Atomic Fermi gas at the unitary limit by quantum Monte Carlo methods: Effects of the interaction range

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We calculate the ground-state properties of unpolarized two-component Fermi gas by the diffusion quantum Monte Carlo (DMC) methods. Using an extrapolation to the zero effective range of the attractive two-particle interaction, we find $E/E_{\text{free}}$ to be $0.212(2)$, $0.407(2)$, $0.409(3)$ and $0.398(3)$ for 4, 14, 38 and 66 atoms, respectively. The obtained energies are lower than those from the previously reported fixed-node DMC studies. In order to test the quality of nodal surfaces and to estimate the impact of the fixed-node approximation we perform released-node DMC calculations for 4 and 14 atoms. Analysis of the released-node and the fixed-node results suggests that the main sources of the fixed-node errors are long-range correlations which are difficult to sample in the released-node approaches due to the fast growth of the bosonic noise. Besides energies, we evaluate the two-body density matrix and the condensate fraction. We find that the condensate fraction for the 66 atom system converges to 0.56(1) after the extrapolation to the zero interaction range.

I. INTRODUCTION

In recent years, the homogeneous Fermi gas with attractive interactions has been studied extensively both theoretically and experimentally due to the success in cooling atoms into ultracold dilute condensates.¹³ By tuning the interaction strength through the Feshbach resonance⁹ the system can cross from the Bardeen-Cooper-Schrieffer (BCS) superfluid phase, where the $s$-wave scattering length $a_s$ is negative, to the Bose-Einstein condensate (BEC), where $a_s$ is positive. Since there is no symmetry change of the quantum state involved, the system exhibits the well-known BCS-BEC crossover.

In the special case corresponding to the diverging scattering length, $a_s \to \infty$, the system is in a strongly interacting regime called the unitary limit. In this regime the interparticle spacing $r_s$ is the only relevant scale, and the rest of the quantities are universal and system independent. The total energy of this system can be conveniently written as $E = \xi E_{\text{free}}$, where $E_{\text{free}}$ is the energy of the non-interacting atomic gas and $\xi$ is a system independent parameter. Experimental measurements of $\xi$ have been performed using $^6\text{Li}$ and $^{40}\text{K}$ atoms by investigating the expansion rate of the atomic cloud and the sound propagation in it.¹³ Simultaneously, a number of theoretical and numerical estimations of $\xi$ have been reported, including diffusion Monte Carlo (DMC)¹³,¹⁵ as well as path integral Monte Carlo, lattice simulations and analytical methods¹⁵,²⁸. The resulting estimates fall between $0.25 - 0.45$ showing that the actual value has not been settled yet and is still of significant interest due to the universal nature of the unitary limit.

One of the most interesting properties of the unitary gas is the robust presence of the pairing condensate which involves a large fraction of the system. The study of pairing effects is thus much more straightforward than, say, in superconducting materials, where only a sliver of the fermions around the Fermi level forms the condensate and the attractive interaction is much more complicated. The quantum Monte Carlo (QMC) methods have the advantage that the condensate can be detected directly, by evaluating the off-diagonal two-particle density matrix and by monitoring its behavior at large distances.⁴¹,⁴⁷–⁵⁵

The goal of our study is twofold. First, any actual simulation involves only a finite system, and the quantities relevant for the thermodynamic limit have to be obtained from appropriate extrapolations. The unitary system is not trivial in this respect, since pairing with infinite scattering length is described by a function with a slow fall-off at large distances. It is necessary to analyze the finite-size scaling of the quantities of interest and to test whether the actual limit of infinite dilution, or, equivalently, of point-like character of the interaction, has indeed been reached. Second, the impact of the fixed-node approximation in the quantum Monte Carlo method is not very well understood for this system since there is nothing to compare with: so far the fixed-node formulation of the QMC methods appears to be the only approach that is able to provide an upper bound for the total energy. This has motivated us to probe the accuracy of the nodes by released-node QMC simulations and by improvements in the variational flexibility of the employed wave functions.

