A variational perturbation scheme for many-particle systems in the functional integral approach

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Abstract

A variational perturbation theory based on the functional integral approach is formulated for many-particle systems. Using the variational action obtained through Jensen-Peierls’ inequality, a perturbative expansion scheme for the thermodynamic potential is established. A modified Wick’s theorem is obtained for the variational perturbation expansions. This theorem allows one to carry out systematic calculations of higher order terms without worrying about the double counting problem. A model numerical calculation was carried out on a nucleon gas system interacting through the Yukawa-type potential to test the efficiency of the present method.

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I. INTRODUCTION

The perturbative approach has been proven widely successful when the interactions between the particles were weak[1-3]. However, when the correlations between the particles are strong, the perturbation approaches are less than satisfactory. In order to overcome such difficulties, many nonperturbative schemes including variational calculation have been developed [4-6]. Although the variational procedure provides a simple and convenient scheme to calculate the physical quantities, it has a serious drawback. Since, it is a basically one-shot process, systematic improvement over the obtained results is not easy to implement.

In this paper, we present a functional integral formulation of variational perturbation scheme for many-particle systems. In fact, this concept has already been used in connection with various research interests such as lattice dynamics, relativistic field theories, and quantum mechanics [7-12]. However, to the authors’ knowledge, it has never been applied to nonrelativistic many-particle systems. For this purpose, we first derive the variation principle for the partition function and the thermodynamic potential in the functional integral formalism using Jensen-Peierl’s inequality [13,14]. Then, this principle is used to obtain a variational action for the functional integral. The difference between the true and the variational action provides a renormalized perturbation. Application of the Wick’s theorem on this renormalized perturbation leads into cancellation of intracell joining diagrams. It will be shown that this modified Wick’s theorem allows us to carry out systematic improvements on the variational result without worrying about the problem of double counting. As a test on the efficiency of the present scheme, we calculate up to the second order contributions to the ground state energy of interacting nucleon gas through the Yukawa-type potential using both the conventional and the present variational perturbation scheme.
II. THE VARIATIONAL PRINCIPLE IN THE FUNCTIONAL INTEGRAL APPROACH

The variational principle for the partition function and the thermodynamic potential can be obtained using Jensen-Peierls' inequality [13,14], which is given as follows for Hermitian operators \( A_0 \) and \( A_1 \):

\[
\frac{\text{Tr} e^{-(A_0 + A_1)}}{\text{Tr} e^{-A_0}} \geq e^{-\langle A_1 \rangle_0},
\]

where

\[
\langle A_1 \rangle_0 = \frac{\text{Tr} A_1 e^{-A_0}}{\text{Tr} e^{-A_0}}.
\]

When \( A_0 \) and \( A_1 \) are normal-ordered operators composed of creation and annihilation operators, \( A_0 = : A_0 (\{ a_\alpha^\dagger, a_\alpha \} ) : \) and \( A_1 = : A_1 (\{ a_\alpha^\dagger, a_\alpha \} ) : \), the trace operation is expressed in the coherent state functional integral form as follows [3],

\[
\text{Tr} e^{-A_0} = \int D[\bar{\psi} \psi] e^{-\int d\tau \left[ \sum_\alpha \bar{\psi}_\alpha (\tau) \partial_\tau \psi_\alpha (\tau) + A_0 (\{ \bar{\psi}_\alpha (\tau), \psi_\alpha (\tau) \} ) \right]}.
\]

Defining the generating function \( K[\bar{\eta}, \eta; A_0] \) with source variables \( \bar{\eta} \) and \( \eta \),

\[
K[\bar{\eta}, \eta; A_0] \equiv \int D[\bar{\psi} \psi] e^{-\int d\tau \left[ \sum_\alpha \bar{\psi}_\alpha (\tau) \partial_\tau \psi_\alpha (\tau) + A_0 (\{ \bar{\psi}_\alpha (\tau), \psi_\alpha (\tau) \} ) + \sum_\alpha \psi_\alpha (\tau) \eta_\alpha (\tau) + \sum_\alpha \eta_\alpha (\tau) \bar{\psi}_\alpha (\tau) \right]},
\]

we can express the above traces as follows,

\[
\text{Tr} e^{-A_0} = K[\bar{\eta}, \eta; A_0]|_{\bar{\eta}, \eta = 0},
\]

