Explicit Energy Functional for Infinite Nuclear Matter with the Tensor Force

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Abstract. We have applied the variational method using explicit energy functionals (EEFs) to energy calculations of infinite nuclear matter. In EEFs, the energy per nucleon is explicitly expressed with spin-isospin-dependent two-body distribution functions, which are regarded as variational functions, and fully minimized energies are conveniently calculated with the EEF. A remarkable feature of this approach is that EEFs guarantee non-negativeness of structure functions. In this study, we extend the EEF variational method so as to consider state-independent three-body forces for neutron matter at finite temperatures following the procedure proposed by Schmidt and Pandharipande. For neutron matter, the free energies obtained with the Argonne v4’ two-body potential and the repulsive part of the Urbana IX (UIX) three-body potential are quite reasonable. Furthermore, we improve the EEF of nuclear matter using the two-body central and tensor forces by considering the main three-body cluster terms and guaranteeing non-negativeness of tensor structure functions. In addition, healing distances are introduced for two-body distribution functions so that Mayer’s condition is satisfied. The obtained energies per neutron of neutron matter with the Argonne v6’ two-body potential and the repulsive part of the UIX potential are in good agreement with those obtained by auxiliary field diffusion Monte Carlo calculations.

1. Introduction
The variational method is one of the most powerful techniques to calculate energies per particle of infinite fermion systems in which fermions interact through strong short-range forces. In the Fermi hypernetted chain (FHNC) method [1], which is a typical variational method, the expectation value of the Hamiltonian with the Jastrow wave function is cluster expanded, and parts of the cluster terms are resummed infinitely. Then, the expectation value of the Hamiltonian is minimized with respect to the correlation functions included in the Jastrow wave function. This method has been applied to liquid $^3$He [2, 3] and nuclear matter [4]. In recent years, quantum Monte Carlo methods have also been applied to these systems [5, 6, 7, 8]. In the case of liquid $^3$He, the intermolecular force between $^3$He atoms is expressed as state-independent two-body central force. In the case of nuclear matter, on the contrary, the two-body nuclear force is strongly state dependent, and the three-body force is also necessary for a realistic nuclear equation of state (EOS). Therefore, in the FHNC calculations for nuclear matter, the correlation functions should be state-dependent operators, and this requirement necessitates a laborious resummation of the cluster terms. In fact, the correlation functions are usually parameterized, and the total energy per nucleon is minimized with respect to these parameters reflecting that...
the full minimization is difficult to perform. Another problem of the FHNC method is that it is
difficult to treat asymmetric nuclear matter with arbitrary proton fractions.

In response to these difficulties associated with the FHNC method, we have been studying
a new type of variational method using explicit energy functionals (EEFs). In this method, we
first propose an EEF in which the energy per particle of an infinite fermion system is explicitly
expressed with variational functions. Once a reliable EEF is acquired, the Euler-Lagrange
equations of the variational functions are derived, and, by solving them, the fully minimized
energy is obtained.

We first applied this variational method to liquid $^3$He and obtained reasonable results [9].
We also applied the EEF to hypothetical neutron matter [9] and symmetric nuclear matter
[10], where, in both cases, two nucleons interact only through static two-body central forces.
By applying this method to more realistic nuclear matter, we next treated the tensor, spin-
orbit, and quadratic-angular-momentum parts of the two-body nuclear force [11]. In this case,
since the extension of the EEF was insufficient with respect to the kinetic energy expression,
the minimized energy was too low, and the obtained two-body distribution functions possessed
unrealistically long tails. In Ref. [11], we also proposed an effective method so as to avoid
these unphysical solutions. Furthermore, we extended this variational method to arbitrarily
spin-polarized liquid $^3$He [12] and (spin-unpolarized) asymmetric nuclear matter with arbitrary
proton fractions [13]. However, it remains to refine the EEF with respect to the tensor, spin-
orbit, and quadratic-angular-momentum parts of the two-body force. Moreover, treatment of
the three-body nuclear force is imperative to obtain a realistic nuclear EOS. Furthermore, it is
of interest to extend the theory to nuclear matter at finite temperatures, as has been performed
with other variational methods [14, 15, 16, 17].

