Spin Condition in the Cluster Variation Method and Its Application to the Neutron Matter

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(Received December 5, 1975)

A kinematical study is made on the relation between the spin-singlet and spin-triplet pair distribution functions in the many-body system of spin-1/2 particles, and a group of inequalities is derived from the positiveness of the square of the “local spin” which is the total spin of a subsystem confined in a certain local region. This spin condition is applied to the neutron matter in the two-body approximation of the cluster variation method, and a conditional Euler-Lagrange equation is derived for the ground state. Although the solution of the Euler-Lagrange equation has a long-range tail, the conditional energy minimum can be obtained from it. Numerical results show that the spin condition compensates the kinematical defects due to the truncation of the cluster series in a fairly wide density region and is useful to eliminate unnatural solutions.

§ 1. Introduction

The cluster variation method for quantum-mechanical many-body problems, which was initiated by Jastrow,\(^a\) Iwamoto and Yamada,\(^b\) has subsequently been studied by many researchers.\(^c\) Among the problems in the application of this method we investigate, in this paper, the truncation of the cluster series and the degree of freedom of the variation as having fundamental importance.

It is practically impossible to calculate all the terms of the cluster series, and some kind of truncation is inevitable. However, Emery\(^d\) pointed out a possible difficulty that the truncation may cause an absence of energy minimum or may yield an unreasonable energy minimum. This difficulty may be caused by imperfect normalization and violation of the Pauli principle in the truncated series. A usual way to remove this difficulty is to exclude unnatural trial functions by imposing subsidiary conditions which compensate the above-mentioned kinematical defects. For example, Yamada\(^e\) derived several geometrical conditions which must always be satisfied by the pair distribution function (necessary condition), and applied them to the nuclear matter.\(^f\) Two other kinds of conditions were used by Clark et al.\(^g\) One is Mayer’s condition\(^h\) which coincides with one of the geometrical conditions in certain cases, and the other is the orthogonality (or average Pauli) condition, which was introduced in the course of their work aimed at a formal connection between the cluster variation method and the reaction-matrix method.

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of Brueckner, Bethe and Goldstone. The importance of the Pauli principle has also been pointed out by many authors.\(^9\) In § 2, we discuss another kinematical feature of the many-body problem, and derive some inequalities related to the spins of the pairs in the many-body system.

Now, we turn to the consideration of the variation procedure. The most popular way is to use a parametrized trial function, which must be chosen \textit{a priori}. Then, there always exists a danger that important variational degrees of freedom are inadvertently omitted resulting in an insufficient minimization. The best way of the minimization is to solve the Euler-Lagrange equation (EL equation). Grypeos\(^1\) derived an EL equation by applying the variation principle to the energy expectation value which was expressed in terms of two kinds of distribution functions.\(^1\) In this paper we derive a different EL equation. We impose the above-mentioned inequalities as subsidiary conditions upon the energy minimization. Those inequalities are infinite in number, and it might appear that the Lagrange multiplier method cannot be used in such a case. In § 3, however, we solve this problem and obtain an EL equation.

We examine the general aspects of the solution of our EL equation in § 4 and apply our method to the neutron matter in § 5. Section 6 is devoted to discussion.

\section*{§ 2. Spin condition}

In this section, we investigate relations among the numbers of the pairs in spin multiplets, and derive a spin condition for the many-body system which consists of one kind of spin-1/2 fermions. We start from an \(n\)-body system. Let \(\mathcal{N}\) and \(\mathcal{N}^3\) be the numbers of the spin singlet and triplet pairs respectively. These numbers are given as the expectation values of the operators

\[
\sum_{i<j}^n \mathcal{P}_{ij},
\]

where \(\mathcal{P}_{ij}\) are the projection operators for the spin singlet \((\nu=1)\) or triplet \((\nu=3)\) pairs, \(\mathcal{P}_{ij} = (1 - \sigma^{(u)} \cdot \sigma^{(v)}) / 4\), \(\mathcal{P}_{ij} = (3 + \sigma^{(u)} \cdot \sigma^{(v)}) / 4\). Expression (1) can be written in terms of the \(n\)-body total-spin operator \(S_n\) (in units of \(\hbar\)) as

\[
\sum_{i<j}^n \mathcal{P}_{ij} = \frac{1}{2} n (n+2) - \frac{1}{2} S_n^z, \quad (2a)
\]

\[
\sum_{i<j}^n \mathcal{P}_{ij} = \frac{3}{2} n (n-2) + \frac{1}{2} S_n^z. \quad (2b)
\]