\[
\text{Tr} e^{-(A_0 + A_1)} = e^{-\int d\tau A_1 (\{ z \frac{\partial}{\partial \eta_\alpha (\tau)}, z \frac{\partial}{\partial \bar{\eta}_\alpha (\tau)} \} )} K[\bar{\eta}, \eta; A_0]|_{\bar{\eta}, \eta = 0},
\]

\[
\text{Tr} A_1 e^{-A_0} = \int d\tau A_1 \left( \{ z \frac{\partial}{\partial \eta_\alpha (\tau)}, z \frac{\partial}{\partial \bar{\eta}_\alpha (\tau)} \} \right) K[\bar{\eta}, \eta; A_0]|_{\bar{\eta}, \eta = 0},
\]

where \( z = -1 (+1) \) and \( \eta \) and \( \bar{\eta} \) are Grassmann (complex) variables for fermion (boson) field. Using the shorthand notation,

\[
\langle F \left( \left\{ \frac{\partial}{\partial \eta_\alpha (\tau)}, \frac{\partial}{\partial \bar{\eta}_\alpha (\tau)} \right\} \right) \rangle_{A_0} \equiv \frac{F \left( \left\{ \frac{\partial}{\partial \eta_\alpha (\tau)}, \frac{\partial}{\partial \bar{\eta}_\alpha (\tau)} \right\} \right) K[\bar{\eta}, \eta; A_0]|_{\bar{\eta}, \eta = 0}}{K[\bar{\eta}, \eta; A_0]|_{\bar{\eta}, \eta = 0}},
\]
we can express Jensen-Peierls’ inequality in the functional integral expression,
\[
\left< e^{-\int d\tau A_1\left(\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}\}\right)} \right>_{A_0} \geq e^{-\left< \int d\tau A_1\left(\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}\}\right) \right>_{A_0}}.
\] (8)

In order to apply this inequality to the partition function, we rewrite the action \(S\) in the form \(S = S_0(\lambda) + (S - S_0(\lambda))\), where \(S_0(\lambda)\) is a variational action and \(\lambda\) is a variational parameter to be determined through the variational calculation. Then the partition function is given by
\[
Z = \int D[\bar{\psi}\psi] e^{-S[\bar{\psi},\psi]}
= \int D[\bar{\psi}\psi] e^{-S_0[\bar{\psi},\psi;\lambda] - (S[\bar{\psi},\psi] - S_0[\bar{\psi},\psi;\lambda])}
= e^{-\left< S[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}\}-S_0[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}};\lambda]\}\right>_{S_0}} \cdot \int D[\bar{\psi}\psi] e^{-S_0[\bar{\psi},\psi;\lambda]}
\geq e^{-\left< (S[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}\]-S_0[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}};\lambda]\])\right>_{S_0}} \cdot \int D[\bar{\psi}\psi] e^{-S_0[\bar{\psi},\psi;\lambda]}. (9)
\]

The thermodynamic potential can be expressed likewise
\[
\Omega \leq -\frac{1}{\beta} \ln \int D[\bar{\psi}\psi] e^{-S_0[\bar{\psi},\psi;\lambda] + \frac{1}{\beta} \left< S \left[ \{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}\} - S_0 \left[ \{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}; \lambda\} \right] \right] \right>_{S_0}}.
\] (10)

We can obtain the variational result by maximizing the fourth line of Eq.(9) or minimizing the righthand side of Eq.(10) with \(\lambda\). Using the above expression, we now obtain the expressions for the variational perturbation process for the partition function and the thermodynamic potential as follows,
\[
Z = \int D[\bar{\psi}\psi] e^{-S_0[\bar{\psi},\psi;\lambda]} e^{-\left< (S[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}\}-S_0[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}};\lambda]\])\right>_{S_0}} \cdot \int D[\bar{\psi}\psi] e^{-S_0[\bar{\psi},\psi;\lambda]}
\geq e^{-\left< (S[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}\]-S_0[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}};\lambda]\])\right>_{S_0}} \cdot \int D[\bar{\psi}\psi] e^{-S_0[\bar{\psi},\psi;\lambda]}. (11)
\]
\[
\Omega = -\frac{1}{\beta} \ln \int D[\bar{\psi}\psi] e^{-S_0[\bar{\psi},\psi;\lambda] + \frac{1}{\beta} \left< S \left[ \{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}\} - S_0 \left[ \{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}; \lambda\} \right] \right] \right>_{S_0}} - \frac{1}{\beta} \ln \left< e^{-\left< (S[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}}\]-S_0[\{\xi, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \tilde{\eta}};\lambda]\])\right>_{S_0}} \cdot \int D[\bar{\psi}\psi] e^{-S_0[\bar{\psi},\psi;\lambda]}. (12)
\]