In this paper, we first report recent extensions of the EEF variational method, such as
treatment of the three-body force and extension to nuclear matter at finite temperatures. We also
report an improvement of the EEF using the two-body central and tensor forces by considering
the proper three-body cluster terms and the non-negativeness of tensor structure functions.

2. Explicit Energy Functional of Neutron Matter at Finite Temperatures

In this section, we review the EEF of neutron matter in which neutrons interact only through spin-
dependent two-body central forces, and extend the EEF so as to treat three-body forces.
Furthermore, we extend this variational method to neutron matter at finite temperatures
following the method proposed by Schmidt and Pandharipande [18].

The EEF of neutron matter at zero temperature proposed in Ref. [9] represents the energy
per neutron as a functional of spin-dependent radial distribution functions $F_s(r)$ defined by

$$
F_s(r) = \Omega^2 \sum_{\text{spin}} \left\langle \Psi_1(x_1, x_2, \ldots, x_N) P_{\text{str}} \Psi(x_1, x_2, \ldots, x_N) \right\rangle dr_1 dr_2 \ldots dr_N,
$$

where $\Omega$ is the volume of the system, and the summation is conducted over spin coordinates
of all the neutrons. The function $\Psi$ in Eq. (1) is the wave function of neutron matter, and $x_i$
represents the space and spin coordinates of the $i$-th neutron. Here $N$ is the total number
of neutrons, and $P_{\text{str}}$ is the spin-projection operator projecting the $(i, j)$ neutron pair state onto
the spin triplet ($s = 1$) or spin singlet ($s = 0$) state. We also introduce the following structure functions:

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

$$
S_{c2}(k) = \frac{1}{3N} \left\langle \sum_{i=1}^N \sigma_i \exp(ik \cdot r_i) \right\rangle^2 = 1 + \frac{S_1(k)}{3} - S_0(k) \geq 0.
$$
\[ S_s(k) = 4\pi \rho \int_0^\infty \left[ F_s(r) - F_s(\infty) \right] j_0(kr)r^2 dr \] (4)

with \( \rho \) being the neutron number density.

Then, the energy per neutron \( E_2/N \) is expressed as follows:

\[ \frac{E_2}{N} = \frac{3}{5} E_F + \frac{E_V}{N} + \frac{E_{TC}}{N}. \] (5)

The first term on the right-hand side of Eq. (5) is the one-body kinetic energy term, and \( E_F \) is the Fermi energy. The second term \( E_V/N \) is the potential energy expressed as

\[ \frac{E_V}{N} = 2\pi \rho \sum_{s=0}^{1} \int_0^\infty F_s(r)V_{Cs}(r)r^2 dr, \] (6)

where \( V_{Cs}(r) \) is the spin-dependent two-body central potential with \( r \) being the distance between two neutrons. The term \( E_{V}/N \) represents the expectation value of the potential energy per neutron exactly. The term \( E_{TC}/N \) in Eq. (5) is the kinetic energy caused by the correlation among neutrons, and given as follows:

\[ \frac{E_{TC}}{N} = \frac{\pi h^2 \rho}{2m} \sum_{s=0}^{1} \int_0^\infty F_s(r) \left[ \frac{1}{F_s(r)} \frac{dF_s(r)}{dr} - \frac{1}{F_s(r)} \frac{dF_{Fs}(r)}{dr} \right] r^2 dr \]

\[ - \frac{\hbar}{16\pi m \rho} \sum_{n=1}^{2} \int_0^\infty (2n-1) \frac{[S_{cn}(k) - 1] [S_{cn}(k) - S_{cF}(k)]^2}{S_{cn}(k)/S_{cF}(k)} \hbar^4 dk, \] (7)

