Quantum Monte Carlo study of dilute neutron matter at finite temperatures

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We report results of fully non-perturbative, Path Integral Monte Carlo (PIMC) calculations for dilute neutron matter. The neutron-neutron interaction in the s channel is parameterized by the scattering length and the effective range. We calculate the energy and the chemical potential as a function of temperature at the density $\rho = 0.003$ fm$^{-3}$. The critical temperature $T_c$ for the superfluid-normal phase transition is estimated from the finite size scaling of the condensate fraction. At low temperatures we extract the spectral weight function $A(p, \omega)$ from the imaginary time propagator using the methods of maximum entropy and singular value decomposition. We determine the quasiparticle spectrum, which can be accurately parameterized by three parameters: an effective mass $m^*$, a mean-field potential $U$, and a gap $\Delta$. Large value of $\Delta/T_c$ indicates that the system is not a BCS-type superfluid at low temperatures.

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Dilute neutron matter is one of the simplest many-body nuclear systems. At sufficiently small densities its properties originate from the two-body s-wave interaction only. It is known that neutron matter has a positive pressure at all densities (contrary to nuclear matter) which prevents fragmentation and it becomes superfluid at low temperatures. From the theoretical point of view, pure and dilute neutron matter is a fascinating system since at a certain density range it becomes a nearly-universal Fermi gas. Such systems are presently of great interest as a result of an extraordinary progress in the field of cold atoms which have taken place over the last few years and in fact opened new chapter in many-body physics (see [1] and references therein). Taking advantage of the Feshbach resonances experimentalists can control the strength of the atom-atom interaction and achieve the so-called unitary regime. It corresponds to the situation where the average distance between fermionic atoms is smaller than the scattering length $a$, which prevents fragmentation and it becomes superfluid at low temperatures.

Since even for the density $\rho = 0.001$ fm$^{-3}$ dilute neutron matter is a strongly correlated Fermi gas ($|k_F a| \gg 1$) only non-perturbative approaches are able to gain reliable insight into physics of this system. The large class of such methods, which are known under the general name of Quantum Monte Carlo (QMC), have been used to date, although most of them concern the zero temperature properties [2]. The finite temperature behavior has been studied in [3]. This work presents the first ab initio, fully non-perturbative evaluation of thermal properties of low-density neutron matter (at about 2% of nuclear saturation density) free of uncontrolled approximations within PIMC method. We focus on the effects generated by the finite effective range.

Contrary to cold atomic gases, in order to capture physics of dilute neutron matter one has to use more realistic interaction than a simple contact, delta-like force. In the present paper we employ the two-body potential of the form:

$$ V(r - r') = \begin{cases} 6g, & r - r' = 0 \\ g, & r - r' \in \mathcal{N}_b \\ 0, & \text{otherwise} \end{cases}, $$

where $\mathcal{N}_b = \{(\pm b, 0, 0), (0, \pm b, 0), (0, 0, \pm b)\}$ represents the set of the nearest neighbor coordinates. This particular form of the interaction is especially designed for the cubic lattice with the lattice constant $b$ and enables to construct a fully non-perturbative approach without the sign problem (for more details see Ref. [9]). It depends on two parameters ($g$ and $b$) which are adjusted to correctly reproduce the scattering length and the effective range of neutron-neutron $^1S_0$ scattering amplitude [10].

Hence we consider the system on a 3D spatial cubic lattice of length $L = N_x b$ with periodic boundary conditions. The lattice spacing $b$ and size $L$ introduce the natural ultraviolet (UV) and infrared (IR) momentum cut-offs given by $p_{cut} = \pi/b$ and $p_0 = 2\pi/L$, respectively.
The momentum space has the shape of a cubic lattice, with size $2\pi/b$ and spacing $2\pi/L$. To simplify the analysis, however, we place the spherically symmetric UV cut-off, including momenta $p \leq p_{\text{cut}}$.

To evaluate numerically expectation values of observables we have followed the path integral approach described in Ref. [11]. Using Trotter expansion and subsequently Hubbard-Stratonovich (H-S) transformation, the evaluation of the emerging path integral was performed using the Metropolis importance sampling. The crucial modification of the procedure described in [11] consists in the construction of such H-S transformation which allow to incorporate the off-site part of the interaction without generation of the sign problem. Namely, we have used the discrete H-S transformation of the form [8]:

$$e^{-\tau \hat{V}} = \prod_{r-r' \in \mathcal{N}_\lambda} \prod_{i=1}^{k} e^{\sigma_i(r,r') [\hat{n}_\lambda(r) + \hat{n}_\lambda(r')]}$$

where $\sigma_i$ are real numbers and $\hat{n}_\lambda(r)$ is the occupation number operator. The notable feature of this H-S transformation is the time reversal invariance of the corresponding imaginary time evolution operator. This property ensures that the probability measure used in the Metropolis algorithm is always positive [9, 12].

