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Rayleigh-Schrödinger-Goldstone variational perturbation theory for many Fermion systems

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Abstract. We present a Rayleigh-Schrödinger-Goldstone perturbation formalism for many Fermion systems. Based on this formalism, variational perturbation scheme which goes beyond the Gaussian approximation is developed. In order to go beyond the Gaussian approximation, we identify a parent Hamiltonian which has an effective Gaussian vacuum as a variational solution and carry out further perturbation with respect to the renormalized interaction using Goldstone's expansion. Perturbation rules for the ground state wavefunctional and energy are found, thus, opening a way for general use of the Schrödinger picture method for many Fermion systems. Useful commuting relations between operators and the Gaussian wavefunctional are also found, which could reduce the calculational efforts substantially. As examples, we calculate the first order correction to the Gaussian wavefunctional and the second order correction to the ground state of an electron gas system with the Yukawa-type interaction.

PACS. 05.30.Fk Fermion systems and electron gas – 71.10.Ca Electron gas, Fermi gas

1 Introduction

Field theories can be constructed from three kinds of pictures which are called Heisenberg, Interaction and Schrödinger pictures [1]. Among them, the Heisenberg picture is known to provide a convenient basis for the study of dynamics of operators and systematic perturbative improvement on physical quantities. On the other hand, the Schrödinger picture approach focuses on the dynamics of wavefunction, which allows detailed study on time evolution. However, in this approach, it is known that systematic improvement on obtained result is rather difficult. Instead, it has a powerful technique which is called a variational method which allows nonperturbative access to problems, so that it could be applied to strongly correlated systems where perturbative approaches break down.

There have been successful applications of the Schrödinger picture to field theories [2–8] and later on to nonrelativistic many-particle systems [9–15]. While it has been proved useful, still the controlable range of trial wavefunctionals has been found to be narrow and further improvement from results of a trial wavefunctional demands much endeavor in field theories. Therefore, recent investigations on the picture have focused on overcoming its drawbacks towards a more managable theory.

Gaussian trial wavefunctional approach in bose fields has been widely applied and proven to be an efficient and powerful method in the Schrödinger picture [3,8]. Further improvements beyond the Gaussian approximation have been investigated mostly in two directions. One is to try it with non-Gaussian wavefunctionals [16,17], and the other is to perform appropriate expansions based on Gaussian trial wavefunctional [18–24].

In Fermi fields, a convenient prescription for operators was proposed by Floreanini and Jackiw [5]. It was shown that this approach gives successful results on Gaussian approximations of Fermi fields as in bose fields. However, in contrast to the bosonic case [1], no successful Rayleigh-Schrödinger type perturbation formalism for Fermi fields has been proposed so far, although several alternative schemes including functional integrals [25] and background field methods [8] have been reported using the Floreanini-Jackiw representation(FJR). Since the Rayleigh-Schrödinger perturbation formalism is the most familiar form of perturbation theories and especially suitable for the Schödinger picture representation in quantum mechanics, it is rather puzzling that it is not so in field theories. Indeed, the Rayleigh-Schrödinger perturbation scheme for bose fields was formulated early [1]. Also, recently, it has been shown to be versatile enough to yield higher order terms which are not attainable by other methods [20]. However, so far there exist no such parallel formalism for Fermi fields.

In this paper, we present a successful perturbation formalism for fermionic many-body systems combining

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the Rayleigh-Schrödinger perturbation with Goldstone's (RSG) expansion. The scheme will be used to formulate a variational perturbation scheme, which provides a systematic improvement beyond the Gaussian approximation. In order to make the presentation compact, we directly formulate a RSG perturbation scheme based on the variational Gaussian wavefunctionals. The formalism is trivially reduced to the conventional perturbation scheme by using a true Gaussian vacuum instead of an effective Gaussian vacuum. This point will be made clear once the formalism is given. It will be shown that the FJR provides surprisingly simple expressions for fermion wavefunctionals. As examples, we calculate the first order correction to the Gaussian wavefunctional and the second order energy of an electron gas with the Yukawa-type interaction.