Conversely, the operator \(S_n^{\pm}\) can simply be expressed as

\[
\frac{3}{2} S_n^z = \frac{1}{2} n - \kappa_n, \quad (3)
\]

where \(\kappa_n\) is defined by

\[
\kappa_n = \sum_{i<j}^n (\mathcal{P}_{ij} - \frac{1}{2} \mathcal{P}_{ij}). \quad (4)
\]
The expectation value of $\kappa_n$ is

$$\tilde{\kappa}_n = \frac{1}{n} - \frac{1}{3} n.$$  \hfill (5)

Since the total-spin quantum number can take the value between 0 and $n/2$, we have the upper and lower limits of the expectation value of $S_n^z$ as

$$\frac{1}{2} n \left( \frac{1}{2} n + 1 \right) \geq S_n^z \geq 0.$$  \hfill (6)

Equation (6) together with Eqs. (3) and (5) gives the inequalities

$$\frac{1}{n} n - \frac{1}{3} n \leq \frac{1}{2} n$$  \hfill (7a)

and

$$\frac{1}{n} n - \frac{1}{3} n \geq - \frac{1}{2} n (n - 1).$$  \hfill (7b)

It is clear that the equality in (7a) holds only in the case of the zero total-spin state. On the other hand, the equality in (7b) corresponds to the totally symmetric (completely polarized) spin state. In most cases the many-body configuration is far from such a state, and we do not pay attention to the relation (7b) any more.

Next, in order to obtain inequalities which are more useful in many-body problems we generalize the above consideration to subsystems of the $N$-body fermion system. In particular, we consider the subsystem which is composed of the particles in a certain spatial region $A$ whose volume is $V_A$. In this case we must pay attention to the fact that the number of particles in $A$ is generally indefinite.

We define the following “local” operator instead of $\kappa_n$:

$$\kappa_A = \frac{1}{2} \sum_{i<j} (P_{ij} - \frac{1}{3} P_{ij}) \xi(A; r_i) \xi(A; r_j).$$  \hfill (8)

The operator $\xi(A; r_i)$ is the projection operator onto the region $A$, and is defined by

$$\xi(A; r_i) = \begin{cases} 1 & r_i \in A \\ 0 & \text{otherwise} \end{cases}.$$  \hfill (9)

We also define the “local spin”\(^{(*)}\) by

$$S_A = \frac{1}{2} \sum_{i=1}^{N} \xi(A; r_i) \sigma^{(z)}.$$  \hfill (10)

Then, by using the commutation relation of the Pauli matrices $\sigma^{(z)}$ and the character of $\xi(A; r_i)$ as a projection operator, we get

$$\kappa_A = \frac{1}{2} \sum_{i=1}^{N} \xi(A; r_i) - \frac{1}{3} S_A^z.$$  \hfill (11)

The expectation value of $\kappa_A$ can be expressed in terms of the spin singlet and

\(^{(*)}\) The “local spin” operator satisfies the commutation relation of the angular momentum, $S_A \times S_A = i S_A$. 

Spin Condition in the Cluster Variation Method
triplet pair distribution functions, which are denoted by $^1F(r_1, r_2)$ and $^3F(r_1, r_2)$ respectively. For a pure quantum-mechanical state, they are expressed as

$$^F = V^2 \int d\gamma \cdots \int d\gamma \sum_e \gamma^* \gamma,$$

where $\gamma = \gamma(r_1; \cdots, r_N; \ldots, \gamma_N)$ is the normalized wave function and $V$ is the volume of the system. The summation $\sum_e$ is taken over all the intrinsic coordinates $\gamma_e$. For a mixed state, $^F(r_1, r_2)$ is the weighted average of those of the pure states. Then, in general, the expectation value of $\gamma_A$ is written as

$$\bar{\gamma}_A = \frac{1}{\rho} \int d\gamma \int d\gamma \{^1F(r_1, r_2) - \frac{1}{3} ^3F(r_1, r_2)\} \gamma(A; r_1) \gamma(A; r_2),$$

where $\rho$ is the number density $N/V$. If the distribution functions depend only on the distance between the two particles, we can write as

$$\bar{\gamma}_A = \frac{1}{\rho} V_A \int d\gamma \{^1F(r) - \frac{1}{3} ^3F(r)\} u_A(r),$$

where $u_A(r)$ is the weight function for the region $A$,

$$u_A(r) = \frac{1}{V_A} \int d\gamma \sum_e \gamma(A; r_1) \gamma(A; r_1 + r).$$

The expectation value of the first term on the right-hand side of Eq. (11) is $\rho V_A/2$, and the second term is certainly positive definite. Thus, we arrive at the spin condition,

$$\bar{\gamma}_A \leq \frac{1}{2} \rho V_A,$$

where the left-hand side is to be calculated by Eq. (13) or (14). This condition must be satisfied for any shape and size of the region $A$. We apply it to the neutron matter in the following section.