We have carried out calculations of the ground-state properties of the dilute unitary Fermi gas by the fixed-node DMC (FN-DMC)²⁵ method for 4, 14, 38 and 66 atoms. By using a more versatile construction of the pair orbital in the BCS wave function and by extrapolating the effective range of the two-particle interactions $R_{\text{eff}}$ to zero, we were able to obtain lower $\xi$ than the previously reported DMC calculations. These results suggest that the extrapolation of $R_{\text{eff}}$ is important, especially for smaller systems. In order to test the quality of the nodal surface of the BCS wave function, we have performed released-node DMC (RN-DMC)²⁹,³⁰ calculations for 4 and 14 atoms. This procedure has been carried out starting from two types of nodal constraints: from the BCS nodes and from the Hartree-Fock (HF) nodes. Our
RN-DMC results indicate that the nodal corrections are driven mainly by long-range correlations which are difficult to sample in the released-node framework due to the rapid growth of the bosonic noise. We have calculated also the two-body density matrix and the condensate fraction for the 66 atom system, and we have estimated the corrections from the effective-range extrapolation on these quantities.

II. METHOD

A. Hamiltonian

We consider a two-component Fermi gas with Hamiltonian

\[ H = -\frac{1}{2} \sum_{i=1}^{N/2} \nabla_i^2 - \frac{1}{2} \sum_{i=1}^{N/2} \nabla_{i'}^2 + \sum_{i,i'} V(r_{ii'}) , \]

where \( N \) is the total number of atoms, \( i \) and \( i' \) correspond to the spin-up and spin-down atoms, and \( r_{ii'} \) denotes the distance \( |r_i - r_{i'}| \). The atoms are located in a cubic box with the side \( L \) and we impose the periodic boundary conditions. The two-particle potential \( V(r_{ii'}) \) is taken in the Pöschl-Teller form

\[ V(r_{ii'}) = -\frac{2\mu^2}{\cosh^2(\mu r_{ii'})} , \]

whose effective range is \( R_{\text{eff}} = 2/\mu \). The s-wave scattering length \( a_s \) is infinite for all values of \( \mu \neq 0 \).

B. Trial wave functions

In the majority of our calculations we employ trial wave functions of the BCS form multiplied with the Jastrow factor (BCS-Jastrow) as given by

\[ \Psi_T(R) = \Psi_{BCS}(R)e^{J(R)} , \]

where

\[ \Psi_{BCS}(R) = A \prod_{i,i'=1}^{N/2} \phi(r_i, r_{i'}) = \det[\phi(r_i, r_{i'})] . \]

Here \( A \) represents the antisymmetrization operator and \( \phi(r_i, r_{i'}) \) is the pair orbital. The vector \( R \) encompasses all atomic coordinates of \( r_i \) and \( r_{i'} \). Additionally, we have carried out a subset of calculations also with the Hartree-Fock-Jastrow (HF-Jastrow) trial functions, in which \( \Psi_{BCS} \) is replaced with a product of two Slater determinants of one-particle orbitals (simple plane waves). The HF-Jastrow wave function reads as

\[ \Psi_{SI}(R) = \det[\varphi_a(r_i)]\det[\varphi_a(r_{i'})]e^{J(R)} . \]

The pair orbital \( \phi(r_i, r_{i'}) \) in \( \Psi_{BCS} \) is written as a linear combination of Gaussian functions

\[ \phi(r_i, r_{i'}) = \sum_{l,m,n=-1}^1 d_k e^{-\alpha_k(x_i-x_{i'}+2l)^2} \times e^{-\alpha_n(y_i-y_{i'}+mL)^2} e^{-\alpha_k(z_i-z_{i'}+nL)^2} , \]

where \( d_k \) are expansion coefficients, and \( r_i = (x_i, y_i, z_i) \) and \( r_{i'} = (x_{i'}, y_{i'}, z_{i'}) \) are coordinates of \( i \) and \( i' \) atoms inside the simulation box of linear size \( L \). We choose sufficiently large exponents \( \alpha_k \) so that only the first neighbor shell of periodic images contributes to the sum, that is, the Gaussian functions are negligible at distances larger than \( 3L/2 \). The pair orbital is smooth with zero derivative at the boundary of the simulation cell. The Jastrow factor \( J(R) \) is constructed in a similar way as the pair orbital \( \phi(r_i, r_{i'}) \) for both different spin atoms and same spin atoms.

A typical trial wave function includes around 30 to 40 variational parameters that are optimized by minimizing a linear combination of the total energy and its variance. Although the Jastrow factor does not change the nodal surface, accurate description of the pair correlations makes the variational optimization much more efficient and robust. When the effective range of the potential approaches zero, more Gaussian functions with larger exponents \( \alpha_k \) are included in the Jastrow factor in order to keep the accuracy of the trial function consistently high. On the other hand, and somewhat surprisingly, we find that similar adjustment of the pair orbital with the changing effective range is relatively minor.