where \( m \) is the neutron mass. The functions \( F_{Fs}(r) \) and \( S_{cF}(k) \) in Eq. (7) are \( F_s(r) \) and \( S_{cn}(k) \) for the Fermi gas, respectively. In order to determine the expression of \( E_{TC}/N \), we first temporarily assume the Jastrow wave function

\[ \Psi = \text{Sym} \prod_{i<j} f_{ij} \phi_F, \] (8)

where Sym[ ] is the symmetrizer with respect to the order of the factors in the products and \( f_{ij} \) is the correlation function for the \((i, j)\) neutron pair, which is given by

\[ f_{ij} = \sum_{s=0}^{1} f_s(r_{ij})P_{sij}. \] (9)

The function \( \phi_F \) in Eq. (8) is the wave function of the Fermi gas. Then, we expand the expectation value of the Hamiltonian per neutron \( \langle H \rangle /N = \langle \Psi | H | \Psi \rangle /N / \langle \Psi | \Psi \rangle \) into cluster terms and construct \( E_{TC}/N \) so as to include the two-body kinetic energy cluster terms and the main part of the three-body cluster (TBC) direct non-nodal kinetic energy terms that are the lowest order in \( h_s(r) = f_s(r) - 1 \). We note that the denominator in the integrand of the last term on the right-hand side of Eq. (7) plays an important role in guaranteeing the non-negativeness of \( S_{cn}(k) \), as shown in Eqs. (2) and (3) [19].

Next, we extend this EEF so as to treat three-body forces. As the first step of this extension, we treat state-independent three-body potential \( V_3(r_1, r_2, r_3) \). To treat this potential, the corresponding three-body distribution function \( F_3(r_1, r_2, r_3) \) is necessary. Here we employ the following extended Kirkwood’s assumption:

\[ F_3(r_1, r_2, r_3) = \frac{F(r_{12})F(r_{23})F(r_{31})}{F_F(r_{12})F_F(r_{23})F_F(r_{31})}, \] (10)
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. Then, the total energy per neutron \( E/N \) is expressed as

\[
\frac{E}{N} = \frac{E_2}{N} + \frac{\rho^2}{6} \int F(r_1, r_2, r_3)V(r_1, r_2, r_3)dr_{12}dr_{23},
\]

and is minimized with respect to \( F_s(r) \), i.e., the Euler-Lagrange equations for \( F_s(r) \) are solved.

Furthermore, we extend this variational method so as to treat neutron matter at finite temperatures following the method proposed by Schmidt and Pandharipande (SP) \[18\]. For this treatment, the free energy per neutron is expressed as \( F/N = \langle H \rangle_T/N - TS/N \) with \( \langle H \rangle_T \), \( T \), and \( S \) being the internal energy, temperature, and entropy, respectively. According to SP, \( \langle H \rangle_T/N \) is constructed by replacing \( F_{Fs}(r) \) and \( S_{EF}(k) \) in \( E/N \) of Eq. (11) at zero temperature by \( F_{Fs}(T, r) \) and \( S_{EF}(T, k) \), respectively. Here \( F_{Fs}(T, r) \) is expressed as

\[
F_{Fs}(T, r) = \frac{(2s + 1)}{4} \{ 1 + (-1)^s |l(T, r)|^2 \},
\]

with \( l(T, r) \) being the Slater function at finite temperature:

\[
l(T, r) = \frac{1}{\pi^2\rho} \int_0^\infty n(k, T)j_0(kr)k^2dk.
\]

In Eq. (13), \( n(k, T) \) is the average occupation probability of single-neutron states expressed as

\[
n(k, T) = \left\{ 1 + \exp \left[ \frac{\epsilon(k) - \mu}{k_BT} \right] \right\}^{-1},
\]

where \( \epsilon(k) = \hbar^2k^2/(2m^*) \) is the single-neutron energy with \( m^* \) being the effective mass, and \( \mu \) is determined by the normalization condition. \( S_{EF}(T, k) \) is constructed through Eqs. (2), (3), and (4) by replacing \( F_s(r) \) in Eq. (4) by \( F_{Fs}(T, r) \). Furthermore, \( S/N \) is expressed as in the case of non-interacting quasi-neutrons with the effective mass \( m^* \). Then, \( F/N \) is minimized with respect to \( F_s(r) \) and \( m^* \).

