Lattice EFT calculation of thermal properties of low-density neutron matter

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Abstract. Thermal properties of low-density neutron matter are investigated by lattice calculation with nuclear effective field theory without pions up to the next-to-leading order. The $^1S_0$ pairing gap is extracted near zero temperature at low densities. We find that the pairing gap is smaller than the BCS approximation with the conventional $NN$ potentials, but not as small as those by various many-body calculations beyond BCS approximation. Our result is consistent with the recent Green’s Function Monte Carlo calculation within the statistical errors. The critical temperature of the normal-to-superfluid phase transition and the pairing temperature scale are also extracted at low densities, and the phase diagram is given. We find that the physics of low-density neutron matter is clearly identified as being BCS-BEC crossover.

Dedicated to Peter Schuck, in celebration of his retirement

1. Introduction
Even though the investigations over many years provided much understanding of the pairing gap $\Delta$, reliable quantitative information has not been fully available, even in the $^1S_0$ channel of the partial wave decomposition, which is the dominant component in low-density neutron matter [1]. For example, $\Delta$ had been firmly established in the BCS approximation, as evident in the fact that various conventional $NN$ potentials have provided nearly the same $\Delta$ as a function of density. Many-body calculations beyond the BCS approximation, however, have yielded $\Delta$ of various magnitudes, generally smaller than BCS $\Delta$. Quantum Monte Carlo calculations have also been used for the determination of $\Delta$. The Green’s function Monte Carlo (GFMC) method has yielded $\Delta$ smaller than BCS $\Delta$ [2], but not as small as those obtained by the many-body calculations beyond the BCS approximation. Another method closely related to GFMC, the auxiliary field diffusion Monte Carlo (AFDMC) method has given $\Delta$ quite close to BCS $\Delta$ [3]. Our motivation is to determine $\Delta$ by a quantum Monte Carlo lattice calculation with the nuclear Effective Field Theory (EFT), which is motivated by the work of Ref. [4] and has been now widely applied to a few- and many-body systems [5, 6, 7, 8, 9, 10, 11, 12, 13]. This contribution of the proceedings is the summary based on our work in Refs. [14, 15].

2. Low-density neutron matter on the lattice
2.1. Lattice Hamiltonian up to the next-to-leading order of pionless EFT
Nuclear EFT is a low-energy effective theory of Quantum Chromodynamics (QCD) [16, 17, 18, 19]. It holds all the symmetries of low-energy QCD such as the approximate chiral symmetry
and its breaking. Below the chiral symmetry breaking scale $\Lambda_\chi \sim 1$ GeV, pions and nucleons are the relevant degrees of freedom to describe the low-energy theory. At low energies sufficiently below the pion mass, even the pions can be integrated out from the theory, the relevant degrees of freedom are only nucleons. At that energy scale, we can describe low-energy nuclear physics by a low-energy effective theory without the pion degrees of freedom referred to as pionless EFT.

Starting with the general second-quantized Hamiltonian with the contact and its derivative interaction terms in the continuous coordinate space, the pionless EFT Hamiltonian up to the next-to-leading order (NLO) can be discretized on the lattice as

$$
\hat{H} = -t \sum_{\langle i,j \rangle} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + 6t \sum_{i\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} + \frac{1}{a^3} \left[ c_0(\Lambda) - \frac{6}{a^2} c_2(\Lambda) \right] \sum_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} + \frac{1}{2a^5} c_2(\Lambda) \sum_{\langle i,j \rangle} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \hat{c}_{j\sigma},
$$

(1)

with the hopping amplitude $t \equiv 1/(2Ma^2)$, the neutron mass $M$, the spatial lattice spacing $a$, and the momentum cutoff scale $\Lambda$ set to be $\pi/a$. $\langle i, j \rangle$ indicates that the summation is restricted to the neighboring pairs of $i$ and $j$. $\hat{c}_{i\sigma}^\dagger$ ($\hat{c}_{i\sigma}$) is the creation (annihilation) operator of the neutron with spin $\sigma = \uparrow, \downarrow$ at the $i$th site.

$c_0$ and $c_2$ are the interaction strengths of the contact and its derivative terms, respectively. As explained later in Sec. 2.2, these coupling constants are determined by solving the coupled equations, Eqs. (3) and (4), so as to reproduce the experimental values of the scattering length and effective range.

