Variational calculations with explicit energy functionals for fermion systems at zero temperature

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Abstract. The variational method with explicit energy functionals (EEFs) is applied to infinite neutron matter. Starting from the Argonne v8’ two-body potential and the repulsive part of the Urbana IX three-body potential, the energy per neutron is expressed explicitly with the spin-dependent central, tensor, and spin-orbit distribution functions. This EEF is constructed as an extension of the previously proposed one for the Argonne v6’ potential, including central and tensor forces. The Euler-Lagrange equations derived from this EEF are solved numerically. The obtained fully minimized energy with this EEF is in good agreement with that obtained from the auxiliary field diffusion Monte Carlo calculation.

1. Introduction

The variational method with explicit energy functionals (EEFs) was proposed in Ref. \cite{1} for calculating energy per particle of spin-1/2 strongly correlated fermion systems, such as nuclear matter and liquid \textsuperscript{3}He at zero temperature. In this method, the energy per particle of a system in which two particles interact through a two-body central force is expressed explicitly with spin-dependent radial distribution functions, which are regarded as variational functions. Then, the Euler-Lagrange equations for these radial distribution functions derived from the EEF are solved numerically, and the fully minimized energy per particle is obtained.

Here we compare this EEF variational method with the Fermi Hypernetted Chain (FHNC) variational method\cite{2}. In the FHNC method, the expectation value of the Hamiltonian per particle \(\langle H \rangle/N\) with the Jastrow wave function is calculated approximately based on the cluster variational method originating from Ref. \cite{3}. Then, the \(\langle H \rangle/N\) is minimized with respect to the correlation function included in the Jastrow wave function. Namely, in the case of the FHNC method, it is clear which cluster terms are included in \(\langle H \rangle/N\). However, the correlation function is usually parameterized for nuclear matter and the minimization of \(\langle H \rangle/N\) is performed with respect to those parameters. This implies that the minimization of \(\langle H \rangle/N\) may be insufficient in the FHNC method. In contrast, the fully-minimized energy per particle is obtained in the variational method with the EEF, which is an advantageous point of this method. Further comparison with the FHNC method is given in Refs.\cite{1, 4}, and is also shown below.
The energy per particle of liquid $^3$He calculated with this variational method is in fairly good agreement with the experimental data \[1\]. Moreover, a refinement of the EEF with respect to a part of the three-body cluster terms was reported in Ref. \[5\]. To treat nuclear matter, in Ref. \[6\], the EEF was extended to include the tensor and spin-orbit forces. Because this extension was observed to be insufficient, further refinements of the EEF were made with respect to the kinetic energy caused by the tensor correlations, as reported in Ref. \[4\]. Furthermore, a state-independent three-body nuclear force was considered, and the EEF of neutron matter at zero temperature was extended to finite temperatures in Ref. \[4\].

In this paper, the variational method with the EEF is applied to infinite neutron matter including the two-body spin-orbit force.

2. Explicit energy functional of neutron matter with the spin-orbit force

In this section, we report on an improvement of the EEF for neutron matter so as to take into account the spin-orbit nuclear force. In a previous study \[4\], we proposed an EEF with the Argonne $v6'$ (AV6) two-body potential \[7\] and the repulsive part of the Urbana IX (UIX) three-body potential \[8\] for neutron matter at zero temperature.

In order to extend the EEF so as to treat the spin-orbit force, we newly introduce the spin-orbit distribution functions $F_{SO}(r)$ in addition to the radial distribution functions $F_{s}(r)$ and tensor distribution function $F_{T}(r)$ employed in the previous EEF. These functions are defined as follows:

$$
F_{s}(r_{12}) = \Omega^2 \sum_{\text{spin}} \int \Psi^{\dagger}(x_{1}, x_{2}, ..., x_{N}) P_{s_{12}} \Psi(x_{1}, x_{2}, ..., x_{N}) dr_{3} dr_{4} ... dr_{N},
$$

$$
F_{T}(r_{12}) = \Omega^2 \sum_{\text{spin}} \int \Psi^{\dagger}(x_{1}, x_{2}, ..., x_{N}) S_{T_{12}} \Psi(x_{1}, x_{2}, ..., x_{N}) dr_{3} dr_{4} ... dr_{N},
$$

$$
F_{SO}(r_{12}) = \Omega^2 \sum_{\text{spin}} \int \Psi^{\dagger}(x_{1}, x_{2}, ..., x_{N}) (L_{12} \cdot s) \Psi(x_{1}, x_{2}, ..., x_{N}) dr_{3} dr_{4} ... dr_{N}.
$$

