Equation of State of Superfluid Neutron Matter and the Calculation of the $^1S_0$ Pairing Gap

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We present a quantum Monte Carlo study of the zero-temperature equation of state of neutron matter and the computation of the $^1S_0$ pairing gap in the low-density regime with $\rho < 0.04$ fm^{-3}. The system is described by a nonrelativistic nuclear Hamiltonian including both two- and three-nucleon interactions of the Argonne and Urbana type. This model interaction provides very accurate results in the calculation of the binding energy of light nuclei. A suppression of the gap with respect to the pure BCS theory is found, but sensibly weaker than in other works that attempt to include polarization effects in an approximate way.

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Superfluidity of neutron matter is currently a subject of great interest across the astrophysics, nuclear physics, and many-body physics communities. Pairing of nucleons may occur in different channels. At densities relevant for the phenomenology of the stellar outer core, a crucial role is played by the energy gap of the $^1S_0$ paired state. It has direct consequences on the low-density equation of state, the cooling process, the phenomenology of glitches [1,2], and on neutrino emission. In addition, the effect of pairing of neutrons in the low-density regime plays an important role also in the pairing effects observed in neutron-rich nuclei, where the energy is sensibly more stable if the total number of nucleons A is even [3] (see, for example, Ref. [1] for a review).

The occurrence of superfluidity in neutron matter is one of the many examples of pairing effects in low-density many-fermion systems. Such systems are often characterized by the parameter $\xi = k_F a$, where k_F is the Fermi momentum, and a is the scattering length, which for neutron matter reaches a value as low as -14.8. At this value we can still regard the system as a weak BCS superfluid [4], but at the same time the nucleon-nucleon interaction induces strong correlations among the neutrons.

This fact leads to a second main reason of interest, i.e., the study of the interplay of the correlations induced by the strong repulsion among neutrons at short distance, and by the spin dependent forces with a strong tensor component, and the occurrence of the BCS state. A clean signature of this effect can be found in the behavior of the BCS energy gap Δ. This quantity has been computed by several authors within many different approximation schemes. A mean-field BCS treatment gives a peak value of the energy gap $\Delta \simeq 3$ MeV at $k_F \sim 0.8$ fm^{-1}, almost irrespective of the nucleon-nucleon (NN) potential [5,6]. This is not surprising because all NN potentials are fitted to reproduce the same S- and P-wave components in the scattering experiments. The situation becomes more intricate when so-called polarization effects, i.e., the interaction with the surrounding medium are introduced. There are two ways to attack the problem. The first is still based on the solution of the BCS equation (a two-body problem) with an effective interaction which approximates the background effects. Alternatively, a more rigorous calculation should include many-body effects by solving the many-body problem with the full interaction, and compute the gap between the BCS and normal state directly as the energy difference. At this level, an accurate computation of the BCS gap can be obtained only if (1) A realistic interaction including all relevant contributions (and, in particular, hard-core repulsion and tensor) and (2) A reliable *ab initio* computational method is employed. The present disagreement among different estimates of the energy gap presently available, and which is shown in Fig. 1, can be explained by the lack of at least one of these two conditions.

The inclusion of polarization effects shows some general trends in the behavior of the BCS gap. It has been pointed out that the screening by the medium could strongly reduce the pairing strength in the $^1S_0$ channel. Actually, the diverse methods used in connection with realistic NN interactions all give a maximum for Δ between 0.7 and 1.0 MeV at a density corresponding to a Fermi momentum between 0.7 and 1.0 fm^{-1} [7,8]. Recent Brueckner theory calculations [9] and Hartree Fock calculations [10] give a remarkably larger value (~ 1.8 MeV). A recent quantum Monte Carlo (QMC) calculation [11], using the AV18 NN potential projected in the $^1S_0$ channel, gave in the very low-density range corresponding to $k_F \leq 0.55$ fm^{-1} a pairing gap sensibly larger with respect to previous results, yet lower than the Brueckner calculation of Ref. [9], and Hartree Fock calculations of Ref. [10].