The lattice Hamiltonian, Eq. (1), corresponds to the extended Hubbard-model Hamiltonian in condensed matter physics [20]. We can apply the Determinantal Quantum Monte Carlo (DQMC) method of the attractive Hubbard model to the low-density neutron matter system on the lattice. After determining the coupling constants, we can perform the DQMC lattice calculation to include the non-perturbative effects or neutron loop contributions as introduced briefly in Sec. 2.3.

### 2.2. Determination of the coupling constants, $c_0$ and $c_2$

The cutoff-dependent neutron-neutron interaction parameters, $c_0(\Lambda)$ and $c_2(\Lambda)$, in Eq. (1) are determined from the neutron-neutron scattering phase shift, using the effective range expansion up to the $p^2$ terms in $^1S_0$ channel,

$$
p \cot \delta_0(p) = -\frac{1}{a_0} + \frac{1}{2} r_0 p^2 + O(p^4),
$$

(2)

with the $^1S_0$ phase shift $\delta_0$, scattering length $a_0$, effective range $r_0$, and relative momentum of two neutrons $p$.

$a_0$ and $r_0$ can be related to $c_0$ and $c_2$ through the coupled equations [21],

$$
\frac{M}{4\pi a_0} = \left[ \frac{1}{c_0(\Lambda)} + \frac{M}{2\pi^2} L_1(\Lambda) \right] + \frac{M}{\pi^2} L_3(\Lambda) \frac{c_2(\Lambda)}{c_0(\Lambda)}
$$

(3)

$$
\frac{M}{16\pi r_0} = \frac{c_2(\Lambda)}{c_0^2(\Lambda)} - \frac{M}{4\pi^2} R \left( \frac{p^2}{\Lambda^2} \right),
$$

(4)

where $L_1$, $L_3$, and $R$ are the quantities related to the choice of the regulator in the momentum integrations. By solving the coupled equations, Eqs. (3) and (4), we can obtain the interaction parameters on the lattice, $c_0$ and $c_2$, from the experimental values of $a_0$ and $r_0$. Note that $c_2$ should be treated perturbatively to keep the power counting rule. The details of the determination of $c_0$ and $c_2$ can be found in Ref. [21].
2.3. Determinantal Quantum Monte Carlo
For the evaluation of the observables, we compute the correlation functions by DQMC method [22]. The essential idea of DQMC is to describe and to compute the observables by the Green’s function. The Green’s function is the fundamental tool of DQMC method, not only for the computation of the observables, but also for the update process of Monte Carlo sampling. For the sake of simplicity, we restrict our discussion to the leading order (LO) case. The concrete introduction including the NLO terms perturbatively can be found in Ref. [14].

By applying the Hubbard-Stratonovich transformation, the expectation value of the observable is written in the form of the functional integral over the auxiliary fields \( \chi \),

\[
\langle \hat{O} \rangle \equiv \frac{1}{Z} \text{Tr} \left( \hat{O} \hat{U} \right) = \frac{1}{Z} \int d[\chi] \langle \hat{O}(\chi) \rangle G(\chi) \xi(\chi),
\]

with the grand partition function,

\[
Z \equiv \text{Tr}(\hat{U}) = \int d[\chi] G(\chi) \xi(\chi),
\]

and the evolution operator,

\[
\hat{U} \equiv \exp \left[ -\beta \left( \hat{H} - \mu \hat{N} \right) \right] \approx \left\{ \exp \left[ -\Delta \beta \left( \hat{H} - \mu \hat{N} \right) \right] \right\}^{N_t} = \int d[\chi] G(\chi) \hat{U}_\chi,
\]

with the inverse temperature \( \beta \equiv 1/T \), the chemical potential \( \mu \), and the number operator \( \hat{N} \). In the second equality, \( \hat{U} \) (and also \( \hat{U}_\chi \)) is discretized into \( N_t \equiv \beta/\Delta \beta \) time slices by using the Torroter-Suzuki approximation. \( G(\chi) \) is the Gaussian factor. \( \xi(\chi) \) is the trace of the one-body evolution operator \( \hat{U}_\chi \), and is related to the Green’s function \( G_{ij} \) through \( \hat{U}_\chi \) in matrix form as \( (U_\chi)_{ij} = (G^{-1})_{ij} \). \( \langle \hat{O}(\chi) \rangle \) is defined as \( \text{Tr}(\hat{O}\hat{U}_\chi)/\xi(\chi) \).