2 Floreanini-Jackiw representation

The action of Fermi field operators on Hilbert space can be represented by product or derivatives of Grassmann variables in the Grassmann function space. Then, Schrödinger equations are transformed into functional differential equations [1]. Among many possible representations preserving the anticommuting relations of Fermi field operators, the simplest one is generated from the fermion coherent states which are defined as eigenstates of annihilation operators [26]. In this representation, annihilation operators $\{a_i\}$ are described by Grassmann variables $\{u_i^*\}$, and creation opeators $\{a_i^\dagger\}$, by Grassmann derivatives $\{\frac{\partial}{\partial u_i^*}\}$. A representation without a complex conjugate notation $*$ is also possible and has been used by Duncan et al. [4,9]. However, we find that the representation proposed by Floreanini and Jackiw is more convenient to formulate the present theory.

In the FJR, the creation and annihilation operators are given as follows [5];

$$a_i^\dagger = \frac{1}{\sqrt{2}}\left(u_i^* + \frac{\partial}{\partial u_i}\right), \quad a_i = \frac{1}{\sqrt{2}}\left(u_i + \frac{\partial}{\partial u_i^*}\right), \quad (1)$$

where u_i and u_i^* are Grassmann variables. In the FJR for free Fermi systems, vacuums are described by Gaussian wavefunctionals just as for bosonic systems. However, the norms between basis states for the FJR are not orthogonal since $\langle u'u'^*|uu^*\rangle = e^{u_i'^* u_i - u_i^* u_i'}$. It can be proven by the fact that four kinds of states relative to a quantum number i are possible. They are represented by 1, u_i^*, u_i and $u_i^* u_i$. Actually, only two kinds of physical states for i exist. One is the occupied state by a fermion and the other unoccupied. Thus, the FJR is a reducible representation and only a subspace of the total Grassmann functional space can be used to describe physically well-defined wavefunctionals. The subspace can be constructed only after a physical vacuum wavefunctional is chosen. The dual space wavefunctional $\bar{\Psi}$ for the wavefunctional Ψ is defined as

$$\bar{\Psi} = \int D[u'u'^*]\Psi e^{u_i'^* u_i - u_i^* u_i'}, \quad (2)$$

where the norm is calculated by $\langle\Psi|\Psi\rangle = \int D[uu^*]\bar{\Psi}\Psi$. It can be easily shown that the free fermion vacuum is described by Gaussian wavefunctional [5] as

$$\Psi_G = e^{G_{ij}u_i^* u_j}, \quad (3)$$

$$\bar{\Psi}_G = \mathrm{Det}G^\dagger e^{\bar{G}_{ij}u_i^* u_j}, \quad (4)$$

where $\bar{G} = {G^\dagger}^{-1}$ and we find the dual wavefunctional is also Gaussian. Gaussian expectation values of some normal ordered operators are calculated as

$$\frac{\langle\Psi_G| : \mathcal{O}(a^\dagger, a) : |\Psi_G\rangle}{\langle\Psi_G|\Psi_G\rangle} = : \mathcal{O}\left(\frac{1}{\sqrt{2}}\frac{\partial}{\partial J_b}\left(I+\bar{G}\right)_{bi}, \frac{1}{\sqrt{2}}(I+G)_{ja}\frac{\partial}{\partial J_a^*}\right) : e^{(G+\bar{G})^{-1}_{ij}J_i^* J_j}|_{J,J^*=0}, \quad (5)$$

where I is an identity matrix and J, J^* are source fields which are inserted into the Gaussian wavefunctional as $e^{G_{ij}u_i^* u_j + J_i^* u_i - u_i^* J_i}$ during the calculation. It allows that the Grassmann integrals are represented by Grassmann derivatives of source fields.