§ 3. The Euler-Lagrange equation

As mentioned in § 1, one of the key points in our variation method with the subsidiary condition is whether we can derive the EL equation or not. It is easy to obtain it for simple conditions, but the spin condition (and the geometrical conditions also) has fairly complicated structures, being represented by an infinite number of inequalities. This infiniteness comes from the arbitrariness of the shape and size of the region $A$. Only a particular shape which is considered to give the severest conditions is adopted in practice. Therefore, we assume a certain shape hereafter. Then, we can derive the EL equation in spite of the remaining arbitrariness of the size.

Let us take up in the present paper the ground state of the infinite neutron matter as an example, and assume the semi-realistic OMY potential and the two-body cluster approximation of the Iwamoto-Yamada expansion. The OMY po-
Spin Condition in the Cluster Variation Method

The potential is specified only for the even states; we adopt a simple hard-core potential for the triplet-odd state. Namely,

\[ V_{ij} = V(r_{ij})^{1+}P_{ij} + V(r_{ij})^{2}P_{ij}, \]

\[ 1+V(r) = \begin{cases} -V_0 \exp \left( -\gamma (r-r_c) \right), & r > r_c, \\ \infty, & r \leq r_c, \end{cases} \]

\[ 2-V(r) = \begin{cases} 0, & r > r_c, \\ \infty, & r \leq r_c. \end{cases} \] (17)

The force parameters and the hard-core radius \( r_c \) are given in Ref. 12).

In the Jastrow-type wave function \( \Psi = \Phi \), the Slater determinant \( \Phi \) composed of plane waves represents the model single-particle configuration. On the other hand, the trial correlation function carries the physical information on the many-body correlation. In connection with the nuclear force (17), we adopt a simple state-dependent pair correlation function,*

\[ f_{ij}(r) = f(r)^{1+} + f(r)^{2}P_{ij}. \] (18)

The boundary condition to be imposed on \( f(r) \) is**

\[ \left. f(r) \right|_{r \to \infty} = 0. \] (19)

Then

\[ \Psi = \Xi \prod_{i<j} f_{ij}(\|r_i-r_j\|). \] (20)

The operator \( \Xi \), which is the symmetrizer with respect to the order of the product, is necessary as \( f_{ij}(\|r_i-r_j\|) \) do not commute with each other. However, this symmetrizer does not change the cluster terms up to the second order, although it causes some additional complication in higher-order terms. Finally, we assume that the pair correlation function \( f_{ij}(r) \) is a real function.

The expression of the energy per neutron is, up to the two-body cluster term,

\[ E = \frac{3}{5} E_F + E_2, \] (21)

where \( E_F \) is the Fermi energy and \( E_2 \) is the two-body energy,

\[ E_2 = \sum_{s=0}^{1}(2s+1)/4 \cdot 2\pi \int_{r_c}^{\infty} L_v \cdot \mathbf{f} H_s \cdot \mathbf{f} r^2 dr. \] (22)

with

\[ H_s = -\hbar^2 \left( \frac{\mathbf{p}^2}{M} + \frac{d}{dr} \ln L_v \cdot \frac{d}{dr} + V(r) \right). \] (23)

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* Hereafter, we distinguish the pair states only by the spin multiplicity \( \nu \).