C. Fixed-node and released-node DMC methods

The DMC method projects out the ground state from a given trial function \( \Psi_T \) by means of an auxiliary evolution in the imaginary time, \( \Phi(\tau) \sim \exp(-\tau H)\Psi_T \). By introducing importance sampling with the aid of a guiding function \( \Psi_G \), we can write an integral equation for \( \Phi(R, \tau) \) in the form

\[ \Psi_G(R)\Phi(R, \tau + \Delta\tau) = \int dR' \Psi_G(R')G(R, R', \Delta\tau)\Psi_G(R')\Phi(R', \tau) . \]

For small \( \Delta\tau \), the propagator \( G(R, R', \Delta\tau) \) can be approximated using the Trotter-Suzuki formula as

\[ \frac{\Psi_G(R)}{\Psi_G(R')}G(R, R', \Delta\tau) \approx G_0(R, R' + \Delta\tau v(R'), \Delta\tau) \times e^{-\Delta\tau(E_L(R)+E_L(R')-2E_T)/2} , \]

where \( v(R') \equiv \nabla \ln |\Psi_G(R')| \) and \( G_0(R, R', \Delta\tau) \) is the Green’s function for non-interacting atoms that takes the
form of the diffusion kernel. The so-called local energy $E_L$ is given by

$$E_L(R) = \frac{H\Psi_G(R)}{\Psi_G(R)}. \quad (9)$$

The product $\Psi_G\Phi$ is represented by a set of samples (also referred to as walkers) and this ensemble is evolved with the aid of a stochastic process simulating Eqs. (7) and (8). In the fixed-node method we set $\Psi_G(R) = \Psi_T(R)$ and the fixed-node condition is imposed by enforcing the sampling points to obey

$$\Psi_G(R)\Phi(R, \tau) \geq 0 \quad (10)$$

at all times. In the limit of long $\tau$ the solution converges towards the lowest-energy state consistent with the boundary conditions given by the fixed nodes.

In the RN-DMC method the guiding function has bosonic symmetry and its square should be close to the square of the fermionic ground state. We have used guiding functions in the form

$$\Psi_G(R) = \sqrt{\Psi_T^2(R) + \alpha \langle \Psi_T^2 \rangle}, \quad (11)$$

where $\langle \Psi_T^2 \rangle$ is the average value of $\Psi_T^2(R_0)$ over all configurations, and $R_0$ are the walker positions right after the nodal release. The tunable parameter $\alpha$ controls the rate of walkers passing through the nodal region. The guiding function is non-negative everywhere and therefore the stochastic process propagates a mix of bosonic and fermionic states. The fermionic component is filtered out by reweighting with the factor $\Psi_T/\Psi_G$ so that the fermionic-state energy is given by

$$\langle \Phi_0 | H | \Psi_T \rangle = \frac{\int dR \Phi_0(R) \Psi_G(R) \Psi_T(R) \Psi_T(R)}{\int dR \Phi_0(R) \Psi_G(R) \Psi_T(R)}, \quad (12)$$

where $\Phi_0(R)$ denotes the exact fermionic ground state.

Since this method is exponentially demanding both in the projection time and in the number of atoms, it is important to choose $\alpha$ so that the statistical information is recovered as quickly as possible. If $\alpha$ is too large the fluctuations from the poor importance sampling overwhelm any useful signal very rapidly. On the other hand, a too small value can bias the results. Since it is difficult to reach reliable error bars in this type of calculations, we have used the method mostly to identify the onset and the amplitude of the energy decrease during the projection period when the stochastic noise was acceptably small.

In the RN-DMC process, we can also pick up the statistical signal from the walkers that have never crossed the nodal surface, and in essence this provides the FN-DMC estimator. By monitoring these paths as well, we can assess the consistency of the estimators and somewhat better tune the parameter $\alpha$ for providing better RN-DMC signal.

### III. RESULTS

For benchmark purposes we first calculate perhaps the smallest nontrivial system—four atoms. Our result is shown in Fig. 1 upper left panel. There is approximately 10% energy drop when $R_{\text{eff}}/r_s$ is reduced from 0.1279 to 0.003998. We extrapolate $R_{\text{eff}}$ to zero using a linear fit and obtain $\xi_{2,2} = 0.212(2)$. Here and in the rest of the paper, the denominator $E_{\text{free}}$ in the ratio $\xi = E/E_{\text{free}}$ is evaluated in the same finite volume subject to the same boundary conditions as the numerator $E$.