The second lines of Eq.(11) and (12) are the perturbations based on the variational basis and, thus, provide systematic improvements over the variational result.
III. VARIATIONAL PERTURBATION ON INTERACTING FERMION SYSTEMS AND MODIFIED WICK'S THEOREM

The above variational perturbation result on the thermodynamic potential can be applied to any strongly correlated systems. In general, the variational result corresponds to the mean field value\[15,16\]. With the expressions given in Eq.(11) and (12), we can readily carry out systematic improvements over the mean field result, since the renormalized perturbation term is generally much smaller than the original one. To see this point clearly, we apply the principle to an interacting fermion gas system through two-body interactions. In the process, we derive a modified Wick’s theorem, which removes the problem of double counting of higher order terms. We also obtain explicit expressions for the thermodynamic potential.

The partition function for two-body interacting fermion systems is generally given by

\[
Z = \int D[\bar{\psi}\psi] e^{-G^{-1}_{ij}\bar{\psi}_i\psi_j - V_{ijkl}\bar{\psi}_i\bar{\psi}_j\psi_k\psi_l} .
\]  

where the subscript stands for all possible quantum numbers and an imaginary time \(\tau\); \(i = (k\sigma\tau)\). The integration or summation symbols are omitted by the summation convention. \(G^o\) is a bare Green’s function matrix and \(V\) is an interaction tensor. For example, for free fermions, \(G^o\) has a form;

\[
G^o_{ij} \rightarrow \langle k\sigma\tau | G^o_{ij} | k'\sigma'\tau' \rangle = (\partial_\tau + \hbar^2 k^2/2m - \mu)\delta(\tau - \tau')\delta_{kk'}\delta_{\sigma\sigma'} .
\]  

The partition function can be rewritten using the variational Green’s function \(G\);

\[
Z = \int D[\bar{\psi}\psi] e^{-G^{-1}_{ij}\bar{\psi}_i\psi_j -(G^o_{ij} - G^{-1}_{ij})\bar{\psi}_i\psi_j - V_{ijkl}\bar{\psi}_i\bar{\psi}_j\psi_k\psi_l - \bar{\eta}_i\psi_i - \bar{\psi}_i\eta_i} |_{\bar{\eta},\eta = 0} = e^{\ln\text{Det}G^{-1} + (G^o_{ij} - G^{-1}_{ij}) \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \bar{\eta}_j} - V_{ijkl} \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \bar{\eta}_j} \frac{\partial}{\partial \eta_k} \frac{\partial}{\partial \bar{\eta}_l} e^{\bar{\eta}_i\psi_i\eta_j} } |_{\bar{\eta},\eta = 0} .
\]  

Here we used the Gaussian integral for the Grassmann variables \[3\];

\[
\int D[\bar{\psi}\psi] e^{-\bar{\psi}_iG^o_{ij}\psi_j + \bar{\eta}_i\psi_i + \bar{\psi}_i\eta_i} = \text{Det}G^{-1}e^{\bar{\eta}_iG^o_{ij}\eta_j} .
\]  

Using the shorthand notation of Eq.(7), the partition function is expressed
Using the variational principle discussed above, we obtain for the partition function

\[ Z \geq e^{\ln \det G^{-1} + (G^{-1}_{ij} - G^{-1}) \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \bar{\eta}_j} \right) G} \cdot (17) \]

It is now necessary to obtain the Green’s function, \( G \), which appears in the variational process. For this purpose, we consider the variational thermodynamic potential.

\[ \Omega \leq \bar{\Omega} = -\frac{1}{\beta} \ln \det G^{-1} - \frac{1}{\beta} (G^{-1}_{ij} - G^{-1}) \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \bar{\eta}_j} \right) G \]

\[ + \frac{1}{\beta} V_{ijkl} \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right) G \]

\[ = -\frac{1}{\beta} \ln \det G^{-1} - \frac{1}{\beta} (G^{-1}_{ij} - G^{-1}) G_{ji} \]

\[ + \frac{1}{\beta} V_{ijkl} (G_{kj} G_{li} - G_{ki} G_{lj}) \cdot (19) \]