In this Letter we propose a systematic computation of the $^1S_0$ pairing gap in neutron matter as a function of the

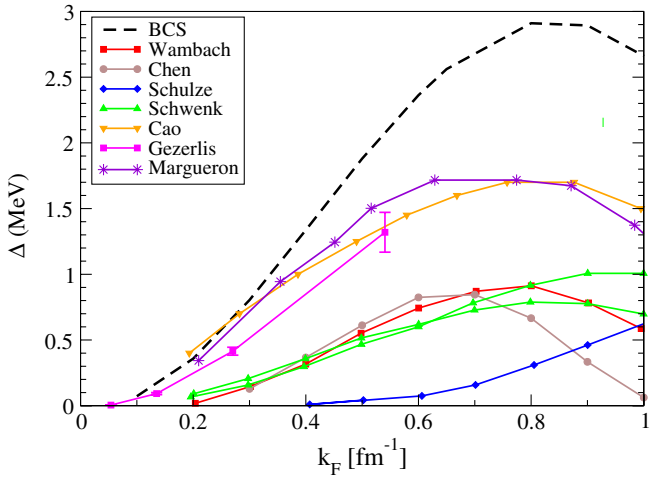

FIG. 1 (color online). The $^1S_0$ pairing gap of neutron matter as a function of the Fermi momentum k_F computed with different methods. In the figure we display works of Wambach *et al.* [27], Chen *et al.* [28], Schulze *et al.* [7], Schwenk *et al.* [8], Cao *et al.* [9], Gezerlis and Carlson [11] and Margueron *et al.* [10]. All the results are compared with a BCS calculation (dashed line).

density of the system in which both the conditions of using a complete realistic interaction (an Argonne-Urbana class potential) and an accurate *ab initio* method (the auxiliary field diffusion Monte Carlo within the fixed phase approximation) are fulfilled, with the aim of benchmarking existing results. QMC techniques have the advantage of accurately solving for the many-body ground state, and provide a powerful tool to study a wide range of systems both finite and homogeneous. The auxiliary field diffusion Monte Carlo (AFDMC) method is particularly well suited to deal with large nucleonic systems [12]. In particular, the AFDMC method gives accurate results for the properties of nuclei [13], symmetric nuclear matter [14], and neutron matter [15], for which studies performed with Green's function Monte Carlo technique are limited to 14 neutrons in a periodic box [16]. The efficiency of the AFDMC method lies in the fact that spin states of nucleons are sampled, rather then explicitly summed, by means of a Hubbard-Stratonovich transformation. It can be extended to systems with over a hundred nucleons. Larger systems are needed to rule out finite-size effects in the estimates. The computations presented in previous AFDMC method works [15,17] were affected by serious technical issues related to the approximations used to cope with the fermion sign problem. In particular, these approximations led to rather poor energy upper bounds in presence of the tensor-tau interaction in the Hamiltonian, and therefore nuclei and nuclear matter could not accurately be simulated. Such technical issues have been totally solved by the use of the fixed phase approximation [13,14,18] instead of the constrained path. For this reason our previous calculations of the energy gap of superfluid neutron matter [17] belongs to an old generation of AFDMC method simulations, which have been much improved upon after the introduction of the fixed phase constraint.

Our calculations for bulk neutron matter are based on a nonrelativistic Hamiltonian of N neutrons in a periodic box:

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}, \qquad (1)$$

where i and j are neutron indices, and v_{ij} and V_{ijk} are, respectively, the two- and the three-nucleon interactions (namely the Argonne v_8' (AV8′) and the Urbana IX (UIX). The AV8′ [19] interaction is a simpler form of the more accurate Argonne v_{18} (AV18) [20]; it contains only 8 operators instead of 18, it preserves the same isoscalar part of AV18 in S and P partial waves as well as in the $^3D_1$ wave and its coupling to $^3S_1$, and it correctly gives the experimental deuteron energy. The advantage of using AV8′ rather than the AV18 interaction is that it has a more suitable form for the AFDMC method calculation. In the low-density regime where $\rho < 0.04$ fm^{-3} the AV8′ gives the same energy as the AV18 interaction within 3% [21]. The Urbana UIX interaction was fitted to correct the overbinding of AV18 in the ground state of light nuclei and to reproduce the empirical value of the equilibrium density of nuclear matter [22].

We consider the *full* nuclear Hamiltonian, instead of projecting in the pairing channel only, in order to include *all* the many-body correlations in the system that the effective bare interactions eventually miss.

The AFDMC method calculations start from a Jastrow BCS trial wave function of the form

$$\psi_T = \left[\prod_{i<j} f_J(r_{ij})\right]\Phi_{\mathrm{BCS}}(\mathbf{R}, S), \qquad (2)$$

where $R = \{\mathbf{r}_1, \ldots, \mathbf{r}_N\}$ and $S = \{s_1, \ldots, s_N\}$ are the space and spin coordinates of the neutrons. The factor f_J is the central component of the Jastrow correlation computed in the Fermi hypernetted chain–single operator chain approximation scheme. Its only role is to avoid the overlap between neutrons, and its detailed form has no influence on the final result. The Φ_{BCS} antisymmetric function is built as a Pfaffian [23] of both paired and single particle orbitals. Paired orbitals are defined by