Calculations were performed on the lattice of size $N_\lambda = 8$ with the lattice constant $b = 3.21$ fm. The chemical potential was chosen in such a way to keep the total number of particles between 53 and 57, which corresponds to the density $k_F \approx 0.45$ fm$^{-1}$. The temperatures span the interval from 0.06 $\epsilon_F$ (0.26 MeV) to 1.0 $\epsilon_F$ (4.3 MeV), where $\epsilon_F$ is the Fermi energy. The number of imaginary time steps required to reach the convergence of the algorithm varies with temperature. At the lowest temperature 2360 imaginary time steps have been applied, whereas for the highest temperature only 216.

The kinetic energy part of the Hamiltonian is defined in the restricted momentum space ($p \leq p_{\text{cut}}$) using the dispersion relation of the form $\epsilon(p) = p^2 / 2m$. Consequently during the imaginary time evolution the FFT algorithm has been used to switch between momentum and coordinate spaces [11]. The number of generated uncorrelated Monte Carlo samples allows to decrease the statistical error below 5%. At low temperatures the Singular Value Decomposition technique was applied to avoid instabilities of the algorithm. In all runs the single-particle occupation probabilities for the highest energy states were below one percent at all temperatures. We have also performed a few exploratory simulations for the lattice of size $N_\lambda = 10$. The results were in a good agreement with those for $N_\lambda = 8$ lattice.

In the Fig. 1 the low temperature behavior of the total energy and the chemical potential is presented for two different lattice sizes. The (shifted) total energy versus temperature for the free Fermi gas at the same particle density has also been plotted (solid line). Note that after shifting of the free Fermi gas energy by 0.52 $\epsilon_{\text{FFG}}$ the curve reproduces Monte Carlo results for $T > 0.15 \epsilon_F$ ($\epsilon_{\text{FFG}} = \frac{3}{2} N \epsilon_F$ is the free Fermi gas energy at $T = 0$). Below this temperature the deviation from the free Fermi gas behavior is clearly visible. The chemical potential is approximately constant for $T < 0.1 \epsilon_F$.

The critical temperature of the superfluid-normal phase transition has been determined using the method based on the finite size scaling of the correlation function. Similar technique was used to determine the critical temperature at the unitary limit (see Refs. [11, 13] for details). The volume-dependent estimation of the critical temperature $T_c^{(ij)}$ was obtained by finding the crossing point of the rescaled condensate fraction for two different lattice sizes $N_{ij}$. As $N_{ij} \to \infty$, the series $T_c^{(ij)}$ converges to $T_c$ and one can extract the limiting value. We have determined $T_c$ using results for two lattices $N_{ij} = 8, 10$. Such large lattices and rather small filling factor which...
in both cases reads $\nu = N/2N_s^3 \approx 5\%$ are enough to estimate the critical temperature with uncertainty smaller than 20\% (in fact this procedure applied to the unitary gas gives estimation of the $T_c$ with the relative error smaller than 10\%). The estimate of the critical temperature reads $T_c \approx 0.09 \varepsilon_F$. Note that $T_c$ is considerably lower than the temperature for the onset of deviation from the free Fermi gas behavior.

Within the PIMC framework one cannot reach directly the $T = 0$ limit. However the ground state energy can be obtained by performing an extrapolation of results to zero temperature limit. In our case this procedure provides the ground state energy $E/FFG = 0.46(2)$ ($E/N = 1.22(5)\text{MeV}$). This value is considerably lower (by about 20\%-40\%) than values obtained by other MC calculations (see for example Ref. [6]). This is most likely due to the fact, that our approach is based on fully unrestricted path integral calculations and, within statistical errors due to the Monte Carlo procedure, gives essentially exact results.