Minimizing \( \bar{\Omega} \) against the variational Green’s function \( G \), we obtain

\[ G^{-1}_{ba} - G^{-1}_{ba} + 2(V_{ibaj} - V_{biaj}) G_{ji} = 0 \cdot (20) \]

In deriving the above result, the symmetry property of \( V_{ijkl} = V_{jilk} \) is used. Defining \( \langle b|\Sigma|a \rangle \equiv 2(V_{ibaj} - V_{biaj}) G_{ji} \), we obtain

\[ G^{-1} - G^{-1} + \Sigma = 0 \cdot (21) \]

Here, we note that \( G \) corresponds to the self-consistent Hartree-Fock Green’s function for the interacting fermion system. Using this variational Green’s function, we rewrite the partition function as follows,

\[ Z = e^{\ln \det G^{-1} + (G^{-1}_{ij} - G^{-1}) \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \bar{\eta}_j} \right) G} \cdot (17) \]

\[ - V_{ijkl} \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right) G \]

\[ \cdot \left( e^{(G^{-1}_{ij} - G^{-1}) \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \bar{\eta}_j} \right) G} - V_{ijkl} \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right) G \right) G \cdot (22) \]

The second line in the above equation is the renormalized perturbation contribution and can be simplified as follows,
expansion. Therefore, we first study contraction rules under the primed operation. We
With the prime defined in Eq.(24), we cannot apply Wick’s theorem directly to the above
Using this primed operation and Eq. (21), the partition function is greatly simplified.
In deriving the above relation, we used the symmetry of the potential \( V_{ijkl} \) and Eq.(20).
Here the primed operation \((\cdots\cdots)'\) is defined to be
\[
\left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \eta_k} \frac{\partial}{\partial \eta_l} \right)' \equiv \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \eta_k} \frac{\partial}{\partial \eta_l} - G_{li} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \eta_k} \frac{\partial}{\partial \eta_l} - G_{kj} \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \eta_l}
\right.
\]
\[\left. + G_{lj} \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_k} \frac{\partial}{\partial \eta_l} + G_{ki} \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} + G_{lj} G_{ki} - G_{lj} G_{ki} \right) . \tag{24} \]
Using this primed operation and Eq. (21), the partition function is greatly simplified.
\[
Z = e^{-\text{tr}\ln G + \frac{1}{2} \text{tr} \Sigma G} \left\langle e^{-V_{ijkl} \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \eta_k} \frac{\partial}{\partial \eta_l} \right)'} \right\rangle_G \tag{25} \]
In order to carry out the perturbation, it is necessary to evaluate terms like
\[
\left\langle \left( \frac{\partial}{\partial \eta_1} \frac{\partial}{\partial \eta_2} \frac{\partial}{\partial \eta_3} \frac{\partial}{\partial \eta_4} \right)' \cdots \left( \frac{\partial}{\partial \eta_n} \frac{\partial}{\partial \eta_1} \frac{\partial}{\partial \eta_2} \frac{\partial}{\partial \eta_3} \right)' \right\rangle_G
\]
\[= \left( \frac{\partial}{\partial \eta_1} \frac{\partial}{\partial \eta_2} \frac{\partial}{\partial \eta_3} \frac{\partial}{\partial \eta_4} \right)' \cdots \left( \frac{\partial}{\partial \eta_n} \frac{\partial}{\partial \eta_1} \frac{\partial}{\partial \eta_2} \frac{\partial}{\partial \eta_3} \right)' e^{\eta_i G_{ij} \eta_j} \mid_{\eta=0} . \tag{26} \]
With the prime defined in Eq.(24), we cannot apply Wick’s theorem directly to the above expansion. Therefore, we first study contraction rules under the primed operation. We rewrite Eq.(24) as follows,
\[
\left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \eta_k} \frac{\partial}{\partial \eta_l} \right)' = (i \jmath \kappa \ell) - (i \jmath \kappa \ell) - (i \jmath \kappa \ell) - (i \jmath \kappa \ell)
\]
\[= -(i \jmath \kappa \ell) + (i \jmath \kappa \ell) + (i \jmath \kappa \ell) , \tag{27} \]
where we used shorthand notations; \( \frac{\partial}{\partial \eta_i} \rightarrow i \) and \( \frac{\partial}{\partial \bar{\eta}_i} \rightarrow \bar{i} \), and the connected pairs represent the contractions; \( \bar{i} j \equiv G_{ji} \). We call one \( (\cdots)' \) a unit cell and mark a contraction with other unit cell elements with dots and a intracell contraction with lines. With these notations, terms in Eq.(27) appear