Here, $\Omega$ represents the volume of neutron matter, and the summations on the right-hand sides of these equations are conducted over the spin coordinates of all the neutrons. In addition, $\Psi$ is the wave function of neutron matter, and $x_{l}$ represents the spatial coordinate $r_{l}$ and the spin coordinate of the $i$-th neutron. Furthermore, $P_{s_{ij}}$ is the spin-projection operator projecting the $(i, j)$ neutron pair state onto the spin triplet ($s = 1$) or spin singlet ($s = 0$) state, $S_{T_{ij}}$ is the tensor operator, and $L_{ij}$ is the relative orbital angular momentum operator.

For convenience, we also introduce the following auxiliary functions, i.e., the intrinsically central distribution functions $F_{Cs}(r)$, the dressed tensor correlation function $g_{T}(r)$, and the dressed spin-orbit correlation function $g_{SO}(r)$, which are defined as the solutions to the following equations\[6\]:

$$
F_{s}(r) = F_{Cs}(r) + 8s \left[g_{T}(r)\right]^2 F_{Fs}(r) + \frac{2}{3} s \left[g_{SO}(r)\right]^2 F_{qFs}(r),
$$

$$
F_{T}(r) = 16 \left[\frac{F_{C1}(r)}{F_{F1}(r)} g_{T}(r) - \left[g_{T}(r)\right]^2 F_{F1}(r)\right] - \frac{2}{3} \left[g_{SO}(r)\right]^2 F_{qF1}(r),
$$

$$
F_{SO}(r) = - 24 \left[g_{T}(r)\right]^2 F_{F1}(r) + \frac{4}{3} \left[\frac{F_{C1}(r)}{F_{F1}(r)} g_{T}(r) - \left[g_{T}(r)\right]^2 \frac{4}{3} - g_{T}(r) g_{SO}(r)\right] F_{qF1}(r).
$$

Here, $F_{Fs}(r)$ ($s = 0, 1$) are the spin-dependent radial distribution functions for the Fermi gas, and $F_{qFs}(r)$ are given by

$$
F_{qFs}(r) = \frac{2s + 1}{4} \left[\frac{(k_{Fr})^2}{5} - (-1)^s 9 j_{2}(k_{Fr}) \frac{j_{1}(k_{Fr})}{k_{Fr}}\right].
$$
Note that without the tensor and spin-orbit forces, $F_{Ca}(r)$ reduce to $F_s(r)$, whereas $g_T(r)$ and $g_{SO}(r)$ vanish.

To construct the EEF, the following structure functions are also necessary:

\[
S_{c1}(k) = \frac{1}{N} \left\langle \sum_{i=1}^{N} \exp(i\mathbf{k} \cdot r_i) \right\rangle^2 = 1 + S_1(k) + S_0(k) \geq 0, \tag{8}
\]

\[
S_{cT1}(k) = \frac{1}{Nk^2} \left\langle \sum_{i=1}^{N} (\sigma_i \cdot \mathbf{k}) \exp(i\mathbf{k} \cdot r_i) \right\rangle^2 = 1 + \frac{1}{3} S_1(k) - S_0(k) - \frac{S_T(k)}{3} \geq 0, \tag{9}
\]

\[
S_{cT2}(k) = \frac{1}{2Nk^2} \left\langle \sum_{i=1}^{N} (\sigma_i \times \mathbf{k}) \exp(i\mathbf{k} \cdot r_i) \right\rangle^2 = 1 + \frac{1}{3} S_1(k) - S_0(k) + \frac{S_T(k)}{6} \geq 0. \tag{10}
\]

Here, $S_s(k)$ and $S_T(k)$ are defined as follows:

\[
S_s(k) = 4\pi \rho \int_0^\infty [F_s(r) - F_s(\infty)] j_0(kr)r^2 dr, \tag{11}
\]

\[
S_T(k) = 4\pi \rho \int_0^\infty F_T(r) j_2(kr)r^2 dr, \tag{12}
\]

with $\rho$ representing the neutron number density. Furthermore, corresponding to the introduction of $F_{SO}(r)$, we also define

\[
S_{SO}(k) = 4\pi \rho \int_0^\infty F_{SO}(r) j_1(kr)k_{TF}^{-1}r^2 dr. \tag{13}
\]

Here, $k_{TF}$ is the Fermi wave number.