Figure 1 shows \( F/N \) of neutron matter with the Argonne v4'(AV4') two-body potential \[21\] and the repulsive part of the Urbana IX (UIX) three-body potential \[22\]. The result without the three-body potential is also shown. Since the repulsive part of the UIX potential is rather strong, \( F/N \) with the three-body force becomes significantly higher than that without the three-body force at high densities. At finite temperatures, \( F/N \) decreases with \( T \): The behavior of \( F/N \) is quite reasonable.

### 3. Improvement of the Explicit Energy Functional with the Tensor Force

In this section, we report on an improvement of the EEF with the tensor force. The previous EEF is reported in Ref. [11], where the tensor distribution function \( F_T(r) \) is introduced.

\[
F_T(r) = \Omega^2 \sum_{\text{spin}} \int \Psi^\dagger(x_1, x_2, ..., x_N)S_{T12}\Psi(x_1, x_2, ..., x_N)dr_3dr_4...dr_N.
\]

Here \( S_{Tij} \) is the tensor operator operating on the \((i, j)\) neutron pair. We also introduce the following auxiliary functions, i.e., the intrinsically central distribution functions \( F_{Cs}(r) \) and the dressed tensor correlation function \( g_T(r) \) defined as the solutions to the following equations:

\[
F_s(r) = F_{Cs}(r) + 8s|g_T(r)|^2F_{Fs}(r),
\]

\[
F_T(r) = 16\sqrt{g_T(r)F_{C1}(r) - 16|g_T(r)|^2F_{F1}(r)}.
\]
We note that, without the tensor force, $F_{Cs}(r)$ reduce to $F_s(r)$, and $g_T(r)$ vanishes.

In the proposed improvement of the EEF with the tensor force, we newly introduce the following tensor structure functions

$$S_{cT1}(k) = \frac{1}{Nk^2} \left( \sum_{i=1}^{N} (\sigma_i \cdot k) \exp(i k \cdot r_i) \right)^2 = S_{c2}(k) - \frac{S_T(k)}{3} \geq 0, \quad (17)$$

$$S_{cT2}(k) = \frac{1}{2Nk^2} \left( \sum_{i=1}^{N} (\sigma_i \times k) \exp(i k \cdot r_i) \right)^2 = S_{c2}(k) + \frac{S_T(k)}{6} \geq 0, \quad (18)$$

with

$$S_T(k) = 4\pi \rho \int_0^\infty F_T(r) j_2(kr) r^2 dr. \quad (19)$$

By using these functions, we propose an improved EEF for neutron matter with the tensor force as in Eq. (5), where $E_V/N$ and $E_{TC}/N$ are expressed, respectively, as

$$\frac{E_V}{N} = 2\pi \rho \int_0^\infty \left[ \sum_{s=0}^1 F_s(r) V_{Cs}(r) + F_T(r) V_T(r) \right] r^2 dr, \quad (20)$$

and

$$\frac{E_{TC}}{N} = \frac{\pi \hbar^2 \rho}{2m} \int_0^\infty \sum_{s=0}^1 F_{Cs}(r) \left[ \frac{1}{F_{Cs}(r)} \frac{dF_{Cs}(r)}{dr} - \frac{1}{F_s(r)} \frac{dF_s(r)}{dr} \right]^2 r^2 dr$$

$$+ \frac{16\pi \hbar^2 \rho}{m} \int_0^\infty \left\{ \frac{dF_T(r)}{dr} + \frac{6}{r^2} g_T(r) \right\} F_{F1}(r) r^2 dr + E_{nod}/N$$