\[
\begin{align*}
( i j k l ) &= ( i j k l ) + ( i j \bar{k} \bar{l} ) + ( i \bar{j} k \bar{l} ) + ( \bar{i} j k \bar{l} ) + ( i \bar{j} \bar{k} \bar{l} ) + ( i j k l ) , \\
-( i j k l ) &= -( i j \bar{k} \bar{l} ) - ( i \bar{j} k \bar{l} ) - ( i j k l ) , \\
-( i j \bar{k} \bar{l} ) &= -( i \bar{j} k \bar{l} ) - ( i j k l ) , \\
-( i \bar{j} k \bar{l} ) &= -( \bar{i} j k \bar{l} ) - ( \bar{i} j k \bar{l} ) , \\
-( \bar{i} j k \bar{l} ) &= -( \bar{i} j k \bar{l} ) - ( i j k l ) .
\end{align*}
\]

(28)

Now adding all contributions within one cell, we find that all intracell contractions cancel and disappear, thus making the perturbation with the variational basis simple and straightforward. The final expression for each primed operation in Eq.(26) appears

\[
\begin{align*}
\left( \frac{\partial}{\partial \eta_n} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right)' &= \left( \frac{\partial}{\partial \eta_1} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right) .
\end{align*}
\]

(29)

Therefore, the contraction rule for higher terms now becomes

\[
\begin{align*}
\left\langle \left( \frac{\partial}{\partial \eta_n} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right)' \cdots \left( \frac{\partial}{\partial \eta_n} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right)' \right\rangle_G \\
= \left\langle ( \bar{i}_1 j_1 k_1 \bar{l}_1 ) \cdots ( \bar{i}_n j_n k_n \bar{l}_n ) \right\rangle_G \\
= \text{Sum of all contractions between different cells.}
\end{align*}
\]

(30)

This modification of Wick’s theorem represents nothing but a requirement that the selfenergy contributions which are included in the variational Green’s function should not contribute
again in the perturbation calculation. This new rule allows one to carry out higher order calculations without worrying about the double counting problem. The perturbation calculations are easily tractable by the diagramatic method. The unit cell with an interaction, $V_{ijkl} \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right)'$ is shown in Fig.1 (a). The modified Wick’s theorem stipulates that diagrams with intracell contractions do not contribute to the thermodynamic potential. Examples of such diagrams are shown in Fig.1 (b).

Since the linked cluster theorem is equally applicable in the present formulation, the thermodynamic potential can now readily be written

$$\Omega = \frac{1}{\beta} \text{tr} \ln G - \frac{1}{2 \beta} \text{tr} \Sigma G - \frac{1}{\beta} \left\langle e^{-V_{ijkl} \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right)'} \right\rangle_{G,C}$$

(31)

where $C$ indicates the connected diagrams only. The first two terms are the variational result and the last is the renormalized perturbation. For example, the second order perturbation terms are given as follows;

$$- \frac{1}{\beta} \cdot \frac{1}{2} V_{ijkl} V_{i' j' k' l'} \left\langle \left( \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \bar{\eta}_k} \frac{\partial}{\partial \bar{\eta}_l} \right)' \left( \frac{\partial}{\partial \eta_{i'}} \frac{\partial}{\partial \eta_{j'}} \frac{\partial}{\partial \bar{\eta}_{k'}} \frac{\partial}{\partial \bar{\eta}_{l'}} \right)' \right\rangle_{G,C}$$

$$= - \frac{1}{\beta} V_{ijkl} V_{i' j' k' l'} G_{li} G_{kj} G_{ki} G_{lj},$$

$$+ \frac{1}{\beta} V_{ijkl} V_{i' j' k' l'} G_{li} G_{kj} G_{ki} G_{lj'},$$

(32)

which correspond to the diagrams in Fig.2 (a).

