}|0\rangle = \frac{3}{5} N_\uparrow \varepsilon_{\mathrm{F}\uparrow} (1 + x^{5/3}) + \frac{g}{V} N_\uparrow N_\downarrow, \quad (4)$$

which is the sum of the noninteracting energy and the mean-field interaction energy; the latter vanishes in the continuum limit $N_k \to \infty$. Thus, the noninteracting and mean-field theories predict $A = F = 0$ and $m^* = m$.

Interaction effects can be accounted for by using a linear combination of determinants that are defined with respect to the filled Fermi sea. Such variational wave functions have been extensively used in the study of Fermi gases [93–96]. Here we will consider the method of configuration interaction with double excitations (CID) with the ground-state wave-function $|\Psi_0\rangle = (c_0 + \hat{C}_2)|0\rangle$, where

$$\hat{C}_2 = {\sum_{\boldsymbol{k}_\uparrow,\boldsymbol{k}_\downarrow\boldsymbol{q}}}' c_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}} \hat{A}^\dagger_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}}, \quad (5a)$$

$$\hat{A}^\dagger_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}} = \hat{a}^\dagger_{\boldsymbol{k}_\uparrow+\boldsymbol{q},\uparrow} \hat{a}^\dagger_{\boldsymbol{k}_\downarrow-\boldsymbol{q},\downarrow} \hat{a}_{\boldsymbol{k}_\downarrow,\downarrow} \hat{a}_{\boldsymbol{k}_\uparrow,\uparrow}, \quad (5b)$$

and the primed summation requires that $k_\sigma < k_{\mathrm{F}\sigma}$, $|\boldsymbol{k}_\uparrow + \boldsymbol{q}| > k_{\mathrm{F}\uparrow}$, and $|\boldsymbol{k}_\downarrow - \boldsymbol{q}| > k_{\mathrm{F}\downarrow}$. The $\hat{C}_2$ operator, thus, creates all possible momentum-conserving double excitations (two particles and two holes), with one excitation for each spin type. Although CID [and CC theory with double excitations (CCD) as we discuss below] can also include same-spin double excitations, our numerical testing showed no significant difference, and so we exclude them in all results that follow. For a normalized wave function, the variational CID energy is

$$E = \langle \Psi_0|\hat{H}|\Psi_0\rangle = E_0 + \frac{g}{V} {\sum_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}}}' c_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}}. \quad (6)$$

In the limit of a single minority atom interacting with a sea of majority atoms (i.e., the Fermi polaron problem), the CID wave function above is the same as Chevy's ansatz [87,97], which provides remarkably accurate energetics even in the limit of strong interactions. For example, at unitarity, Chevy's ansatz gives a polaron energy of $E_{\mathrm{p}} \approx -0.6066\varepsilon_{\mathrm{F}\uparrow}$, which is extremely close to the diagrammatic Monte Carlo energy of $E_{\mathrm{p}} \approx -0.6157\varepsilon_{\mathrm{F}\uparrow}$ [66,71]. Configuration interaction calculations are systematically improvable by considering additional particle-hole excitations as was performed in Ref. [98]. In quantum chemistry, such calculations would be described as configuration interaction with double, triple, quadruple, etc., excitations.

In principle, such variational wave functions 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 wave functions 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 [79,80,99,100]. 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 wave-function ansatz to partially polarized Fermi gases, which we demonstrate numerically in this paper (*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 wave functions discussed above. For example, the (right-hand) wave function used in coupled-cluster theory with double excitations (CCD) is $|\Psi_0\rangle = e^{\hat{T}_2}|0\rangle$, where

$$\hat{T}_2 = {\sum_{\boldsymbol{k}_\uparrow,\boldsymbol{k}_\downarrow\boldsymbol{q}}}' t_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}} \hat{A}^\dagger_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}}. \quad (7)$$

Variational minimization with this ansatz would have a computational cost that scales combinatorially with the number of particles and basis functions. Therefore, the amplitudes $t_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}}$ are determined by projection to satisfy the nonlinear CCD equations [75,79,80],

$$0 = \langle 0|\hat{A}_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}} e^{-\hat{T}_2} \hat{H} e^{\hat{T}_2}|0\rangle, \quad (8)$$

from which the energy is evaluated as

$$E = \langle 0|e^{-\hat{T}_2} \hat{H} e^{\hat{T}_2}|0\rangle = E_0 + \frac{g}{V} {\sum_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}}}' t_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}}. \quad (9)$$

Equations (8) and (9) can be derived by assuming that the CCD wave-function $|\Psi_0\rangle$ is an exact eigenstate, although, in general, it is not. Alternatively, Eqs. (8) and (9) can be derived by demanding that the Fermi sea state $|0\rangle$ is an eigenstate of the similarity-transformed Hamiltonian $e^{-\hat{T}_2}\hat{H}e^{\hat{T}_2}$ when projected into the Hilbert space spanned by the Fermi sea $|0\rangle$ and all momentum-conserving doubly excited determinants $\hat{A}^\dagger_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}}|0\rangle$. 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 Eq. (8) is $O(N_\uparrow N_\downarrow N_k^2)$. The iterative solution of Eq. (8) is achieved with a nonlinear generalization of Jacobi iteration with convergence acceleration via the direct inversion in the iterative subspace algorithm.