Using these functions, we propose an improved EEF for neutron matter with the spin-orbit force as follows:

\[
\frac{E_2}{N} = \frac{3}{5} E_F + \frac{E_V}{N} + \frac{E_{TF}}{N} + \frac{E_{TS}}{N} + \frac{E_{TN}}{N}. \tag{14}
\]

Here, the first term on the right-hand side of Eq. (14) represents the one-body kinetic energy, and $E_F$ corresponds to the Fermi energy. The second term $E_V/N$ represents the potential energy given by

\[
\frac{E_V}{N} = 2\pi \rho \int_0^\infty \left\{ \sum_{s=0}^{1} F_s(r) V_{Ca}(r) + F_T(r) V_T(r) + F_{SO}(r) V_{SO}(r) \right\} r^2 dr, \tag{15}
\]

with $V_{Ca}(r)$, $V_T(r)$, and $V_{SO}(r)$ being the two-body central, tensor, and spin-orbit potentials, respectively. The remaining terms $E_{TF}/N$, $E_{TS}/N$, and $E_{TN}/N$ on the right-hand side of Eq. (14) represent the kinetic energy caused by the correlations among neutrons expressed as

\[
\frac{E_{TF}}{N} = \frac{\pi \hbar^2}{2m} \int_0^\infty \left\{ \sum_{s=0}^{1} \left[ \frac{dF_s(r)}{dr} - \frac{dF_{Ca}(r)}{dr} \right] \right\} r^2 dr \frac{2}{r^2} dr \tag{16}
\]

\[
+ \frac{2\pi \hbar^2}{m} \int_0^\infty \left\{ \frac{dF_T(r)}{dr} \right\}^2 + \frac{6}{r^2} \left[ g_T(r) \right]^2 \right\} F_{F1}(r) + \frac{2}{3} \left[ \frac{dF_{SO}(r)}{dr} \right] F_{qF1}(r) \right\} r^2 dr, \tag{16}
\]

\[
\frac{E_{TS}}{N} = -\frac{\hbar^2}{16\pi m \rho} \int_0^\infty \frac{[S_{c1}(k) - S_{ex}(k)] \left\{ [S_{c1}(k) - S_{cF}(k)]^2 + \frac{15}{2} [S_{SO}(k)]^2 \right\}}{S_{c1}(k)/S_{cF}(k)} k_4 dk, \tag{17}
\]

\[
- \frac{\hbar^2}{16\pi m \rho} \int_0^\infty \sum_{n=1}^{2} \frac{[S_{cTn}(k) - S_{ex}(k)] \left\{ [S_{cTn}(k) - S_{cF}(k)]^2 + \frac{15}{4} (n - 1) [S_{SO}(k)]^2 \right\}}{S_{cTn}(k)/S_{cF}(k)} k_4 dk,
\]
with $S_{ex}(k) = 2S_{cF}(k) - 3$, and

$$\frac{E_{TN}}{N} = \frac{\hbar^2 \rho^2}{2m} \sum_{n=1}^{4} c_n a_n b_n, \quad (18)$$

$$a_1 = \rho \int \left\{ \left[ \frac{dG_C(r)}{dr} \right]^2 + 2G_T(r) \right\} dr, \quad b_1 = \rho \int \left\{ \left[ \frac{dG_C(r)}{dr} \right]^2 + \frac{2}{5} G_T(r) \right\} dr,$$

$$a_2 = b_2 = k_F \rho \int g_T(r) g_{SO}(r) dr, \quad a_3 = \rho \int \left\{ \frac{1}{20} \left[ \frac{dG_C(r)}{dr} \right]^2 + \frac{2}{5} G_T(r) \right\} dr,$$

$$b_3 = \rho \int [g_{SO}(r)]^2 (k_F r)^2 dr, \quad a_4 = \rho \int \left\{ \left[ \frac{d(g_{SO}(r))}{dr} \right]^2 + \frac{6}{r^2} [g_{SO}(r)]^2 \right\} (k_F r)^2 dr,$$