For the free field Hamiltonian, $H_0 = h_{ij}a_i^\dagger a_j$, the functional Schrödinger equation in the FJR is

$$\frac{1}{2}h_{ij}\left(u_i^* + \frac{\partial}{\partial u_i}\right)\left(u_j + \frac{\partial}{\partial u_j^*}\right)\Psi = E_0\Psi. \quad (6)$$

This equation contains second order derivatives and a quadratic term which are similar to the harmonic oscillator problem. Thus, we expect the Gaussian wavefunctional, equation (3), as a vacuum. In order for equation (3) to be an eigenfunctional with an eigenvalue $E_0 = \frac{1}{2}\mathrm{Tr}h(I+G)$ in equation (6), G should satisfy the following condition;

$$(I-G)h(I+G) = 0. \quad (7)$$

Equation (7) has trivial and non-trivial solutions. Trivial solutions are $G = \pm I$ and non-trivial ones, $G = \pm\frac{h}{\sqrt{h^2}}$. Here, we note that the number of particles N is given by $N = \frac{1}{2}\mathrm{Tr}(I+G)$. Therefore, G can be expressed as $G = -\frac{h-\mu I}{\sqrt{(h-\mu I)^2}}$, where μ is a chemical potential. Diagonalized, diagonal elements of G become 1 (-1) below (above) μ. In the case of free Dirac fields, μ is zero and all the negative energy states are fully filled in the Dirac vacuum.

3 Gaussian approximation and the state wavefunctionals

When interactions between fermions exist, exact eigenfunctionals are different from the above Gaussian. Variational method or perturbation theory is applied in order to approximate true eigenfunctionals. Although the variational method depends largely on intuition in contrast

to the systematic perturbative approach, it could provide excellent results if trial states are chosen carefully.

In the Gaussian approximation, Gaussian wavefunctional with variational parameters is used as a trial functional. We now consider the case of interacting fermion system where the Hamiltonian has a general form,

$$H = h_{ij}a_i^\dagger a_j + v_{ijkl}a_i^\dagger a_j^\dagger a_k a_l. \tag{8}$$

Trial wavefunctional is chosen to be

$$\Psi_G = e^{G_{ij}u_i^* u_j}, \tag{9}$$

where G is a variational parameter matrix. Then, the energy expectation value is readily calculated with the aid of equation (5)

$$E = \frac{\langle\Psi_G|H|\Psi_G\rangle}{\langle\Psi_G|\Psi_G\rangle} = \frac{1}{2}(h+\Sigma)_{ij}\Omega_{ji} - \frac{1}{4}\Sigma_{ij}\Omega_{ji}, \tag{10}$$

where $\Sigma_{ij} = (v_{kijl} - v_{ikjl})\Omega_{lk}$ and $\Omega = (I+G)(G+\bar{G})^{-1}(I+\bar{G})$. Minimization of the energy under a fixed number of particles is achieved through the relation, $\frac{\partial}{\partial G_{ij}}\left[E - \mu(\frac{1}{2}\mathrm{Tr}\Omega - N)\right] = 0$, where μ, the chemical potential, is introduced as a Lagrange's multiplier. Thus, the solution G should satisfy the following condition;

$$(I-G)\,(h+\Sigma-\mu I)\,(I+G) = 0. \tag{11}$$

The equivalent condition for $\bar{G}$ is obtained by minimizing with respect to G, and is given by $(I+\bar{G})\,(h+\Sigma-\mu I)\,(I-\bar{G}) = 0$ which provides the same G as in equation (11). As in equation (7), the nontrivial solution G of equation (11) is given by

$$G = -\frac{h+\Sigma-\mu I}{\sqrt{(h+\Sigma-\mu I)^2}}. \tag{12}$$

With this solution, the ground state energy E_0 is given as $E_0 = \frac{1}{2}\mathrm{Tr}(h+\Sigma)(I+G)$. The parent Hamiltonian $\tilde{H}_0$ which has the above Gaussian vacuum is easily found to be $\tilde{H}_0 = (h+\Sigma)_{ij}a_i^\dagger a_j$. In order to obtain excitations based on the Gaussian wavefunctional, we should have a unitary matrix U which diagonalizes G as $UGU^\dagger = \tilde{I}$, where $\tilde{I}$ is a diagonal matrix with elements of $+1(-1)$ below (above) the Fermi level μ. Thus, G can be rewritten as follows;

$$G = \begin{pmatrix} G_1 & G_2 \\ G_2^\dagger & G_4 \end{pmatrix} = \begin{pmatrix} U_1^\dagger & U_3^\dagger \\ U_2^\dagger & U_4^\dagger \end{pmatrix}\begin{pmatrix} -I & 0 \\ 0 & I \end{pmatrix}\begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}. \tag{13}$$