$$\phi(\mathbf{r}_{ij}, s_i, s_j) = \sum_{\alpha}\frac{v_{k_\alpha}}{u_{k_\alpha}} e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_{ij}}\chi(s_i, s_j), \qquad (3)$$

where χ is a spin function coupling two neutrons in the singlet state. The single particle orbitals are plane waves fitting Born–von Kármán periodic boundary conditions. The coefficients u and v entering the paired orbitals are provided by a correlated basis functions (CBF) calculation [5]. In the case of even N, no single particle wave functions are considered in the Pfaffian, while if N is odd the single particle plane wave accommodating the unpaired neutron is chosen in order to minimize the energy of the system. Finite-size effects due to the truncation of the potential are

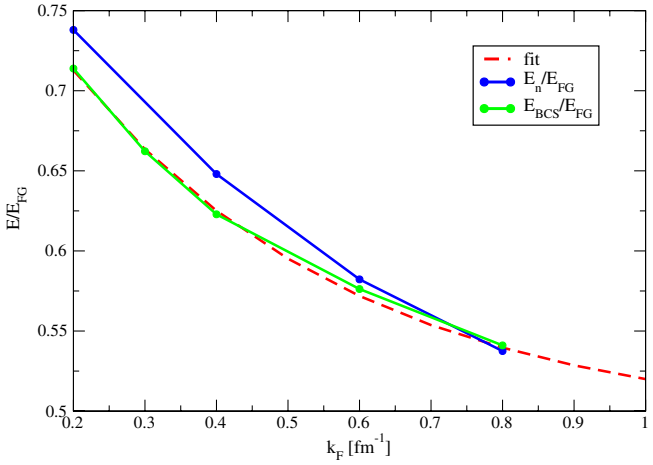

FIG. 2 (color online). The EOS of neutron matter in the low-density regime. The two calculations were performed using different trial wave functions modeling a normal and a BCS state. The fit is a guide to the eye.

reduced following the common procedures described in [15].

Because the AFDMC method projects out the lowest energy state with the same symmetry and phase of the trial wave function from which the projection is started, once the character of the initial state (BCS or normal Fermi liquid) is given, the computed energy will refer to that particular phase. It is therefore possible to compare the two equations of state, and discuss the relative stability. In Fig. 2 we display the resulting values as a function of k_F normalized to the corresponding Fermi gas energy. In almost all of the range of densities considered the BCS phase is stable with respect to the normal Fermi liquid, although the relative energy difference never exceeds 4%.

When the Fermi wave vector increases beyond $k_F = 0.6$ fm^{-1} the normal state is energetically more favorable than the BCS state, with an energy difference smaller than 1% of the total energy. We can therefore conclude that in the low-density regime neutron matter is in a $^1S_0$ superfluid phase. In this regime the neutron-neutron interaction is dominated by this channel, having a scattering length of about $a = -18.5$ fm. Quantum Monte Carlo calculations of the equation of state (EOS) of dilute cold fermions showed that in the unitary limit (when $ak_F \rightarrow -\infty$), the ratio between the energy of the system and the energy of the Fermi gas is $\xi = 0.42(1)$ [24–26]. The deviation from this asymptotic value is a measure of the relevance of the details of the interaction in determining the equation of state of the system in the range of densities considered. One should also consider the fact that at larger densities the effect of pairing in scattering channels other than the $^1S_0$ becomes important.

In a full many-body calculation the superfluid gap can be evaluated by using the difference

$$\Delta(N) = E(N) - \tfrac{1}{2}[E(N+1) + E(N-1)], \qquad (4)$$

where N is taken to be odd. It should be noted that the above expression is valid only if $E(N)$, $E(N+1)$, and $E(N-1)$ are computed by keeping the volume V of the system fixed. This means that the density would be different in the N, $N+1$, $N-1$ neutron systems. Because our simulations are usually performed at fixed density, we checked the dependence of the energy on the constraint used. Considering a number of particles around $N = 14$, which is the lowest number of neutrons used in the simulations, and therefore the worst case scenario, we evaluated the gap at fixed volume first, and then at fixed density. The difference in the results is well within statistical errors.