$$- \frac{\hbar^2}{16\pi \rho m} \int_0^\infty \frac{[S_{c1}(k) + 2S_{cF}(k) - 3][S_{c1}(k) - S_{cF}(k)]^2}{S_{c1}(k)/S_{cF}(k)} k^4 dk$$

$$- \frac{\hbar^2}{16\pi \rho m} \int_0^\infty \sum_{n=1}^2 \frac{[S_{cTn}(k) + 2S_{cF}(k) - 3][S_{cTn}(k) - S_{cF}(k)]^2}{S_{cTn}(k)/S_{cF}(k)} k^4 dk. \quad (21)$$

In Eq. (20), $V_{Cs}(r)$ and $V_T(r)$ are the two-body central and tensor potentials, respectively. The term $E_{nod}/N$ in Eq. (21) is given by

$$E_{nod}/N = \frac{\hbar^2 \rho^2}{2m} \int_{d(r_{12})} \frac{3}{4} \left[ \frac{dG(r_{12})}{dr_{12}} \right]^2 + \frac{1}{18} \left[ \frac{dF_T(r_{12})}{dr_{12}} \right]^2 + \frac{6}{r_{12}^2} [F_T(r_{12})]^2 \right]$$

$$\times \int_{d(r_{23})} \left[ \left[ G(r_{23}) \right]^2 + \frac{1}{18} \left[ F_T(r_{23}) \right]^2 \right], \quad (22)$$

**Figure 1.** Free energy per neutron of neutron matter with the AV4’ two-body potential and the repulsive part of the UIX three-body potential as a function of the number density $\rho$. 
with
\[ G(r) = \frac{1}{3} F_1(r) - F_0(r) - \frac{1}{3} F_{F1}(r) + F_{F0}(r). \] (23)

As in the case of the central forces alone, the expectation value of the potential energy is exactly expressed with Eq. (20). The functional form of \( E_{TC}/N \) representing the kinetic energy caused by the correlations among neutrons is the improved form, which is constructed by considering the following two points:

i) When we temporarily assume the Jastrow wave function given in Eq. (8) with the following correlation function
\[ f_{ij} = \sum_{s=0}^{1} f_s(r_{ij}) P_{sij} + f_T(r_{ij}) S_{Tij}, \] (24)

\( E_{TC}/N \) then properly includes the two-body kinetic-energy cluster terms and the main part of the TBC kinetic-energy terms that are the lowest order in \( h_s(r) \) and \( f_T(r) \) as cluster terms of the expectation value of the Hamiltonian per neutron \( \langle H \rangle /N \). Here we note that the EEF proposed in Ref. [11] is insufficient with respect to the inclusion of the TBC terms that consist of \( f_T(r) \). Furthermore, in this refinement of the EEF, we correctly consider the TBC two-particle exchange terms as well as the direct terms that are the lowest order in the correlations. We have studied, in Ref. [23], the effect of the TBC two-particle exchange terms on the EEF in a more sophisticated way. However, in the present improvement, we simply include all the TBC two-particle exchange terms in \( E_{TC}/N \). Other TBC terms included in this refinement are the so-called nodal diagrams, which have not been considered in the previous studies. Though it is well known that the nodal diagrams cancel out in the case of state-independent central forces, it is found that they play an important role in the present improvement. Therefore, we consider the TBC nodal diagrams that are the lowest order in the correlations as \( E_{nod}/N \).

ii) We guarantee non-negativity of the tensor structure function \( S_{C2Tn}(k) \). It is obvious that the relation \( S_{C2}(k) \geq 0 \) is automatically guaranteed when \( S_{C2Tn}(k) \geq 0 \) \((n = 1, 2)\) is satisfied. Therefore, rather than employing \( S_{C2}(k) \) as the denominator of the integrand of the last term of Eq. (7), the denominators \( S_{C2Tn}(k) \) are adopted in the integrand of the last term of Eq. (21).