Our calculations with 14, 38 and 66 atoms are carried out analogously to the 4-atom case, and the extrapolated values of $\xi$ are 0.407(2), 0.409(3) and 0.398(3), respectively, as plotted in Fig. 1. In these calculations, the smallest effective range is $R_{\text{eff}}/r_s = 0.003125$. It should be noted that in the previous DMC calculations, the range of $R_{\text{eff}}/r_s$ was between 0.1 to 0.2, and within this range our DMC results agree well with the previously obtained values. Reduction of $R_{\text{eff}}$ decreases the energy in all cases although the decrease per atom is smaller in larger systems.

To test the quality of the nodal surfaces, we have carried out released-node calculations for 4-atom and 14-atom systems. The RN-DMC calculations for 4 atoms were done with $R_{\text{eff}}/r_s = 0.06397$. In a typical released-node run the number of walkers was about two million so that the error bars were initially very small. In Fig. 2 the upper row shows the pair orbital along three distinct
FIG. 2. The pair orbitals and FN-DMC and RN-DMC energies of the 4-atom unitary system with \( R_{\text{eff}}/r_s = 0.06397 \). The upper row shows the pair orbitals with the lowest (left), intermediate (middle) and optimal (right) accuracy with regard to the variational optimization. The lower row shows the corresponding DMC energies as functions of the projection time starting from the variational estimate. Note that the resolution of the left and right panels differs by an order of magnitude. The vertical dotted lines indicate the instant of the nodal release.

directions (100, 110 and 111) of the interparticle distance vector \( \mathbf{r}_i - \mathbf{r}_j \). The lower row shows the FN-DMC and RN-DMC energies as they evolve with the projection time. The plots show convergence of the FN-DMC energy followed by the nodal release. This is accomplished by switching the guiding wave function from \( \Psi_T(\mathbf{R}) \) to the bosonic function \( \Psi_G(\mathbf{R}) \) defined in Eq. (11).

The released-node signal reflects the quality of the nodal surface of the trial wave function employed in the FN-DMC simulation. We have tested wave functions with intentionally varied accuracy by employing suboptimal pair orbitals. The plot of the energy evolution in the left panel of Fig. 2 shows a clear and pronounced drop after the nodal release. As the quality of the pair orbital improves, this drop shrinks. For the fully optimized BCS-Jastrow wave function (the right panel in Fig. 2) the energy is reduced by less than 0.002 within the longest projection time we have tried. This fact as well as comparison with other methods indicate that our BCS wave functions are very accurate in this small system and that the fixed-node error is marginal.

We observe an unexpectedly high sensitivity of the nodal quality to the details of the pair orbital at large distances. This suggests an explanation for the relatively slow convergence of the released-node energy: the long-range tails of the pair orbital affect the nodal hypersurfaces, although their contribution to the total energy is relatively small. One can further deduce that this makes the released-node method quite challenging to apply since it requires sampling of long distances and the corresponding correlations. This is, however, difficult to achieve because the diffusive motion of walkers is slow, proportional to \( t^{1/2} \), while the growth of the noise is fast, proportional to \( \exp(\Delta_{BF}t) \) where \( \Delta_{BF} \) is the difference between the bosonic and fermionic ground-state energies.

The time step \( \Delta_T \) was set to \( 4 \times 10^{-5}r_s^2 \) in all runs and we have verified that the time-step bias of the RN-DMC results is negligible. The converged RN-DMC energy should not depend on the parameter \( \alpha \) in the bosonic guiding function \( \Psi_G \) provided one would be able to evolve the stochastic process with the error bars under control until the full convergence. In the same time, the parameter \( \alpha \) crucially affects the growth of the fluctuations with the projection time as illustrated in Fig. 2.

The RN-DMC energy for 14 atoms with \( R_{\text{eff}}/r_s = 0.2 \) is shown in Fig. 3. The error bars are estimated from eight independent runs with two million walkers each. In the interval of \( E_Ft \leq 0.2 \) after the nodal release the RN-DMC energy gain appears to be very small and the error bars preclude to make any statistically sound estimation for longer projection times. The rapid loss of resolution is expected since the difference between the bosonic and
fermionic ground states grows with the number of atoms. Again, the RN-DMC signal exhibits little dependence on \( \alpha \) we choose.