The functional integral, Eq. (5), is evaluated by Monte Carlo integration with the Metropolis algorithm, regarding \( G(\chi) \xi(\chi) \) as the weight,

\[
\langle \hat{O} \rangle = \frac{\sum_{i=1}^{N} \langle \hat{O} \rangle_i \Phi_i}{\sum_{i=1}^{N} \Phi_i},
\]

with the sign of the weight \( \Phi_i \equiv G(\chi) \xi(\chi)/|G(\chi) \xi(\chi)| \) and the number of samples \( N \).

3. Results
3.1. Setup
The DQMC framework is based on the grand canonical ensemble. To measure the observables at some fixed neutron number, the neutron number for the observables that we compute is determined by interpolation of the observables for various values of chemical potential. To take the thermodynamic and continuum limits, we perform the calculations with the spatial lattice sizes \( N_s \) of \( 4^3 \), \( 6^3 \), \( 8^3 \), and \( 10^3 \), and the filling fraction of neutrons in the cubic box \( n \) ranging from \( 1/16 \) to \( 1/2 \). By using these results in \( N_s \) and \( n \), the final observables are extrapolated in the thermodynamic (\( N_s \rightarrow \infty \)) and continuum limits (\( n \rightarrow 0 \)). To observe the phase transition, we set the temporal lattice sizes \( N_t \) ranging from 2 to 128.

3.2. \(^{1}S_0 \) pairing gap near zero temperature
\( \Delta \) is extracted directly from the off-diagonal long-range order of the spin pair-pair correlation function \( P_s \) [23],

\[
P_s(R) = \frac{1}{N_s} \sum_i \langle \hat{\Delta}_{i+R}^\dagger \hat{\Delta}_i \rangle = \frac{1}{N_s} \sum_{i,j=i+R} (\delta_{ij} - G_{ij})^2,
\]
where \( \hat{\Delta}_i \equiv \hat{c}_i \hat{c}_i \) is the two-neutron spin-pairing operator at the \( i \)-th site, and \( R \) is the separation of the neutron pairs in the lattice spacing unit. \( G_{ij} \equiv G^\sigma_{ij} = \langle \hat{c}_i \sigma \hat{c}_j \sigma \rangle \) is the equal-time Green’s function for \( \sigma = \uparrow, \downarrow \). From the diminishing asymptotic behavior of \( P_s \) at sufficiently large \( R \), \( \Delta \) near zero temperature is evaluated by \( \Delta = \left| \frac{c_0}{\sigma} \right| \sqrt{P_s} (T \approx 0, R \gg 1) \).

Figure 1 shows comparison of our \( \Delta \) at low densities with other selected calculations in the literature. In the figure, the density \( \rho \) is described by the Fermi momentum \( k_F \) through the relation in the system of non-interacting neutrons, \( k_F = \left( \frac{3 \pi^2 \rho}{2} \right)^{1/3} \). The solid curve is the typical BCS result with realistic two-nucleon interactions. Note that all BCS results with various realistic \( NN \) forces fall into this curve. The other curves are some selected many-body calculations beyond BCS approximation. Calculations in random phase approximation are labeled by R1 [24], R2 [25] and R3 [26], those with correlated basis functions by C1 [27] and C2 [28], and the renormalization group method by RG [29]. These results are scattered, but show the trend of the drastic suppression of \( \Delta \) from the BCS results, except for R3 [26] and C2 [28]. Symbols are the quantum Monte Carlo results. The open squares are the recent GFMC [2], the open circles are the AFDMC [3], and the open diamonds are our DQMC lattice results [14]. It has been pointed out that the AFDMC results may not have been converged to the ground state and would become consistent with the GFMC and our results by using an appropriate initial wave function [30]. These quantum Monte Carlo results imply that \( \Delta \) is suppressed with respect to the BCS results, but is not much smaller than BCS results as predicted by most of the other many-body calculations beyond BCS approximation. Note that the recent path integral Monte Carlo calculation seems to confirm our \( \Delta \) at \( k_F \sim 0.46 \text{ fm}^{-1} \) [31].

![Figure 1](image1.png)

**Figure 1.** Comparison of our Monte Carlo \( \Delta \) to other calculations as a function of the neutron matter density (represented by the Fermi momentum \( k_F \)). The solid diamonds show our results, with statistical uncertainties. The other calculations consist of three types: quantum Monte Carlo (shown by symbols with statistical uncertainties), BCS (shown by the solid curve), and the many-body calculations beyond BCS approximation (R’s, C’s, and RG; shown by dotted and dashed curves). See text for the description of each calculation shown.