The gap in the fermionic spectrum, related to superfluidity, has been computed from the spectral weight function $A(p, \omega)$ by performing the analytic continuation of the imaginary time propagator $\mathcal{G}(p, \tau)$ to real frequencies [14]. This procedure is equivalent to solving the integral equation:

$$\mathcal{G}(p, \tau) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega A(p, \omega) \frac{\exp(-\omega \tau)}{1 + \exp(-\omega/\beta)}, \quad (3)$$

where $\mathcal{G}(p, \tau)$ is known from the Monte Carlo calculations for 51 different values of $\tau \in [0, \beta = 1/T]$. The inverse problem is however numerically ill-posed i.e. there is an infinite class of solutions for $A(p, \omega)$ which satisfy Eq. (3) within uncertainties generated by the Monte Carlo method. Therefore we have used two independent methods based on completely different mathematical approaches.

The first one, the maximum entropy method, is based on Bayes’ theorem [15]. It treats the values of $\hat{\mathcal{G}}(p, \tau_i)$ ($i = 0, 1, \ldots, 50$) provided by QMC simulation as normally distributed random numbers, around the true values $\mathcal{G}(p, \tau_i)$, and searches for the most probable solution assuming some $a\ priori$ knowledge concerning the spectral function. As an $a\ priori$ information we have used constraints:

$$A(p, \omega) \geq 0, \quad \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} A(p, \omega) = 1, \quad (4)$$

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} A(p, \omega) \frac{1}{1 + \exp(\omega/\beta)} = n(p), \quad (5)$$

and we have assumed a Gaussian-like structure for $A(p, \omega)$. In the formula (5) $n(p)$ represents the occupation probability of the state with momentum $p$ which is known from the Monte Carlo simulation.

The second method is based on the singular value decomposition (SVD) of the integral kernel $\mathcal{K}$ of Eq. (3), which can be rewritten in the operator form as $\hat{\mathcal{G}}(p, \tau_i) = (\mathcal{K}A)(p, \tau_i)$. The operator $\mathcal{K}$ possesses the singular system which forms a suitable basis for the expansion of the projected spectral weight function $\hat{A}(p, \omega)$ onto a subspace where the inverse problem is well-posed [16]. Since the method provides only projection of the “true” solution, it does not require any $a\ priori$ information, contrary to the maximum entropy method. However, since $\mathcal{G}(p, \tau_i)$ include statistical errors due to the Monte Carlo procedure, the projected solution $\hat{A}(p, \omega)$ is also affected by this uncertainty. One can use this flexibility by choosing the solution satisfying the constraints (4) (17). The details of both methods will be discussed elsewhere [18].

The spectral weight function for the lowest temperature $T = 0.06 \varepsilon_F$ obtained for $N_s = 10$ lattice is shown in the Fig. 2. The same outcome has been generated by both methods (maximum entropy and SVD) independently. The presence of a “pairing” gap is clearly visible for this temperature.

Figure 3 presents the quasiparticle excitation spectrum extracted from the spectral weight function for $T = 0.06 \varepsilon_F$. We have found that the quasiparticle excitations can be accurately parameterized by the BCS-like formula:

$$E(p) = \pm \sqrt{\left(\frac{p^2}{2m^*} - \mu + U\right)^2 + \Delta^2}, \quad (6)$$

where $m^*$ is an effective mass, $U$ the mean field potential and $\Delta$ is the “pairing” gap. The values of these parame-
Comparison of our results with those obtained in the limit $r_{\text{eff}} \to 0$ provides an information about the influence of the effective range. From the data reported in Ref. 11 we infer that the effects of the effective range do not significantly alter the ground state energy. The value of the energy gap and the critical temperature decreases considerably (at $r_{\text{eff}} \to 0$: $\Delta^{(0)}/T_c \approx 0.41$ and $T^{(0)}/T_c \approx 0.13$). However, surprisingly the ratio $\Delta^{(0)}/T_{c}^{(0)} \approx 3.2$ remains approximately constant (taking into account uncertainties of our estimation) when increasing $r_{\text{eff}}$ to the value associated with $^1S_0$ neutron-neutron interaction. Note also that the equation of state exhibits the existence of the second temperature scale, which can be attributed to the onset of deviations of $E/E_{\text{Fermi}}$ from the (shifted) energy of the free Fermi gas. It bears similarity to the case of the unitary Fermi gas, where the existence of the so-called “pseudogap” above $T_c$ is reported.20

Summarizing, our results do not indicate the presence of qualitative changes in comparison to the case of zero effective range. In conclusion the main aspects of physics at the unitary regime survive in the limit of dilute neutron matter.

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quasiparticles energies from $A(p, \omega)$
fit $E(p)$: $m^*/m = 1.29$, $\Delta/\varepsilon_F = 0.29$, $U/\varepsilon_F = -0.36$
model of independent quasiparticles