$$b_4 = \rho \int \left\{ \frac{1}{20} G_C(r)^2 + \frac{2}{5} G_T(r)^2 + \frac{17}{4800} [g_{SO}(r)]^2 (k_F r)^2 \right\} dr \quad (19)$$

with

$$G_C(r) = \frac{1}{3} F_{C1}(r) - F_{C0}(r) - \frac{1}{3} F_{F1}(r) + F_{F0}(r), \quad G_T(r) = \left[ \frac{dG_T(r)}{dr} \right]^2 + \frac{6}{r^2} [g_T(r)]^2, \quad (20)$$

and $(c_1, c_2, c_3, c_4) = (3/4, -1/60, 1, 1)$.

The EEF given in Eq. (14) is constructed with the following procedure. The first and the second terms are the exact expressions regardless of the explicit functional form of the wave function $\Psi(x_1, x_2, ..., x_N)$. In order to construct the rest of the kinetic-energy terms, we "temporarily" assume the following Jastrow wave function

$$\Psi = \text{Sym} \left\{ \prod_{i<j} \left[ \sum_{k=0}^{1} f_{C_s}(r_{ij}) P_{sij} + f_T(r_{ij}) S_{Tij} + f_{SO}(r_{ij}) (L_{ij} \cdot s) \right] \right\} \Phi_F. \quad (21)$$

Here, $\Phi_F$ is the wave function of the Fermi gas. The meaning of "temporarily" will be discussed below. Then, $E_{TF}/N$ is constructed so that $E_2/N$ properly includes the two-body cluster kinetic energy terms in $\langle H \rangle/N$. It is noted that $E_{TF}/N$ also includes a part of the three-body cluster and higher-order cluster kinetic energy terms in $\langle H \rangle/N$, because it is expressed with $F_s(r), F_T(r)$, and $F_{SO}(r)$ rather than $f_{C_s}(r), f_T(r)$, and $f_{SO}(r)$. In fact, the three-body cluster kinetic energy direct terms that are the lowest order in $h_{C_s}(r) = f_{C_s}(r) - 1, F_T(r)$, and $f_{SO}(r)$, which are denoted by $E_{3d}/N$, are included partially in $E_{TF}/N$. The rest of $E_{3d}/N$ is expressed as the form of $E_{TS}/N$ with the denominators $S_{c1}(k)$ and $S_{cTn}(k)$ being replaced by unity. Then, we introduce the denominators into $E_{TS}/N$ for the following two reasons. (i) $E_{TS}/N$ without the denominators is a harmful term which goes to negative infinity when the $E_2/N$ without these denominators is minimized with respect to $E_s(r), F_T(r)$ and $F_{SO}(r)$: The harmful term is converted into a harmless term by the introduction of the denominators. (ii) $S_{c1}(k)$ and $S_{cTn}(k)$ $(n = 1, 2)$ are non-negative functions as shown in Eqs. (8)-(10)[9], and the introduction of the denominators in the expression of $E_{TS}/N$ guarantees the non-negativity of those structure functions. It is noted that in $E_{3d}/N$ including the spin-orbit operator $(L_{ij} \cdot s)$, we consider for simplicity only the terms in which $L_{ij}$ operates on $\Phi_F$. In addition, as reported in Ref. [4], the two-particle exchange three-body cluster terms that are the lowest order in $h_{C_s}(r)$ and $F_T(r)$ are included in $E_{TF}/N$ and $E_{TS}/N$. The last term on the right-hand side of Eq. (14), $E_{TN}/N$, represents the three-body cluster direct nodal diagrams that are the lowest order in $h_{C_s}(r), f_T(r)$, and $f_{SO}(r)$. 

\[4\]
In addition to the two-body potential given above, we consider the state-independent three-body potential \( V_3(r_i, r_j, r_k) \) by introducing the corresponding three-body distribution function \( F_3(r_1, r_2, r_3) \). Then, the total energy per neutron \( E/N \) is expressed as follows:

\[
\frac{E}{N} = \frac{E_2}{N} + \frac{\rho^2}{6} \int F_3(r_1, r_2, r_3) V_3(r_1, r_2, r_3) \, dV_{12} \, dV_{23}.
\]  

(22)

Here, as in Ref. [4], we employ the following extended Kirkwood’s assumption:

\[
F_3(r_1, r_2, r_3) = F(r_{12}) F(r_{23}) F(r_{31}) \frac{F_{3F}(r_1, r_2, r_3)}{F_{F}(r_{12}) F_{F}(r_{23}) F_{F}(r_{31})},
\]

(23)

where \( F(r) = F_1(r) + F_0(r) \), and \( F_{3F}(r_1, r_2, r_3) \) is the three-body distribution function \( F_3(r_1, r_2, r_3) \) for the Fermi gas.