** We impose another boundary condition (Eq. (47)) later on.
where \( k_F \) is the Fermi wave number. We consider the variation of \( E \) as a functional of \( \vec{f} \) and \( \vec{f} \) and for convenience put

\[
\partial \vec{f} = \eta \vec{\phi},
\]

where \( \vec{\phi} \) are functions satisfying the boundary condition

\[
\vec{\phi} = 0 \quad \text{for } r \leq r_e \quad \text{or} \quad r \to \infty,
\]

and \( \eta \) is a real parameter. Actually we need another boundary condition associated with the derivative at \( r \to \infty \), which will be specified later as Eq. (46). Expanding the variation \( \delta E = \delta E_2 \) in powers of \( \vec{\phi} \), we have the first-order variation \( \delta^{(1)} E_2 \) as

\[
\delta^{(1)} E_2 = \eta \sum_{s=0}^{1} \frac{(2s+1)}{4 \cdot 4\pi \rho} \int_{r_e}^{\infty} L_s \vec{\phi} H_s \vec{f}^2 dr - \eta \sum_{s=0}^{1} \frac{(2s+1)}{4 \cdot 2\pi \rho} \lim_{r \to \infty} r^2 L_s \left( \vec{f} \frac{d^2 \vec{\phi}}{dr^2} - \vec{\phi} \frac{d^2 \vec{f}}{dr^2} \right).
\]

Here, the last term is the surface term arising from partial integration. In order that \( E_2 \) may have a minimum this term should vanish, and we neglect it in this section, although it requires further discussion as given in § 4. Without this term the EL equation for the unconditional variation can be immediately obtained from \( \delta^{(1)} E_2 = 0 \) as

\[
H_s \vec{f} = 0, \quad (s = 0, 1).
\]

Now, we impose the spin condition (16) by choosing the sphere as the shape of the region A. Denoting its radius by \( b \), we can write the condition in a form

\[
K(\vec{f}, \vec{f}; b) \geq 0 \quad \text{for all } b.
\]

If we use the two-body cluster approximation of the pair distribution functions,

\[
\vec{F} = \frac{(2s+1)}{4} \vec{L}_s,
\]

then \( K(\vec{f}, \vec{f}; b) \) is expressed as

\[
K(\vec{f}, \vec{f}; b) = 1 - \pi \rho \int_{r_e}^{\infty} (\vec{f}^2 \vec{L}_0 - \vec{f}^2 \vec{L}_0) u(r, b) r^2 dr
\]

with

\[
u(r, b) = \begin{cases} 
1 - \frac{3r}{4b} + \frac{r^3}{16b^3}, & r \leq 2b, \\
0, & \text{otherwise}.
\end{cases}
\]

When the solution of Eq. (28) satisfies the inequalities (29), it is the final solution. On the other hand, when it violates the inequalities (29), the condition to be imposed is also written as
Spin Condition in the Cluster Variation Method

\[ K(f, \phi; b_0) = 0, \]  

where \( b_0 \) is the value of \( b \) which minimizes \( K(f, \phi; b) \):

\[ K(f, \phi; b_0) = \min K(f, \phi; b). \]  

Thus, by the use of the Lagrange multiplier \( \lambda \), our conditional problem of variation can be reduced to the minimization (or stationalization) of the functional

\[ I(f, \phi) = E_0(f, \phi) - \lambda K(f, \phi; b_0). \]  

It should be noted that the value of \( I(f, \phi) \) is equal to that of \( E_0(f, \phi) \) as far as the condition (33) is satisfied. The variation of \( K(f, \phi; b) \) is written as

\[ \delta K = K(f + \eta \phi, \phi + \eta ^* \phi; b_0) - K(f, \phi; b_0), \]  

where \( b_0 \) and \( b_1 \) satisfy the following equations from the requirement of (34):

\[ \frac{d}{db} K(f, \phi; b) \bigg|_{b=b_1} = 0, \]  

\[ \frac{d}{d\eta} K(f + \eta \phi, \phi + \eta ^* \phi; b) \bigg|_{\eta=0} = 0. \]  

First, we deal with the part of \( \delta K \) caused by the change of the parameter from \( b_0 \) to \( b_1 \). By keeping only the first-order term for this part, we get

\[ \delta K \approx K(f + \eta \phi, \phi + \eta ^* \phi; b_0) - K(f, \phi; b_0) \]  

\[ + \eta \frac{db}{d\eta} \bigg|_{\eta=0} \cdot \frac{d}{db} K(f, \phi; b) \bigg|_{b=b_0}. \]  

Fortunately, however, the last term vanishes because of Eq. (37). Then, the remaining part is merely the variation of \( K(f, \phi; b) \) at the fixed point \( b = b_0 \), and we get the first order variation,

\[ \delta^{(1)} K = -\gamma 2\pi \rho \int_{r_e}^{\infty} \left( \phi ^* f L_0 - \phi ^* f L_1 \right) u(r, b_0) r^2 dr. \]  