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

$$t_{\boldsymbol{k}_\uparrow\boldsymbol{k}_\downarrow\boldsymbol{q}} = \frac{g}{V}(\varepsilon_{\boldsymbol{k}_\uparrow+\boldsymbol{q}} + \varepsilon_{\boldsymbol{k}_\downarrow-\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}_\downarrow} - \varepsilon_{\boldsymbol{k}_\uparrow})^{-1}, \tag{10}$$

which, together with Eq. (9), just gives the second-order perturbation theory energy. This perturbative energy expression was used to provide a picture of interacting Fermi polarons in Ref. [92].

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 [86]. 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) [84,85,101–103]. This ppRPA energy can be obtained as an approximation to CCD by only including a subset of the terms in Eq. (8). Such t-matrix or ppRPA approaches have been extensively used in the study of dilute Fermi gases [104–111], 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 $x = N_\downarrow/N_\uparrow$. To avoid breaking spatial symmetries in the Fermi sea determinant, we limit our calculations to closed shell configurations with $N_\sigma = 1, 7, 19, 27, 33, 57$. To obtain continuum predictions, we performed calculations using two different mesh sizes N_k and extrapolated the energies to $N_k \to \infty$, assuming $N_k^{-1/3}$ convergence [91,112]. For CID, we used $N_k = 8^3, 10^3$; whereas for CCD and ppRPA, we used $N_k = 10^3, 12^3$. In principle, the thermodynamic limit also requires $N_\sigma \to \infty$ while maintaining the zero-density limit of $N_\sigma/N_k \to 0$. This is nearly impossible within the additional constraint imposed by closed shell configurations, and so we limit ourselves to fixed particle numbers. This is the same approach taken by other studies of polarized Fermi gases [40,52]. Based on QMC results of unpolarized Fermi gases [53,55,58,113] where finite-size effects are simpler to study, we estimate that the finite-size errors in our energies are on the order of a few percent or less.

The Fermi polaron problem is defined by the choice $N_\downarrow = 1$ and $N_\uparrow \to \infty$, i.e., $x \to 0$. For this problem, with all values of $N_\uparrow$ and N_k, we find that CCD and CID give numerically identical results, which are, therefore, identical to those of Chevy's ansatz [87,97] 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 [98]. At polarizations away from the polaron limit, the equivalence between CID and CCD no longer holds, which will be the main focus of our paper.

In Figs. 1(a)–1(d), we show the total energies as a function of x for four values of the interaction strength, $1/k_{\mathrm{F}\uparrow}a = -0.5, 0, 0.2, 0.4$, where $1/k_{\mathrm{F}\uparrow}a = 0$ corresponds to unitarity. For the latter three values of the interaction strength, we also compared to fixed-node DMC (FN-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 FN-DMC results. In contrast, the CID results do not, and overall they show a significantly smaller correlation energy, consistent with the method's lack of size extensivity.

We fit our CCD results to the Landau-Pomeranchuk equation of state (3). Because A and m^* can be extracted from the polaron problem, for which CCD gives results identical to Chevy's ansatz, we use the latter's parameters [66,97] and have only the interaction parameter F as a free parameter to be fit. In Fig. 1(e), we show the extracted value of F over the full range of interaction strengths we studied. Since the overall fit is relatively insensitive to F especially for lower values of x where CCD can converge more easily, we include error bars indicating two standard deviations from the fit value. The resulting range of fitted energy curves are plotted in Figs. 1(a)–1(d) as shaded regions along with the raw data. We have also carried out an identical fitting procedure to the FN-DMC results from Ref. [40] with $x < 1$ using the same values of A and m^* for consistency. Within error bars, we find very good agreement between CCD and FN-DMC, indicating that both provide an accurate description of quasiparticle interactions. Finally, in Fig. 1(e), we include results from Ref. [92], which argued that the interaction parameter F can be obtained from polaron properties via $F = (5/9)(d\mu/d\varepsilon_{\mathrm{F}\uparrow})^2$, where μ is the chemical potential of a single polaron. The agreement is good especially in the weakly interacting BCS limit $1/k_{\mathrm{F}\uparrow} \to -\infty$ that is accurately described by lowest-order perturbation theory.