It is worth noting that a variational method which treats more cluster terms in \( \langle H \rangle/N \) with the Jastrow wave function is not necessarily a better variational method, because the Jastrow wave function is an approximate one which cannot express the exact ground-state wave function of neutron matter: As more cluster terms are included, \( \langle H \rangle/N \) approaches the exact expectation value with the Jastrow wave function, which is just the upper bound of the true ground-state energy, even if the minimization is performed sufficiently. Furthermore, the Jastrow wave function Eq. (21) is not appropriate for representing the spin dependence of the correlation among neutrons, as pointed out in Ref.[1]. This shortcoming is found in the three-body cluster and higher-order cluster terms: It is not necessarily a better approximation to taking into account more cluster terms sophisticatedly. In the present EEF method, therefore, the energy per neutron \( E/N \) is directly connected to the two-body distribution functions \( F_1(r), F_T(r), \) and \( F_{SO}(r) \) (or practically, \( F_{CS}(r), g_T(r), \) and \( g_{SO}(r) \)). We do not persist in treating the three-body cluster and higher-order cluster kinetic energy terms rigorously in the present EEF variational method: A part of the three-body cluster kinetic-energy terms in \( \langle H \rangle/N \) are used just as a reference for the construction of the corresponding part of EEF. This is the reason why we "temporarily" assume the Jastrow wave function.

3. Results and Future Perspectives

Using the new EEF shown above, we derive the Euler-Lagrange (EL) equations for \( F_{CS}(r), g_T(r), \) and \( g_{SO}(r) \) and solve them numerically for the Argonne v8’ two-body potential [10] and UIX three-body potential to obtain fully minimized \( E/N \). The EL equations are the coupled integrodifferential equations, and are solved in the iterative way: Detailed procedure of the numerical calculations is similar to those given in Ref.[6]. The result is presented in Figure 1 together with the result by the auxiliary field diffusion Monte Carlo (AFDMC) calculation [11]. The present result is in good agreement with that obtained from the AFDMC calculation. We note that in the AFDMC calculation, the 2\( \pi \)-exchange part of the UIX potential is also included. Therefore, this agreement implies that the contribution from the 2\( \pi \)-exchange part of the UIX potential is negligibly small in \( E/N \) of neutron matter. We note that the numerical calculations for the EEF variational method is possibly much less the CPU demanding than the AFDMC calculation, which is an advantageous point for the present variational method.

In future work, the evaluation of the three-body cluster terms excluded in the present energy expression is important. Furthermore, it is interesting to include the 2\( \pi \)-exchange part of the UIX potential to directly evaluate its contribution. Another important future problem would be to extend the present EEF to symmetric nuclear matter. In addition, it is interesting to apply the present EEF variational method to low dimensional systems, such as a two-dimensional (2D) \(^3\)He system. In the strictly 2D \(^3\)He system, the Monte Carlo calculations show no negative-energy point at finite number density, which implies that the 2D \(^3\)He system is a gas state at zero
Figure 1. Energy per neutron of neutron matter with the AV8′ two-body potential and the repulsive part of the UIX three-body potential as a function of the number density \( \rho \). The result obtained from the AFDMC calculation with the full UIX potential is also shown.

temperature[12, 13]. Here, it is pointed out that the Fermi statistics play a crucial role. On the other hand, recent experiments observed a self-bound liquid state in the 2D \(^3\)He system, by using \(^3\)He atoms absorbed on graphite [14]. Under these paradoxical circumstances, we extended our simplest EEF given in Ref. [1] to strict 2D \(^3\)He system, and obtained a negative-energy minimum point as a preliminary numerical result. In order to examine whether this minimum point is an artifact stemming from the insufficiency with respect to the Fermi statistics, the EEF is now being improved with respect to the three-body cluster exchange terms, as reported in Ref. [5] for 3D liquid \(^3\)He. The results will be reported elsewhere in the near future.

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