### IV. A MODEL CALCULATION

A sample calculation was carried out to test the efficiency of the present method using a three dimensional nucleon gas system interacting through the two-body Yukawa-type potential. The model Hamiltonian is given by

$$H = \sum_{k\sigma} \epsilon_k a_{k\sigma}^\dagger a_{k\sigma} + \frac{1}{2} \sum_{kk'q\sigma\sigma'} v(q) a_{k\sigma}^\dagger a_{k'\sigma'}^\dagger a_{k'-q\sigma'} a_{k+q\sigma},$$

(33)

where
\[ \epsilon_k = \frac{\hbar^2 k^2}{2m_n} \]

\[ v(q) = \frac{4\pi\gamma}{V(q^2 + \lambda^2)} . \]  

(34)

Here, \( m_n \) is the nucleon mass and \( \gamma \) and \( \lambda \) are model parameters which should be fixed for numerical calculations. The primed summation indicates that the \( q = 0 \) term is renormalized away because this divergent energy term has the same contribution for both the conventional and the variational perturbation methods. With this model Hamiltonian, we calculate the ground state energy at zero temperature using both the variational perturbation theory and the conventional perturbation theory up to the second order. The bare Green’s function and the interaction of this model is expressed as

\[ G_{ij}^{\sigma^{-1}} \rightarrow G_{k\sigma k'\sigma'}^{\sigma^{-1}} = (\partial_\tau + \epsilon_k - \mu)\delta(\tau - \tau')\delta_{kk'}\delta_{\sigma\sigma'} , \]

(35)

\[ V_{ijkl} \rightarrow V_{k_1\sigma_1 k_2\sigma_2 k_3\tau_3 k_4\sigma_4} = \frac{1}{2} v(||k_4 - k_1||)\delta_{k_1+k_2+k_3+k_4}\delta_{\sigma_1\sigma_4}\delta_{\tau_1-\tau_2}\delta_{\tau_3-\tau_4}\delta_{\tau_2-\tau_3} , \]

(36)

where \( \mu \) is the chemical potential. Denoting \( G_{k\sigma k'\sigma'} \) as \( G_{k\sigma}(\tau - \tau') \) for a homogeneous system, the equation of \( G \), Eq.(21) is expressed as follows,

\[ G_{k\sigma}(\tau - \tau') = G_{k\sigma}^0(\tau - \tau') - \int d\tau'' G_{k\sigma}^0(\tau - \tau'') \sum_q v(q)G_{k+q\sigma}(0)G_{k\sigma}(\tau'' - \tau') . \]

(37)

Fourier transforming of this equation with respect to time, we easily obtain the variational Green’s function \( G_{k\sigma}(i\omega_n) \) as

\[ G_{k\sigma}(i\omega_n) = -\frac{1}{i\omega_n - (\tilde{\epsilon}_{k\sigma} - \mu)} , \]

(38)

where \( \omega_n \) is the fermion Matsubara frequency, \( \frac{(2n+1)\pi}{\beta} \) and \( \tilde{\epsilon}_{k\sigma} \) is the renormalized nucleon energy value given by \( \epsilon_k - \sum_q v(q)n_{k+q\sigma} \). \( n_{k\sigma} \) is the Fermi distribution function, \( \frac{1}{e^{\beta(\tilde{\epsilon}_{k\sigma} - \mu)} + 1} \) with the renormalized energy. Therefore, the variational result of the thermodynamic potential, \( \bar{\Omega}_{\text{min}} \) is

\[ \bar{\Omega}_{\text{min}} = \frac{1}{\beta} \text{trln}G - \frac{1}{2\beta} \text{tr}\Sigma G \]

\[ = -\frac{1}{\beta} \sum_{k\sigma} \ln \left( 1 + e^{-\beta(\epsilon_k - \sum_q v(q)n_{k+q\sigma} - \mu)} \right) + \frac{1}{2} \sum_{kq\sigma} v(q)n_{k+q\sigma}n_{k\sigma} . \]