Now, we can express the first-order variation of \( I(f, \phi) \) (Eq. (35)) using Eqs. (27) and (40), and then, with the variation principle \( \delta^{(1)} I = 0 \), we get the conditional EL equations,

\[ (H_e + U_s) f = 0, \quad (s = 0, 1) \]  

where

\[ U_0 = 2\lambda u(r, b_0), \]  

\[ U_1 = -\frac{\gamma}{2} \lambda u(r, b_0). \]  

These equations should be solved simultaneously with Eqs. (33) and (34). Equations (41) show that the subsidiary condition acts as a kind of effective interaction. Here, we add that the conditional EL equation for the state-independent pair correlation function can be obtained in a similar way. In this case \( K(f, b) \) is
usually minimized at $b \to \infty$, and the EL equation becomes

$$\left\{ -\frac{\hbar^2}{M} \left( \frac{d^2}{dr^2} \ln L \right) + V + U \right\} f = 0 \quad (43)$$

with

$$L = L_0/4 + 3L_1/4,$$
$$V = (L_0^1 V + 3L_1^3 - V)/4L,$$
$$U = \lambda (L_0 - L_1)/2L. \quad (44)$$

§ 4. General behavior of the solution

4.1 Long-range behavior and the energy limit

We denote the solution of the EL equations (41) with the boundary condition (19) by $f_E$, where we attach the subscript E for convenience of discussion. The asymptotic form of $f_E$ is easily obtained as

$$f_E \approx 1 - a/r. \quad (r > 1) \quad \text{as} \quad r \to \infty \quad (45)$$

The integration constant $a$ (the singlet scattering length) tends to the singlet scattering length in the limits of $k_F \to 0$ and $\infty$. *

In order to examine in what sense this long-range behavior can be accepted, let us recall the surface term in Eq. (27). With the above correlation functions and the boundary condition (26), the surface term is written as

$$-\eta \sum_{s=0}^{1} (2s + 1)/4 \cdot 2\pi \rho \frac{\hbar^2}{M} \lim_{r \to \infty} r^s \frac{d^s \phi}{dr^s}.$$ 

In order that $I(f, \phi)$ may have a minimum, this term, and accordingly $\lim_{r \to \infty} r^s \cdot (d^s \phi/dr)$, must vanish:

$$\lim_{r \to \infty} r^s \frac{d^s \phi}{dr} = 0, \quad \text{as} \quad r \to \infty \quad \text{(46)}$$

and as a natural extension of this,** we also impose an additional condition on $d^s f/dr$ as

$$\lim_{r \to \infty} r^s \frac{d^s f}{dr} = 0. \quad (47)$$

Here, we encounter a problem that the solution of the EL equation generally

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* This result ($a \to a_{\text{singlet (free)}}$ for $r \to \infty$) comes from masking of the Fermi correlation (which is represented by $L_0$) by the hard-core repulsion.

** Various other arguments are possible for the necessity of this condition, but we give no account of them in this paper because they rather deviate from the subject of this paper.
violates the condition (47) because it has the asymptotic form as given by (45). However, this does not constitute a real obstacle; all we have to do are to introduce infinitesimal modifications of the \( f \)'s so as to make the \( f \)'s satisfy Eq. (47) and to pay proper attention to these modifications in calculating the energy. In order to prove it we consider the following functional \( I'(f, f) \):

\[
I'(f, f) = \sum_{s \geq 0} \frac{1}{4} \cdot \frac{2\pi \rho}{4} \int R \left[ \frac{h^2}{M} \left( \frac{d}{dr} \ln f \right)^2 + \frac{\nu}{2} \right] f^2 \rho^2 dr
- \lambda K(f, f; b_0)
= E_f'(f, f) - \lambda K(f, f; b_0). \tag{48}
\]

This expression differs from \( I(f, f) \) in the kinetic energy part, and the partial integration reduces the difference to a surface term:

\[
I'(f, f) = I(f, f) + \sum_{s \geq 0} \frac{1}{4} \cdot \frac{2\pi \rho}{4} \int R \frac{h^2}{M} \lim_{r \to \infty} r^2 L_r f \frac{df}{dr}. \tag{49}
\]