In order to make a comparison with a case displaying a clear fixed-node bias, we have carried out RN-DMC runs using the Slater-Jastrow trial wave function, see Fig. 4. Since this wave function has the nodal surface of the non-interacting Fermi gas, the nodal surface is strongly distorted. As a result, we see a very pronounced released-node signal. However, within the projection time interval of \( E_F t \leq 0.2 \), the energy drops by only \( \approx 0.015 \) for the largest \( \alpha \) we tested. This is very small considering that the true ground-state energy is at least an order of magnitude lower. This again illustrates the challenges of efficient application of the released-node method, at least for present cases. Comparison of the Slater and BCS wave functions shows a significant effect of pairing as was demonstrated in earlier studies.\(^{13}\)

In order to quantify the pairing effects we calculate the two-body density matrix which enable us to evaluate the condensate fraction. The projected two-body density matrix for spin-up and spin-down atoms is defined as

\[
\rho^{(2)}(r) = \frac{N^2}{4V^2} \int dR \Phi(R) \Psi_T(R) \frac{\Psi_T(r_1+r_2+r) \Psi_T(r_1, r_2)}{\Psi_T(r_1, r_2)} ,
\]

where \( N \) is the total number of atoms and \( V \) is the volume of the simulation cell. The density matrices have been calculated for the fixed-node wave functions and hence they correspond to the mixed estimators.\(^{25}\) Nevertheless, the mixed-estimator bias is negligible since the variational Monte Carlo and DMC estimates of \( \rho^{(2)} \) coincide within error bars. This is a further evidence of the high accuracy of our trial wave functions.

The condensate fraction can be extracted from the two-body density matrix as

\[
c = \frac{2V^2}{N} \lim_{r \to \infty} \rho^{(2)}(r) .
\]

The calculated density matrices are shown in Fig. 5 with the condensate fraction estimated from the long-range limit. The condensate fraction saturates for \( R_{\text{eff}} \leq 0.5 \) at \( c = 0.56(1) \). This value is not too far from the results obtained previously.\(^{10,15}\)

To illustrate the character of the nodal surfaces in the BCS-BEC systems, we present three-dimensional scans of the nodes for three wave functions corresponding to the following scattering regimes: the free atomic gas with no pairing, our best unitary-limit wave function, and the wave function with enhanced pairing from the BEC side of the BCS-BEC phase diagram \((\alpha, k_F = 0.6592)\). The left column of Fig. 6 displays the nodal surface of the free atomic Fermi gas. The delocalized nature of the system is apparent. At the unitary limit, shown in the middle column of Fig. 6, the shape of the nodal surface is significantly different as the pairing effects clearly dominate and lead to a localized character of the nodes from the
FIG. 6. Three-dimensional subsets of the nodal hypersurfaces for three types of wave functions and corresponding phases in the 14-atom system. The node is obtained by scanning the simulation cell with a pair of spin-up and spin-down atoms sitting on the top of each other while keeping the rest of the atoms at fixed positions (tiny spheres). From the left to the right, the columns show the nodal surfaces of the wave functions corresponding to the free Fermi gas, the unitary limit and the BEC side of the crossover. The lower row displays the same surfaces rotated by 45 degrees around the z-axis.

perspective of a pair of up and down spin atoms. The nodes on the BEC side (the right column) do not differ much from the unitary limit, except for a slightly more pronounced localization.

IV. CONCLUSIONS

We have carried out QMC calculations of the zero-temperature, spin-unpolarized atomic Fermi gas in the unitary limit. We show that the interaction range impacts the resulting total energies significantly. By extrapolating the interaction range to zero we obtain the ratio $E/E_{\text{free}}$ for 4, 14, 38 and 66 atoms to be 0.212(2), 0.407(2), 0.409(3) and 0.398(3), respectively. Our results agree well with the previous fixed-node DMC calculations when we employ similar simulation parameters such as the atom density, the interaction range and the number of atoms. From the released-node DMC calculations for 4 and 14 atoms we have found that the convergence to the correct and asymptotically exact ground-state energies is unfavorably slow compared to the growth of the statistical noise. We were able to identify only small energy gains within the simulation times that allowed for acceptable signal to noise ratio. We have calculated the two-body density matrix and the condensate fraction in the limit of zero interaction range, and we have found only small changes in these quantities when compared with the previous calculations. Our condensate fraction from the fixed-node DMC simulations is 0.56(1).

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