B. Tan's contact density

From our ground-state energy results, we can extract a system property called the contact density C, which has units of [length]^4 and roughly measures how many pairs of opposite-spin fermions are close together [2,114]. 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 [114–120]. For example, the contact

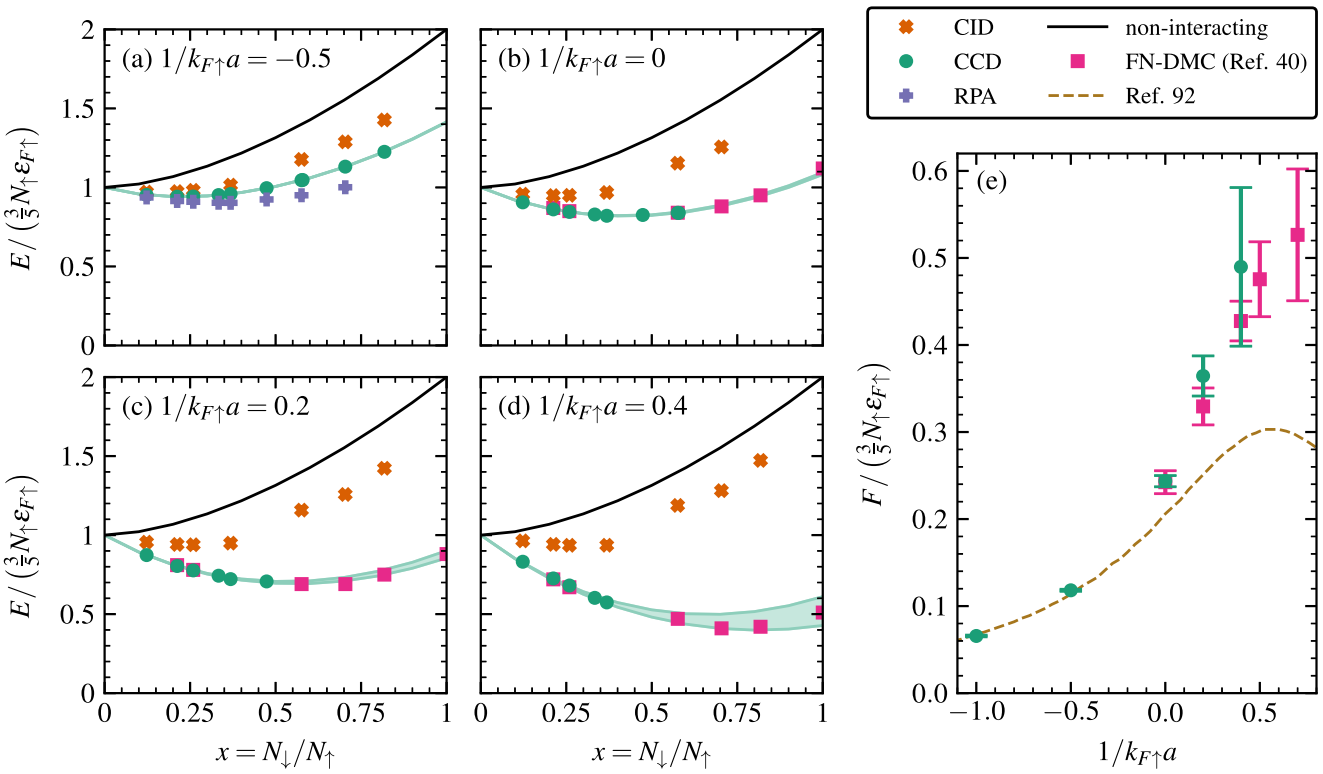

FIG. 1. Energetics of the normal state of attractive Fermi gases over a range of spin polarizations and interaction strengths. (a)–(d) Total energy (scaled by the noninteracting energy of the spin-up particles) as a function of the concentration of minority spin-down particles at respective interaction strengths of $1/k_{F\uparrow}a = -0.5, 0, 0.2, 0.4$. 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. [92]. Error bars indicate two standard deviations of the F parameter fit.

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 [41,114,121,122],

$$\frac{C}{k_{F\uparrow}^4} = -(5\pi)^{-1}\frac{\partial\left(E/\frac{3}{5}N_\uparrow\varepsilon_{F\uparrow}\right)}{\partial(1/k_{F\uparrow}a)}. \tag{11}$$

We calculated the derivative by fitting our data to the functional form $E = A - B/C^{1/k_{F\uparrow}a}$. In Fig. 2, we show our results for the dimensionless contact density as a function of the interaction parameter $1/k_{F\uparrow}a$ 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 ($1/k_{F\uparrow}a \to +\infty$) limit to leading order in $k_{F\uparrow}a$ [41,114,121].

C. Phase boundary

As can be seen in Figs. 1(a)–1(d), we cannot obtain CCD results beyond a critical interaction-dependent concentration $x_c(1/k_{F\uparrow}a)$. In practice, this occurs when the iterative method used to solve Eq. (8) does not converge. This behavior