Thus, as far as the \( f \)'s satisfying Eq. (47) are concerned, \( I'(f, f) \) and \( I(f, f) \) are equivalent. However, it happens that we have to consider the \( f \)'s having long-range tails because such functions can be obtained as limits of appropriate sequences of functions satisfying Eq. (47) and also because they have actually occurred as the solutions of the EL equation. For such \( f \)'s, the integral \( I'(f, f) \) is much easier to handle since it has a far well-behaved functional dependence as compared with \( I(f, f) \) at large distances. The EL equation which is obtained from the variation procedure on \( I'(f, f) \) is the same as Eqs. (41), and no additional boundary condition is necessary because of the absence of a surface term such as the last term in Eq. (27). Therefore, the stationary value of \( I'(f, f) \) is given by \( I'(f, f) \). In order to calculate this value, we rewrite \( I(f, f) \) by putting Eqs. (22) and (31) into Eq. (35) and by using Eqs. (42),

\[
I'(f, f) = \sum_{s \geq 0} \frac{1}{4} \cdot \frac{2\pi \rho}{4} \int R L_r f (H_r + U_r) f \rho^2 dr - \lambda. \tag{50}
\]

For the solution of the EL equations (41), the first term on the right-hand side vanishes, and we have

\[
I'(f, f) = -\lambda. \tag{51}
\]

Then, \( I'(f, f) \) is obtained from Eq. (49) by the use of Eqs. (45) and (51) as

\[
I'(f, f) = \sum_{s \geq 0} \frac{1}{4} \cdot \frac{2\pi \rho}{4} \frac{h^2}{M} \nu \sigma - \lambda. \tag{52}
\]

*) It cannot immediately be decided from which expression one should start. The expression \( I'(f, f) \) might rather be superior to \( I(f, f) \) because \( I'(f, f) \) clearly shows the positive-definiteness of the kinetic energy. If we start from \( I'(f, f) \), we do not need most of the arguments in this subsection.
The difference between $I_2(f, g)$ and $I_2'(f, g)$ is due to the singular behavior of $I_2(f, g)$ around $f = f_E$. In the following we show that the expression (52), not (51), should be taken as the two-body cluster energy.

Let $R_0$ and $R_1$ be the function spaces which are specified by the asymptotic behavior as

$$
R_0 = \{\text{functions which tend to unity faster than } 1 - a/r\},
R_1 = \{\text{functions with } 1 - a/r \text{ tails}\}.
$$

In the space $R_0 \cup R_1$ the functional $I_2'(f, g)$ has the stationary value which is given by Eq. (52). Here, we assume that this stationary value of $I_2'(f, g)$ is the conditional minimum of the energy $E_2'(f, g)$.\(^{*)}\) This stationary point actually lies in $R_1$ unless $a$ are zero. However, since $I_2'(f, g)$ is insensitive to the long-range parts of $f$ and $g$, we can always find functions $f_0$ in $R_0$ which are arbitrarily close to $f_E$ and make $I_2'(f_0, g_0)$ arbitrarily close to $I_2'(f_E, g_0)$. This statement holds even if we restrict $f_0$ within those satisfying the condition $K(f_0, g_0; b_0) = 0$; this either follows simply from the fact that $K(f, g; b_0)$ is independent of the long-range parts of $f$ as in the case of a finite $b_0$ value, or is inferred from the cancellation of the long-range parts in $K(f, g; b_0)$ as in the case $b_0 = \infty$.

Namely, we have

$$
\begin{align*}
&f_0 \rightarrow f_E, \\
&I_2'(f_0, g_0) \rightarrow I_2'(f_E, g_E), \\
&K(f_0, g_0; b_0) = 0.
\end{align*}
$$

Thus, if we use only the functions in $R_0$, we get $I_2'(f_E, g_E)$ as a certain limit, which indeed is the lower limit of $E_2'(f, g)$ for conditional variations. For the functional $I_2(f, g)$ we must restrict, according to the condition (47), $f$ and $g$ within $R_0$, where $I_2(f, g)$ takes the same value as $I_2'(f, g)$, and $E_2(f, g)$ the same value as $E_2'(f, g)$. Then we have

$$
I_2(f_0, g_0) = I_2'(f_0, g_0) \rightarrow I_2'(f_E, g_E).
$$

This indicates that the value $I_2'(f_E, g_E)$ as a limit\(^{**)\) of $I_2'(f, g)$ is the lower limit of $E_2(f, g)$ for conditional variations in $R_0$, and, in this sense, we accept $f_E$ as the solution for the ground-state pair correlation functions and $I_2'(f_E, g_E)$ (Eq. (52)) as the two-body cluster energy in the ground state. Namely, the ground-state energy per particle is given by

$$
E = \frac{3}{5} E_F + \sum E_A - \lambda
$$

\(^*)\) From Eq. (48) and $K(f_0, g_0; b_0) = 0$, we get $I_2'(f_0, g_0) = E_2'(f_0, g_0)$.