(39)
The first order contribution is absent due to the modified Wick’s theorem and the relevant second order diagrams are shown in Fig.2 (a), while conventional diagrams of the same order are also shown in Fig.2 (b) for the comparison, where double lines represent the variational $G$ and single lines the bare $G^0$. The details of the calculations are exactly the same for both cases except that the double line Green’s function has the one particle energy, $\tilde{\epsilon}_{k\sigma}$ instead of the bare energy, $\epsilon_k$. For the nucleon gas interacting with the potential given in Eq.(34), at zero temperature, the energy $\tilde{\epsilon}_{k\sigma}$ can be evaluated analytically to be given by

$$\tilde{\epsilon}_{k\sigma} = \frac{\gamma}{2r} \left[ \left( \frac{9\pi}{8} \right)^{\frac{\gamma}{2}} \frac{\hbar^2}{\gamma rm_t} \left( \frac{k}{k_F^0} \right)^2 - \frac{4}{\pi} \left( \frac{9\pi}{8} \right)^{\frac{\gamma}{2}} F \left( \frac{k}{k_F^0} \left( \frac{\lambda r}{(9\pi/8)^{1/3}} \right) \right) \right], \quad (40)$$

where $r$ is the average distance between nucleons which is defined by $V = \frac{4}{3}\pi r^3 N$ with the volume $V$ and the number of nucleons $N$ of the system. $k_F^0$ is the Fermi wave vector and $F(x, b)$ is given by

$$F(x, b) = \frac{1}{2} + \frac{1+b^2-x^2}{8x} \ln \frac{b^2+(x+1)^2}{b^2+(x-1)^2} - \frac{1}{2} \left[ \tan^{-1} \frac{1-x}{b} + \tan^{-1} \frac{1+x}{b} \right]. \quad (41)$$

Using the above prescriptions and following standard textbook steps [1], we calculated the total energy at zero temperature numerically. The result is shown in Fig.3 and compared to the conventional calculation. Since the exact solution is not available, it is not possible to access the accuracy of the present method directly. It is known that, for the homogeneous fermion gas, the variational Hartree-Fock result corresponds to the standard first order calculation [18]. Therefore, a convergence test can be carried out by comparing the second order contributions from both methods with the Hartree-Fock result. The result in Fig.3 clearly shows that the magnitude of the second order contribution is substantially reduced in the variational perturbation calculation. For example, at $r = 2.5$ Fermi, the renormalized contribution is 60.2% of the bare contribution. This renormalization clearly originates from the higher order terms included in the variational perturbation process [12].

The simple Yukawa-type potential considered here allows an analytic expression for the variational one-particle energy $\tilde{\epsilon}_{k\sigma}$. However, in real systems, the interaction between nucleons is more complicated and, thus, generally does not yield a closed expression. We note
that, although an analytic expression for $\tilde{\epsilon}_{k\sigma}$ is convenient to carry out the calculation, a numerical form of $\tilde{\epsilon}_{k\sigma}$ does not pose a fundamental difficulty, once whole spectrum of the energy values is known.

V. SUMMARY

In conclusion, we have presented a variational perturbation scheme for many particle systems using the functional integral formulation. It is shown that the Green’s function obtained through the variational process corresponds to the Hartree-Fock Green’s function. A modified Wick’s theorem for renormalized perturbation based on the variational Green’s function is obtained. A model calculation with a nucleon gas interacting with the Yukawa type potential shows that the present formalism provides an efficient and convenient formalism to study strongly correlated systems.

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FIGURES

FIG. 1. (a) Unit cell to construct Feynman diagrams, (b) Diagrams which do not appear in the variational perturbation calculation. The double line indicates the variational Green’s function.

FIG. 2. Second order diagrams (a) for the present variational perturbation scheme and (b) for the conventional perturbation theory. Note that the last diagram in (b) does not appear in (a) due to the modified Wick’s theorem.

FIG. 3. The ground state energy per particle calculated up to the second order; (a) solid line represents the present variational perturbation result, (b) dotted line the conventional perturbation upto the second order, and (c) dashed line the Hartree-Fock result. Here, $\frac{\hbar}{m_\pi c}$ is the Compton wavelength of the pion [17].
\[ r \text{ (Fermi)} \]

| Energy (MeV) |
|--------------|
| -20          |
| -16          |
| -12          |
| -8           |
| -4           |
| 0            |
| 4            |
| 8            |

\( \gamma = 0.189 \, \hbar c, \, \lambda = 0.1 m_n c/\hbar \)