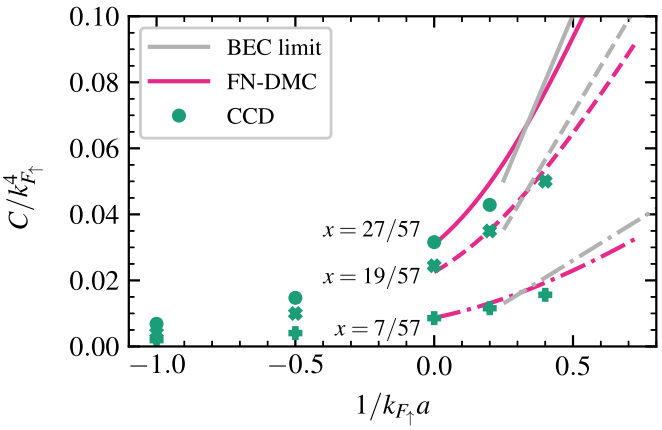

FIG. 2. Universal contact as a function of the interaction parameter $1/k_{F\uparrow}a$ at $x = 27/57, 19/57, 7/57$ (top to bottom). Gray (solid, dashed, and dashed-dot, top-to-bottom) lines on the right give, to leading order in $k_{F\uparrow}a$, the BEC limit (at $a \to 0^+$). Pink (solid, dashed, and dashed-dot, top-to-bottom) lines come from the analytic, parametrized formulas of Ref. [42] that were constructed to match FN-DMC results. Green circles, crosses, and plusses (top to bottom) are calculated from our CCD data as described in the main text.

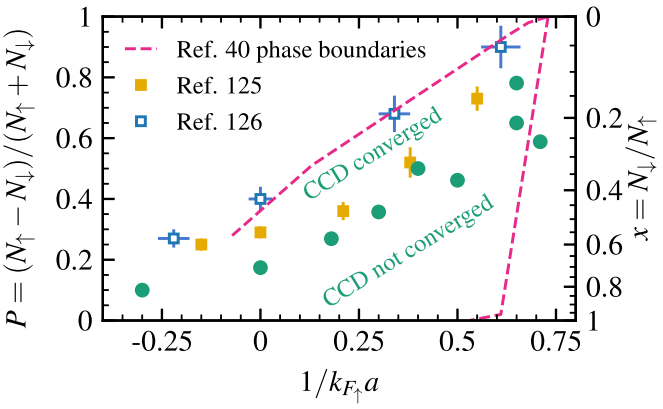

FIG. 3. Phase diagram of CCD convergencewhere the green circles give the maximum value of $1/k_{F\uparrow}a$ for which CCD converged at each polarization. The pink dotted lines indicate the boundaries for the coexistence region of the partially polarized normal state with several superfluid states as determined in Ref. [40] on the basis of FN-DMC data. The closed and open squares indicate the experimentally determined normal state boundary from Refs. [125,126].

suggests (but does not guarantee) that Eq. (8) has no solution. Similar to the use of the Thouless criterion for the vertex function [104,123,124] 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 does not converge for a system of fixed size $N_k = 1000$. It is known from previous works [9,10,40,44,49] that with increasing interaction strength, the partially polarized normal state undergoes a first-order phase transition to a region of coexistence with a superfluid state. At a subsequent second-order phase transition, the coexisting partially polarized normal state evolves into a coexisting fully polarized normal state. These two phase boundaries as determined in previous theoretical work are also plotted in Fig. 3 along with experimentally determined normal-state boundaries from Shin and co-workers [125] and from Olsen and co-workers [126]. For large polarizations, the CCD convergence boundary is in good agreement with these phase boundaries. At smaller polarizations, we see that the CCD iterations fail to converge in the region of coexistence of normal and superfluid states. Fuller insight into the phase diagram would require a CCD study of the partially and fully polarized superfluid phases as performed via FN-DMC in Ref. [40].

IV. CONCLUSION

To summarize, we have described coupled-cluster theory as a promising computational method for the study of dilute Fermi gases. We have established the performance of 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 [127–134] as performed recently for the uniform electron gas with long-range repulsive Coulomb interactions [135,136]. 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 [81,82], precluding the local-density approximation for trapped gases as well as at nonzero temperature [137–142] and in nonequilibrium settings [143–145]. Lastly and perhaps most importantly, CC theory can be formulated with respect to a BCS reference wave function as opposed to the normal Fermi sea wave function used here, allowing a more accurate study of pairing and superfluidity [146–151]. Work along all of these lines is currently in progress.

ACKNOWLEDGMENTS

We thank F. Werner for helpful discussions. J.M.C. was supported by the Department of Defense (DoD) through the National Defense Science and Engineering Graduate (NDSEG) Fellowship Program. J.S. acknowledges support from the National Science Foundation (NSF) Materials Research Science and Engineering Centers (MRSEC) program through Columbia University in the Center for Precision Assembly of Superstratic and Superatomic Solids under Grant No. DMR-1420634. J.S. also acknowledges the hospitality of the Center for Computational Quantum Physics (CCQ) at the Flatiron Institute. We acknowledge computing resources from Columbia University's Shared Research Computing Facility project, which is supported by NIH Research Facility Improvement Grant No. 1G20RR030893-01, and associated funds from the New York State Empire State Development, Division of Science Technology and Innovation (NYSTAR) Contract No. C090171 both awarded April 15, 2010. The Flatiron Institute is a division of the Simons Foundation.