\(^{**)\) By comparing (54) with Eqs. (51) and (52), we see that $I_2'(f_0, g_0)$ does not converge to $I_2(f_E, g_E)$.
Spin Condition in the Cluster Variation Method

\[ E_F = \frac{3}{5} E_f + \sum (\mu E_A + \mu E_U) \]  \hfill (55)

with

\[ \mu E_A = (2s+1)/4 \cdot 2\pi \rho \frac{\hbar^2}{M} a \]  \hfill (56a)

\[ \mu E_U = - (2s+1)/4 \cdot 2\pi \rho \int_{r_c}^{\infty} L_\mu f_E^2 U \rho^2 dr \]  \hfill (56b)

In deriving the expression (56b) we have used

\[ \lambda K(f_E, f_E'; b_0) = \lambda + \mu E_U = 0 \]  \hfill (57)

4.2 Correlation functions with nodes

Here, we make brief comments on the second-order variation. In the case of unconditional variation (\(\lambda = 0\)), the second-order variation is given by

\[ \delta^{(2)} = \delta^{(2)} I = \delta^{(2)} E_\mu = \delta^{(2)} E_z \]

\[ = q^2 \sum_{\mu=0}^1 (2s+1)/4 \cdot 2\pi \rho \int_{r_c}^{\infty} L_\mu \phi H_\mu \phi r^2 dr \]  \hfill (58)

The right-hand side of this equation is positive unless the operator \(H_w\) has negative eigenvalues. Figure 1 shows the unconditional singlet scattering length in the neutron matter. The positive value of \(\lambda\) is associated with a correlation function with a node, showing the existence of pair bound states. If this bound state function is taken to be \(\phi_n\), the second-order variation is negative. Thus, the pair correlation functions with positive scattering lengths as in Fig. 1 have nothing to do with the ground state. Furthermore, the large absolute values of \(\lambda\) around \(k_F \approx 2 \text{ fm}^{-1}\) give an unusually deep minimum value of \(I(f, f)\) for unconditional variations. This kind of singular behavior of the scattering length does not appear if a state-independent trial function is used. Its occurrence in our case of state-dependent pair correlation functions is due to the allowance of more variational

Fig. 1. Singlet-even scattering lengths in the neutron matter which are defined by Eq. (45). These curves are calculated from the unconditional equation (28) (or Eq. (41) with \(\lambda = 0\)). The numbers attached to the curves denote the hard-core radius \(r_c\). The dashed parts correspond to the densities higher than the closest packing. The spin condition is violated in the whole density region.
degrees of freedom. However, this difficulty can be removed by the spin condition as seen in the next section. This indicates that the role of the subsidiary condition becomes more important as the degrees of freedom increase.

§ 5. Numerical calculations for the neutron matter

In § 3 we have derived the EL equations (41) which are to be solved simultaneously with Eqs. (33) and (34). In the numerical calculations we proceed as follows: First, by assuming some values for $\lambda$ and $b_0$, we solve Eqs. (41) obtaining the first approximation of $f$. Next, we calculate the second approximation of $b_0$ by minimizing $K(f, f; b)$ as Eq. (34) in which we use the first approximation for $f$. This procedure is repeated until $b_0$ converges. The value of $K(f, f; b_0)$ thus obtained is generally different from zero and does not satisfy Eq. (33). However, we can adjust $\lambda$ with comparative ease so that Eq. (33) may be satisfied. This completes our numerical calculation.

Fig. 2. Scattering lengths in the neutron matter which are calculated from the conditional EL equation (41). The solid curves are for $\rho_s=0.4$ fm, while the dashed curves are for $\rho_s=0.6$ fm.

Fig. 4. Radius of the region $\Lambda$.

Fig. 3. Lagrange multiplier.
Calculations are made for the two sets of force parameters of the OMY potential corresponding to the hard-core radii 0.4 and 0.6 fm. The scattering length and the parameters of effective potential arising from the spin condition are plotted in Figs. 2-4, where we put $r_0 = (4\pi \rho / 3)^{-1/3}$. It is seen in Fig. 2 that the main factor determining the scattering length is the hard core in the high density

Fig. 5. Examples of the pair correlation functions for $r_s = 0.4$ fm. The numbers in parentheses denote the density parameter $r_0$. The state-independent pair correlation function is fairly close to $f'(0.8)$ for $r_0 = 0.8$ as well as 1.2 fm.