![Figure 2](image2.png)

**Figure 2.** The \( ^1S_0 \) phase diagram of low-density neutron matter. The solid and open symbols with statistical uncertainties show the LO and NLO results, respectively. The dashed curves for \( T_c \) and \( T^* \) are drawn by interpolation. Neutron matter is in the superfluid phase below the critical temperature \( T_c \) of the second-order phase transition. Above \( T_c \), neutron matter is in the pseudo-gap phase, in which pairing remains locally without forming long-range order, and undergoes a smooth transition from the pseudo-gap phase to the normal phase around \( T^* \), as pairing gets much less.
3.3. Phase diagram at finite temperature

To investigate the phase diagram of low-density neutron matter, we evaluate the critical temperature $T_c$ of the normal-to-superfluid phase transition and the pairing temperature scale $T^*$. $T_c$ is measured from the spin pair-pair correlation sum \[ C_\Delta(T) = \frac{1}{N_s} \sum_{i,j} \langle \Delta_i \Delta_j \rangle + \Delta \langle \Delta_i \rangle = \frac{1}{N_s} \sum_{i,j} (G_{ij})^2 + (\delta_{ij} - G_{ji})^2 \]. \[ (10) \]

$T_c$ is then extracted from the inflexion point of $C_\Delta(T)$ by fitting an assumed functional form near the inflexion point.

$T^*$ is extracted from the Pauli spin susceptibility $\chi_P$, which is given by

\[ \chi_P(T, N_s) = \frac{1}{T} \frac{1}{N_s} \sum_{i,j} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \frac{1}{T} \frac{1}{N_s} \sum_{i,j} 2G_{ij} (\delta_{ij} - G_{ji}) , \]

(11)

where $\mathbf{S}_i = \sum_{\mu,\nu=\uparrow,\downarrow} c^\dagger_{i\mu} \sigma_{\mu\nu} c_{j\nu}$ and $\sigma$ is the vector of Pauli matrices. $T^*$ is evaluated by identifying the maximum point of $\chi_P$ as a function of $T$ [32].

Figure 2 shows the phase diagram. As in Figure 1, the density is described by the Fermi momentum. The solid and open symbols with statistical uncertainties show the LO and NLO results. The dashed curves are drawn for $T_c$ and $T^*$. Note that $T^*$ is just the pairing temperature scale, not the signature of the phase transition, and is related to the pseudo gap phase.

Table 1 summarizes our results of the $^1S_0$ pairing gap $\Delta$ near zero temperature, the critical temperature of the normal-to-superfluid phase transition $T_c$, and the pairing temperature scale $T^*$. In the table, the first and second columns are for the Fermi momenta $k_F$ and the corresponding densities $\rho$, respectively. $\rho_0$ is the normal nuclear density, $\rho_0 = 0.16 \text{fm}^{-3}$. Our results of $\Delta$ at $T \approx 0$, $T_c$, and $T^*$ are listed in the third, fourth, and fifth columns, respectively. These results have been extrapolated to the thermodynamic ($N_s \to \infty$) and continuum limits ($n \to 0$). The values in the parentheses are only the statistical errors. (The systematic and theoretical errors are not included here.)

| $k_F$ (MeV) | $\rho$ ($\rho_0$) | $\Delta$ (MeV) | $T_c$ (MeV) | $T^*$ (MeV) |
|------------|------------------|----------------|-------------|-------------|
| 15         | $9 \times 10^{-5}$ | 0.021(1)       | 0.014(3)    | 0.014(1)    |
| 30         | $7 \times 10^{-4}$ | 0.13(1)        | 0.067(5)    | 0.091(9)    |
| 60         | $6 \times 10^{-3}$ | 0.49(3)        | 0.29(5)     | 0.45(5)     |
| 90         | $2 \times 10^{-2}$ | 1.10(7)        | 0.76(9)     | 1.1(1)      |
| 120        | $5 \times 10^{-2}$ | 1.7(1)         | 1.4(2)      | 2.8(1)      |

4. Summary

In summary, we have investigated thermal properties of low-density neutron matter by determinantal quantum Monte Carlo lattice calculations with the pionless EFT up to the NLO. The $^1S_0$ pairing gap at $T \approx 0$, the critical temperature of normal-to-superfluid phase transition, and the pairing temperature scale have been extracted directly from the correlation functions,
and have provided the phase diagram for densities of \((10^{-4} - 10^{-1})\rho_0\). The thermodynamic limit was taken, and the continuum limit was examined in the determination. The pairing gap was found to be suppressed by approximately one third from the BCS value. The physics of neutron matter in this density region has clearly been identified as a BCS-BEC crossover.

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