[1] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008).
[2] M. Randeria and E. Taylor, Annu. Rev. Condens. Matter Phys. **5**, 209 (2014).
[3] P. Massignan, M. Zaccanti, and G. M. Bruun, Rep. Prog. Phys. **77**, 034401 (2014).
[4] M. W. Zwierlein, *Novel Superfluids* (Oxford University Press, Oxford, 2014), Vol. 2, pp. 269–422.
[5] J. Kinast, S. L. Hemmer, M. E. Gehm, A. Turlapov, and J. E. Thomas, Phys. Rev. Lett. **92**, 150402 (2004).
[6] J. Kinast, A. Turlapov, and J. E. Thomas, Phys. Rev. Lett. **94**, 170404 (2005).
[7] M. W. Zwierlein, J. R. Abo-Shaeer, A. Schirotzek, C. H. Schunck, and W. Ketterle, Nature (London) **435**, 1047 (2005).
[8] M. W. Zwierlein, A. Schirotzek, C. H. Schunck, and W. Ketterle, Science **311**, 492 (2006).

[9] Y. Shin, M. W. Zwierlein, C. H. Schunck, A. Schirotzek, and W. Ketterle, Phys. Rev. Lett. **97**, 030401 (2006).

[10] G. B. Partridge, W. Li, R. I. Kamar, Y.-a. Liao, and R. G. Hulet, Science **314**, 54 (2006).

[11] Y.-i. Shin, C. H. Schunck, A. Schirotzek, and W. Ketterle, Nature (London) **451**, 689 (2008).

[12] M. Horikoshi, S. Nakajima, M. Ueda, and T. Mukaiyama, Science **327**, 442 (2010).

[13] S. Riedl, E. R. Sánchez Guajardo, C. Kohstall, J. Hecker Denschlag, and R. Grimm, New J. Phys. **13**, 035003 (2011).

[14] M. J. H. Ku, A. T. Sommer, L. W. Cheuk, and M. W. Zwierlein, Science **335**, 563 (2012).

[15] K. Levin and R. Hulet, *Contemporary Concepts Condensed Matter Science* (Elsevier, Amsterdam, 2012), Vol. 5, pp. 69–94.

[16] K. Fenech, P. Dyke, T. Peppler, M. G. Lingham, S. Hoinka, H. Hu, and C. J. Vale, Phys. Rev. Lett. **116**, 045302 (2016).

[17] B. Mukherjee, Z. Yan, P. B. Patel, Z. Hadzibabic, T. Yefsah, J. Struck, and M. W. Zwierlein, Phys. Rev. Lett. **118**, 123401 (2017).

[18] C. Carcy, S. Hoinka, M. G. Lingham, P. Dyke, C. C. N. Kuhn, H. Hu, and C. J. Vale, Phys. Rev. Lett. **122**, 203401 (2019).

[19] L. Sobirey, N. Luick, M. Bohlen, H. Biss, H. Moritz, and T. Lompe, Science **372**, 844 (2021).

[20] M. Greiner, C. A. Regal, and D. S. Jin, Nature (London) **426**, 537 (2003).

[21] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, S. Gupta, Z. Hadzibabic, and W. Ketterle, Phys. Rev. Lett. **91**, 250401 (2003).

[22] G. B. Partridge, K. E. Strecker, R. I. Kamar, M. W. Jack, and R. G. Hulet, Phys. Rev. Lett. **95**, 020404 (2005).

[23] M. Bartenstein, A. Altmeyer, S. Riedl, S. Jochim, C. Chin, J. H. Denschlag, and R. Grimm, Phys. Rev. Lett. **92**, 203201 (2004).

[24] C. A. Regal, M. Greiner, and D. S. Jin, Phys. Rev. Lett. **92**, 040403 (2004).

[25] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, A. J. Kerman, and W. Ketterle, Phys. Rev. Lett. **92**, 120403 (2004).

[26] T. Bourdel, L. Khaykovich, J. Cubizolles, J. Zhang, F. Chevy, M. Teichmann, L. Tarruell, S. J. J. M. F. Kokkelmans, and C. Salomon, Phys. Rev. Lett. **93**, 050401 (2004).

[27] M. W. Zwierlein, C. H. Schunck, A. Schirotzek, and W. Ketterle, Nature (London) **442**, 54 (2006).

[28] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).

[29] J. T. Stewart, J. P. Gaebler, and D. S. Jin, Nature (London) **454**, 744 (2008).

[30] A. Schirotzek, C.-H. Wu, A. Sommer, and M. W. Zwierlein, Phys. Rev. Lett. **102**, 230402 (2009).

[31] N. Navon, S. Nascimbene, F. Chevy, and C. Salomon, Science **328**, 729 (2010).

[32] M. Feld, B. Fröhlich, E. Vogt, M. Koschorreck, and M. Köhl, Nature (London) **480**, 75 (2011).

[33] I. Bloch, J. Dalibard, and S. Nascimbène, Nat. Phys. **8**, 267 (2012).

[34] A. T. Sommer, L. W. Cheuk, M. J. H. Ku, W. S. Bakr, and M. W. Zwierlein, Phys. Rev. Lett. **108**, 045302 (2012).