Fig. 6. Contents of the two-body cluster energy $E_2$ for $r_s = 0.4$ fm. The pure potential energies are denoted by $E_P$, and other symbols are defined in the text.

Fig. 7. Contents of the two-body cluster energy $E_2$ for $r_s = 0.6$ fm.
region while it is the state dependence of the nuclear force in the low density region. It should be noted that the spin condition has remarkably reduced the absolute values of the scattering lengths as compared with Fig. 1 and has eliminated the unphysical pair bound state. Some examples of the calculated pair correlation functions are also shown in Fig. 5. The energy expectation values are calculated with those parameters by the use of Eqs. (55), (56a) and (56b). Figures 6 and 7 show the contents of the two-body energy. These results are summarized in Fig. 8.

Fig. 8. Fermi gas, two-body cluster and total energies. The numbers in parentheses denote the hard-core radius \( r_c \). The solid curves are for the state-dependent correlation functions, while the dashed curves are for the state-independent functions. The fourth geometrical condition in Ref. 5) is violated in the dotted parts of these curves.

Fig. 9. Energy per particle of the neutron matter. The curve \( F \) is for the Fermi gas. The curves \( E_1 \) and \( E_2 \) are our results for the state-dependent pair correlation functions with \( r_c = 0.4 \) and 0.6 fm respectively, while \( E_3 \) and \( E_4 \) are for the state-independent pair correlation functions. Other curves are taken from references: BL: K. Bleuler et al., BR: K. A. Brueckner et al., M: W. D. Myers, N: J. Nemeth and D. W. L. Sprung, P: V. R. Pandharipande and H. A. Bethe, S: E. E. Salpeter, W: C. T. P. Wang.
Spin Condition in the Cluster Variation Method

It is observed that a minimum of $E_2$ appears in the case of the larger hard core but not in the case of the smaller one. The geometrical condition is violated in the dotted part. If we impose it in addition to the spin condition, we shall get a minimum of $E_2$ even for the smaller-core potential.

Finally, we compare our results on the neutron matter with some of other calculations in Fig. 9.

§ 6. Discussion

It is found in § 5 that the spin condition moderates the strong state dependence of the pair correlation functions. This is the consequence of the repulsion (for the singlet-even state) and the attraction (for the triplet-odd state) of the effective potential (42). Thus, this condition is useful to avoid unnatural solutions. It will be interesting to see whether this is the case with more realistic potentials. Incidentally, our method of deriving the EL equation can easily be applied to the cases of more realistic potentials and more complicated correlation functions.

The consideration as was made in § 2 is extendible to the many-fermion system composed of spin-1/2 isospin-1/2 particles, and we can obtain some spin-isospin conditions, which will be published elsewhere. These conditions will be important for the discussion of the nuclear matter. On the other hand, while the spin condition discussed in the present paper is referred to one local region, we can get other conditions referring to two regions like those of the geometrical conditions. It is probable that such conditions are severer than the present one.

Meanwhile, in the high density region, higher-order cluster terms are important. Although handling of them offers a difficult problem, we expect that the geometrical conditions, when incorporated into the two-body cluster formulation, will compensate the neglect of higher terms fairly well. While one of the geometrical conditions, which is considered to be severest among them in most cases, contains three variable parameters referring to the sizes and relative distance of two local regions, the EL equation with this condition can be obtained by the method discussed in § 3. This EL equation includes additional state-independent effective potentials due to the geometrical conditions. As for the numerical handling of this equation we may gain useful information from the treatment of the boson systems, e.g., a $^4$He liquid.

The authors express their thanks to Mr. M. Uno and Mr. M. Hirano for their valuable discussions. The numerical work has been carried out with the aid of the electronic computer HITAC 8800/8700 at the Computer Center, the University of Tokyo. This study has been supported financially in part by the Institute for Nuclear Study, the University of Tokyo.

*) In the case of the state-independent function, the solution of the unconditional EL equation violates the spin condition at $r_i \geq 0.9 \text{ fm}$ for $r_e = 0.4 \text{ fm}$, and at $r_i \geq 1.3 \text{ fm}$ for $r_e = 0.8 \text{ fm}$.
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