Several simulations at different values of N were performed in order to evaluate the gap and the corresponding statistical error bars. A first check concerned the dependence of the gap estimate on the number of neutrons used in evaluating the difference in Eq. (4). The values of Fermi momentum considered for the check were 0.4, 0.6, and 0.8 fm^{-1}, and the numbers of neutrons were taken in the ranges $N = 12$–18 and $N = 62$–68. For each case, we evaluated the gap around the odd N according to Eq. (4). At each density $\Delta(66)$ (the averaged gap between $N = 62$ and 68) is always smaller than $\Delta(14)$. The same behavior was also observed in the QMC calculation of Gezerlis and Carlson [11] using the simple interaction projected in the pairing channel. In that paper computations were extended also to $N = 92$. The gap values $\Delta(66)$ and $\Delta(92)$ are equal within error bars and approach the infinite limit in the same way as in the mean-field BCS calculation. Unfortunately in QMC simulations, in the absence of a correlated sampling scheme, it is impossible to use arbitrarily large values of N, because the gap has to be evaluated as the difference among total energies. This means that the accuracy required in the evaluation of the energy makes the computational time increase with $\sqrt{N}$, in addition to the N^3 standard scaling for Fermion simulations.

A finite-size effect might be connected to the relative size of the neutrons' Cooper pair and the simulation box. The Heisenberg uncertainty principle can be used to estimate the dimension of a Cooper pair as $\delta x \simeq \epsilon_F/(\Delta k_F)$ where ϵ_F is the Fermi energy per particle. Taking $\Delta = 2$ MeV, and $k_F = 0.8$ fm^{-1}, we have therefore $\delta x \simeq 6.6$ fm, much smaller than the typical box size, which for 66 neutrons is $\sim$16 fm. A consequence of this analysis is also that relevant correlation lengths should be all contained in the simulation box, implying that an explicit inclusion in the wave function of long range effects (which are automatically included in mean-field calculations) should not lead to significant differences in the results.

We report in Fig. 3 the estimate of the $^1S_0$ superfluid gap as a function of the Fermi momentum k_F. The AFDMC method points are compared with results of the CBF calculation [5] used to determine the BCS coefficients entering the trial wave function. We also display, for the sake of comparison, the family of more recent calculations. As can be seen, the AFDMC method calculations give values of Δ

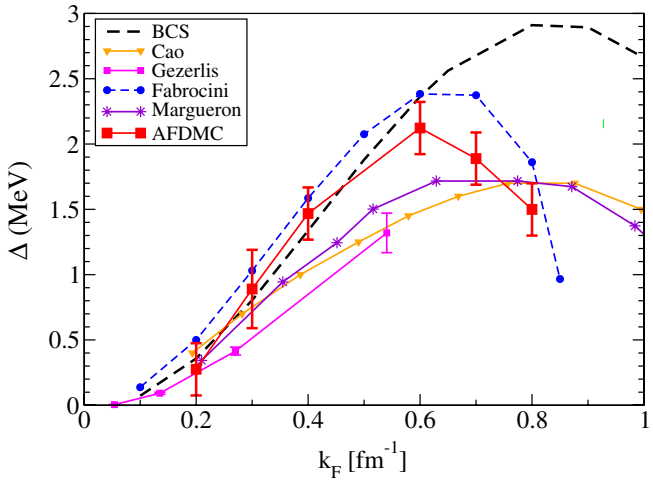

FIG. 3 (color online). AFDMC method calculation of the $^1S_0$ pairing gap of neutron matter as a function of the Fermi momentum k_F and compared with more recent results. The AFDMC method results are indicated by large squares with statistical error bars. Other results are some of those displayed in Fig. 1, and the dashed line with circles is the CBF calculation of Fabrocini *et al.* [5].

lower than those of the CBF calculation. This behavior is opposite to that reported in a previous paper in which the same comparison was made [17]. The difference can be attributed both to the larger number of neutrons used in the present work, and to the use of the fixed phase approximation instead of the constrained path approximation to keep the sign problem under control.

We confirm the depletion of the superfluid gap with respect the BCS result. However, our results are leaning towards the calculations giving a maximum value of the gap of order 2 MeV. The other available QMC calculations by Gezerlis and Carlson [11] differ within error bars for densities corresponding to $k_F < 0.3$ fm^{-1}. At $k_F = 0.55$ fm^{-1} they predict a gap about 30% smaller with respect to the AFDMC method estimate. We believe that such difference comes from the fact that when increasing the density, the correlations induced by the interactions in channels others than $^1S_0$ become more and more important, and give a sizeable contribution to the value of the energy, and consequently to the gap.

In conclusion, we have presented the results of accurate AFDMC method simulations for evaluating the superfluid gap in neutron matter with a realistic nucleon-nucleon potential. The present calculations are qualitatively and quantitatively improved over previous diffusion Monte Carlo results, and are to be regarded as a benchmark for other methods. While at very low densities the results agree with the Green's function Monte Carlo results of Gezerlis and Carlson, at higher densities the gap turns out to be of about 2 MeV, in qualitative agreement with recent Brueckner-Hartree-Fock estimates.

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