[35] M. Koschorreck, D. Pertot, E. Vogt, B. Fröhlich, M. Feld, and M. Köhl, Nature (London) **485**, 619 (2012).

[36] G. C. Strinati, P. Pieri, G. Röpke, P. Schuck, and M. Urban, Phys. Rep. **738**, 1 (2018).

[37] G. Ness, C. Shkedrov, Y. Florshaim, O. K. Diessel, J. von Milczewski, R. Schmidt, and Y. Sagi, Phys. Rev. X **10**, 041019 (2020).

[38] A. Bulgac and M. M. Forbes, Phys. Rev. A **75**, 031605(R) (2007).

[39] A. Schirotzek, Y.-i. Shin, C. H. Schunck, and W. Ketterle, Phys. Rev. Lett. **101**, 140403 (2008).

[40] S. Pilati and S. Giorgini, Phys. Rev. Lett. **100**, 030401 (2008).

[41] M. Punk, P. T. Dumitrescu, and W. Zwerger, Phys. Rev. A **80**, 053605 (2009).

[42] G. Bertaina and S. Giorgini, Phys. Rev. A **79**, 013616 (2009).

[43] F. Chevy and C. Mora, Rep. Prog. Phys. **73**, 112401 (2010).

[44] L. Radzihovsky and D. E. Sheehy, Rep. Prog. Phys. **73**, 076501 (2010).

[45] A. Gezerlis and R. Sharma, Phys. Rev. C **85**, 015806 (2012).

[46] M. G. Ries, A. N. Wenz, G. Zürn, L. Bayha, I. Boettcher, D. Kedar, P. A. Murthy, M. Neidig, T. Lompe, and S. Jochim, Phys. Rev. Lett. **114**, 230401 (2015).

[47] E. J. Mueller, Rep. Prog. Phys. **80**, 104401 (2017).

[48] H. Caldas, J. Phys. B: At., Mol. Opt. Phys. **53**, 085301 (2020).

[49] M. M. Parish, H. S. Adlong, W. E. Liu, and J. Levinsen, Phys. Rev. A **103**, 023312 (2021).

[50] T.-L. Ho, Phys. Rev. Lett. **92**, 090402 (2004).

[51] S. Nascimbène, N. Navon, K. J. Jiang, F. Chevy, and C. Salomon, Nature (London) **463**, 1057 (2010).

[52] C. Lobo, A. Recati, S. Giorgini, and S. Stringari, Phys. Rev. Lett. **97**, 200403 (2006).

[53] G. Bertaina and S. Giorgini, Phys. Rev. Lett. **106**, 110403 (2011).

[54] G. E. Astrakharchik, J. Boronat, E. Krotscheck, and T. Lichtenegger, J. Phys.: Conf. Ser. **529**, 012009 (2014).

[55] A. Galea, H. Dawkins, S. Gandolfi, and A. Gezerlis, Phys. Rev. A **93**, 023602 (2016).

[56] A. Galea, T. Zielinski, S. Gandolfi, and A. Gezerlis, J. Low Temp. Phys. **189**, 451 (2017).

[57] L. M. Schonenberg, P. C. Verpoort, and G. J. Conduit, Phys. Rev. A **96**, 023619 (2017).

[58] J. Carlson, S. Gandolfi, K. E. Schmidt, and S. Zhang, Phys. Rev. A **84**, 061602(R) (2011).

[59] H. Shi, S. Chiesa, and S. Zhang, Phys. Rev. A **92**, 033603 (2015).

[60] S. Bour, D. Lee, H.-W. Hammer, and U.-G. Meißner, Phys. Rev. Lett. **115**, 185301 (2015).

[61] E. Vitali, H. Shi, M. Qin, and S. Zhang, Phys. Rev. A **96**, 061601(R) (2017).

[62] S. Jensen, C. N. Gilbreth, and Y. Alhassid, Phys. Rev. Lett. **124**, 090604 (2020).

[63] S. Jensen, C. N. Gilbreth, and Y. Alhassid, Phys. Rev. Lett. **125**, 043402 (2020).

[64] N. Prokof'ev and B. Svistunov, Phys. Rev. B **77**, 020408(R) (2008).

[65] E. Burovski, E. Kozik, N. Prokof'ev, B. Svistunov, and M. Troyer, Phys. Rev. Lett. **101**, 090402 (2008).

[66] J. Vlietinck, J. Ryckebusch, and K. Van Houcke, Phys. Rev. B **87**, 115133 (2013).