Using the new EEF shown above, we derive the Euler-Lagrange equations for \( F_{Cs}(r) \) and \( g_T(r) \). When we solve them, Mayer’s condition \( S_{C1}(0) = 0 \) is considered. Since this condition is not explicitly imposed in the present variational method, the solutions obtained may violate the condition. In general, when Mayer’s condition is violated, the distribution functions exhibit long tails. This corresponds to the problem of treating long-range correlations in neutron matter. As reported in Ref. [3], it is difficult to treat long-range correlations exactly in the FHNC method. Therefore, in FHNC calculations [4, 8], healing distances with respect to the correlation functions in the Jastrow wave function are introduced as so as to avoid unphysical long-range correlation. In the present EEF variational method, we adopt a similar technique, i.e., we introduce healing distances \( r_{hCs} \) and \( r_{hT} \) for \( F_s(r) \) and \( F_T(r) \), respectively, so that \( F_s(r) \) and \( F_T(r) \) satisfy the following conditions: \( F_s(r_{hCs}) = F_T(r_{hCs}) \), \( dF_s(r)/dr|_{r=r_{hCs}} = dF_T(r)/dr|_{r=r_{hCs}} \), and \( F_T(r_{hT}) = dF_T(r)/dr|_{r=r_{hT}} = 0 \). Furthermore, we set \( F_s(r) = F_{Ps}(r) \) at \( r \geq r_{hCs} \) and \( F_T(r) = 0 \) at \( r \geq r_{hT} \). In order to guarantee these conditions, following the FHNC method, we replace \( V_{Cs}(r) \) and \( V_T(r) \) in the Euler-Lagrange equations by \( V_{Cs}(r) - \lambda_{Cs} \) and \( V_T(r) - \lambda_T \), respectively, where the constants \( \lambda_{Cs} \) and \( \lambda_T \) represent corrections with respect to the long-range correlations. The values of \( \lambda_{Cs} \) and \( \lambda_T \) are chosen so that the above-mentioned continuity conditions of \( F_s(r) \) at \( r = r_{hCs} \) and \( F_T(r) \) at \( r = r_{hT} \) are satisfied. Finally, the values of the healing distances \( r_{hCs} \) and \( r_{hT} \) are determined so that the quantity \( E_2/N + \lambda|S_{C1}(0)|^2 \) is minimized. Here, we choose \( \lambda = 1000 \text{ MeV} \). This choice is similar to the method adopted in the FHNC calculations [8, 20].

The obtained \( E_2/N \) of neutron matter with the Argonne v6’ (AV6’) potential [21] is shown in Fig. 2. \( E/N \) calculated with the AV6’ and the repulsive part of the UIX three-body potential is also shown in this figure. In this calculation, the contribution from the three-body force is
considered as shown in Eq. (11). It is seen that, in both cases, the present results are in good agreement with those obtained by auxiliary field diffusion Monte Carlo (AFDMC) calculations [7, 8]. Here we note that, in the AFDMC calculations, the rest of the UIX potential, i.e., the $2\pi$-exchange part, is also considered. The agreement observed between our $E/N$ calculations and that by AFDMC may imply that the contribution from the $2\pi$-exchange part of the UIX potential is negligibly small. It is also noted that we have improved the EEF for symmetric nuclear matter using the two-body central and tensor forces in a manner similar to that for neutron matter reported here, and that the improved $E/N$ are also in good agreement with those obtained by the AFDMC method, as will be reported in detail elsewhere.

4. Concluding Remarks

In this study, we have extended the EEF variational method for simplified neutron matter to finite temperatures including the three-body force. Furthermore, we have improved the EEF using the two-body central and tensor forces. The extension and improvement were successful. In order to treat the full Argonne v18 two-body potential [24] and the UIX three-body potential, the next improvement is to treat the spin-orbit forces and corresponding correlations. Then, we will proceed further to consider asymmetric nuclear matter toward systematic calculations of hot asymmetric nuclear EOS with the EEF variational method.

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