[67] P. Kroiss and L. Pollet, Phys. Rev. B **90**, 104510 (2014).
[68] P. Kroiss and L. Pollet, Phys. Rev. B **91**, 144507 (2015).
[69] O. Goulko, A. S. Mishchenko, N. Prokof'ev, and B. Svistunov, Phys. Rev. A **94**, 051605(R) (2016).
[70] K. Van Houcke, F. Werner, T. Ohgoe, N. V. Prokof'ev, and B. V. Svistunov, Phys. Rev. B **99**, 035140 (2019).
[71] K. Van Houcke, F. Werner, and R. Rossi, Phys. Rev. B **101**, 045134 (2020).
[72] S. Y. Chang, V. R. Pandharipande, J. Carlson, and K. E. Schmidt, Phys. Rev. A **70**, 043602 (2004).
[73] M. Kolodrubetz and B. K. Clark, Phys. Rev. B **86**, 075109 (2012).
[74] E. R. Anderson and J. E. Drut, Phys. Rev. Lett. **115**, 115301 (2015).
[75] R. F. Bishop, Theor. Chim. Acta **80**, 95 (1991).
[76] F. Coester and H. Kümmel, Nucl. Phys. **17**, 477 (1960).
[77] G. Hagen, T. Papenbrock, M. Hjorth-Jensen, and D. J. Dean, Rep. Prog. Phys. **77**, 096302 (2014).
[78] T. D. Crawford and H. F. Schaefer, in *Reviews in Computational Chemistry*, Vol. 14 (Wiley, New York, 2000) pp. 33–136.
[79] R. J. Bartlett and M. Musiał, Rev. Mod. Phys. **79**, 291 (2007).
[80] I. Shavitt and R. J. Bartlett, *Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory* (Cambridge University Press, Cambridge, UK, 2009).
[81] T. Grining, M. Tomza, M. Lesiuk, M. Przybytek, M. Musiał, R. Moszynski, M. Lewenstein, and P. Massignan, Phys. Rev. A **92**, 061601(R) (2015).
[82] T. Grining, M. Tomza, M. Lesiuk, M. Przybytek, M. Musiał, P. Massignan, M. Lewenstein, and R. Moszynski, New J. Phys. **17**, 115001 (2015).
[83] I. Y. Zhang and A. Grüneis, Front. Mater. **6**, 123 (2019).
[84] R. Bishop, Ann. Phys. (NY) **77**, 106 (1973).
[85] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (Dover, New York, 2003).
[86] J. J. Shepherd, T. M. Henderson, and G. E. Scuseria, J. Chem. Phys. **140**, 124102 (2014).
[87] F. Chevy, Phys. Rev. A **74**, 063628 (2006).
[88] C. Mora and Y. Castin, Phys. Rev. A **67**, 053615 (2003).
[89] L. Pricoupenko and Y. Castin, J. Phys. A: Math. Theor. **40**, 12863 (2007).
[90] W. Ketterle and M. W. Zwierlein, Riv. del Nuovo Cim. **31**, 247 (2008).
[91] F. Werner and Y. Castin, Phys. Rev. A **86**, 013626 (2012).
[92] C. Mora and F. Chevy, Phys. Rev. Lett. **104**, 230402 (2010).
[93] C. J. M. Mathy, M. M. Parish, and D. A. Huse, Phys. Rev. Lett. **106**, 166404 (2011).
[94] C. Trefzger and Y. Castin, Phys. Rev. A **85**, 053612 (2012).
[95] M. M. Parish and J. Levinsen, Phys. Rev. A **87**, 033616 (2013).
[96] X. Cui, Phys. Rev. A **102**, 061301(R) (2020).
[97] R. Combescot, A. Recati, C. Lobo, and F. Chevy, Phys. Rev. Lett. **98**, 180402 (2007).
[98] R. Combescot and S. Giraud, Phys. Rev. Lett. **101**, 050404 (2008).
[99] R. J. Bartlett and I. Shavitt, Int. J. Quantum Chem. **14**, 543 (2009).
[100] R. J. Bartlett and G. D. Purvis, Int. J. Quantum Chem. **14**, 561 (1978).
[101] G. E. Scuseria, T. M. Henderson, and I. W. Bulik, J. Chem. Phys. **139**, 104113 (2013).
[102] D. Peng, S. N. Steinmann, H. van Aggelen, and W. Yang, J. Chem. Phys. **139**, 104112 (2013).
[103] T. C. Berkelbach, J. Chem. Phys. **149**, 041103 (2018).
[104] M. Jin, M. Urban, and P. Schuck, Phys. Rev. C **82**, 024911 (2010).
[105] M. Urban and P. Schuck, Phys. Rev. A **90**, 023632 (2014).
[106] H. Hu, B. C. Mulkerin, J. Wang, and X.-J. Liu, Phys. Rev. A **98**, 013626 (2018).
[107] H. Tajima and S. Uchino, New J. Phys. **20**, 073048 (2018).
[108] B. C. Mulkerin, X.-J. Liu, and H. Hu, Ann. Phys. (NY) **407**, 29 (2019).
[109] M. Pini, P. Pieri, and G. C. Strinati, Phys. Rev. B **99**, 094502 (2019).
[110] D. Durel and M. Urban, Phys. Rev. A **101**, 013608 (2020).
[111] H. Hu and X.-J. Liu, Phys. Rev. A **105**, 043303 (2022).
[112] E. Burovski, N. Prokof'ev, B. Svistunov, and M. Troyer, New J. Phys. **8**, 153 (2006).
[113] M. M. Forbes, S. Gandolfi, and A. Gezerlis, Phys. Rev. Lett. **106**, 235303 (2011).
[114] Edited by W. Zwerger, *The BCS-BEC Crossover and the Unitary Fermi Gas*, Lecture Notes in Physics, Vol. 836 (Springer, Berlin/Heidelberg, 2012).
[115] S. Tan, Ann. Phys. (NY) **323**, 2952 (2008).
[116] S. Tan, Ann. Phys. (NY) **323**, 2971 (2008).
[117] S. Tan, Ann. Phys. (NY) **323**, 2987 (2008).
[118] E. Braaten and L. Platter, Phys. Rev. Lett. **100**, 205301 (2008).
[119] F. Werner, L. Tarruell, and Y. Castin, Eur. Phys. J. B **68**, 401 (2009).
[120] S. Zhang and A. J. Leggett, Phys. Rev. A **79**, 023601 (2009).
[121] R. Haussmann, M. Punk, and W. Zwerger, Phys. Rev. A **80**, 063612 (2009).
[122] J. Levinsen, P. Massignan, S. Endo, and M. M. Parish, J. Phys. B: At., Mol. Opt. Phys. **50**, 072001 (2017).
[123] D. J. Thouless, Ann. Phys. (NY) **10**, 553 (1960).
[124] P. Noziöres and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1985).
[125] Y.-i. Shin, A. Schirotzek, C. H. Schunck, and W. Ketterle, Phys. Rev. Lett. **101**, 070404 (2008).
[126] B. A. Olsen, M. C. Revelle, J. A. Fry, D. E. Sheehy, and R. G. Hulet, Phys. Rev. A **92**, 063616 (2015).
[127] H. Koch and P. Jorgensen, J. Chem. Phys. **93**, 3333 (1990).
[128] M. Nooijen and J. G. Snijders, Int. J. Quantum Chem. **44**, 55 (1992).
[129] M. Nooijen and J. G. Snijders, Int. J. Quantum Chem. **48**, 15 (1993).
[130] J. F. Stanton and R. J. Bartlett, J. Chem. Phys. **98**, 7029 (1993).
[131] K. Bhaskaran-Nair, K. Kowalski, and W. A. Shelton, J. Chem. Phys. **144**, 144101 (2016).
[132] B. Peng and K. Kowalski, J. Chem. Theory Comput. **14**, 4335 (2018).
[133] B. Peng and K. Kowalski, Mol. Phys. **116**, 561 (2018).
[134] B. Peng, N. P. Bauman, S. Gulania, and K. Kowalski, *Annual Reports in Computational Chemistry*, 1st ed. (Elsevier B.V., 2021), Vol. 17, pp. 23–53.
[135] J. McClain, J. Lischner, T. Watson, D. A. Matthews, E. Ronca, S. G. Louie, T. C. Berkelbach, and G. K.-L. Chan, Phys. Rev. B **93**, 235139 (2016).
[136] A. M. Lewis and T. C. Berkelbach, Phys. Rev. Lett. **122**, 226402 (2019).
[137] F. Hummel, J. Chem. Theory Comput. **14**, 6505 (2018).

[138] A. F. White and G. K.-L. Chan, J. Chem. Theory Comput. **14**, 5690 (2018).
[139] A. F. White and G. Kin-Lic Chan, J. Chem. Phys. **152**, 224104 (2020).
[140] R. Peng, A. F. White, H. Zhai, and G. Kin-Lic Chan, J. Chem. Phys. **155**, 044103 (2021).
[141] M. R. Hermes and S. Hirata, J. Chem. Phys. **143**, 102818 (2015).
[142] G. Harsha, T. M. Henderson, and G. E. Scuseria, J. Chem. Theory Comput. **15**, 6127 (2019).
[143] A. A. Dzhioev and D. S. Kosov, J. Phys. A: Math. Theor. **48**, 015004 (2015).
[144] A. F. White and G. K.-L. Chan, J. Chem. Theory Comput. **15**, 6137 (2019).
[145] P. Shushkov III and T. F. Miller, J. Chem. Phys. **151**, 134107 (2019).
[146] W. A. Lahoz and R. F. Bishop, Z. Phys. B: Condens. Matter **73**, 363 (1988).
[147] A. Signoracci, T. Duguet, G. Hagen, and G. R. Jansen, Phys. Rev. C **91**, 064320 (2015).
[148] T. Duguet and A. Signoracci, J. Phys. G: Nucl. Part. Phys. **44**, 049601 (2017).
[149] T. M. Henderson, G. E. Scuseria, J. Dukelsky, A. Signoracci, and T. Duguet, Phys. Rev. C **89**, 054305 (2014).
[150] T. M. Henderson, I. W. Bulik, and G. E. Scuseria, J. Chem. Phys. **142**, 214116 (2015).
[151] Y. Qiu, T. M. Henderson, T. Duguet, and G. E. Scuseria, Phys. Rev. C **99**, 044301 (2019).