Therefore, we obtain an expression for U,

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{I-G_1} & -\frac{1}{\sqrt{I-G_1}}G_2 \\ \frac{1}{\sqrt{I+G_4}}G_2^\dagger & \sqrt{I+G_4} \end{pmatrix}. \tag{14}$$

The Gaussian wavefunctional is diagonalized by the new Grassmann variables $\tilde{u}_i = U_{ij}u_j$ and $\tilde{u}_i^* = u_j^* U_{ji}^\dagger$. We use capital (small) letters above(below) the Fermi see, so that

$$\Psi_G = e^{G_{ij}u_i^* u_j} = e^{\tilde{u}_a^*\tilde{u}_a - \tilde{u}_A^*\tilde{u}_A} \quad (a < k_F,\ A > k_F). \tag{15}$$

We define new creation and annihilation operators as follows;

$$\tilde{a}_i^\dagger = \frac{1}{\sqrt{2}}\left(\tilde{u}_i^* + \frac{\partial}{\partial\tilde{u}_i}\right), \quad \tilde{a}_i = \frac{1}{\sqrt{2}}\left(\tilde{u}_i + \frac{\partial}{\partial\tilde{u}_i^*}\right). \tag{16}$$

Excited wavefunctionals and their duals are obtained by these operations to the Gaussian as

$$\Psi_{\mathrm{excited}} = \tilde{u}_{A_1}^* \cdots \tilde{u}_{A_n}^* \tilde{u}_{a_1} \cdots \tilde{u}_{a_n} e^{G_{ij}u_i^* u_j}, \tag{17}$$

$$\bar{\Psi}_{\mathrm{excited}} = \tilde{u}_{a_n}^* \cdots \tilde{u}_{a_1}^* \tilde{u}_{A_n} \cdots \tilde{u}_{A_1} e^{G_{ij}u_i^* u_j}, \tag{18}$$

which has an excitation energy of $\tilde{\epsilon}_{A_1} + \cdots + \tilde{\epsilon}_{A_n} - (\tilde{\epsilon}_{a_1} + \cdots + \tilde{\epsilon}_{a_n})$ where $\tilde{\epsilon}_i$ is the ith matrix element of $U(h+\Sigma)U^\dagger$. We note here that any physical wavefunctional in the FJR could be represented by multiplying only some combinations of $\tilde{u}_A^*$ and $\tilde{u}_a$ to the Gaussian, while in other representations, wavefunctionals should also contain Grassmann derivatives for describing hole states and, thus, are quite complicated in general. An important aspect of the present result is that equations (17) and (18) have same structures to those in bose systems [1].

4 Rayleigh-Schrödinger-Goldstone perturbation formalism beyond the Gaussian approximation

In order to go beyond the Gaussian approximation by a perturbative method based on the parent Hamiltonian $\tilde{H}_0$, Hamiltonian is rearranged as

$$\begin{aligned} H &= \tilde{H}_0 + \left(H - \tilde{H}_0\right) \\ &= (h+\Sigma)_{ij}a_i^\dagger a_j + \left(V_{ijkl}a_i^\dagger a_j^\dagger a_k a_l - \Sigma_{ij}a_i^\dagger a_j\right) \\ &= \left(\tilde{h}+\tilde{\Sigma}\right)_{ij}\tilde{a}_i^\dagger\tilde{a}_j + \left(\tilde{V}_{ijkl}\tilde{a}_i^\dagger\tilde{a}_j^\dagger\tilde{a}_k\tilde{a}_l - \tilde{\Sigma}_{ij}\tilde{a}_i^\dagger\tilde{a}_j\right), \end{aligned} \tag{19}$$

where $\tilde{h} = UhU^\dagger$, $\tilde{\Sigma} = U\Sigma U^\dagger$ and $\tilde{V}_{ijkl} = U_{il}U_{jm}V_{lmpq}U_{pk}^\dagger U_{ql}^\dagger$. Here, we note that the whole formalism simply reduces to the conventional perturbation if Σ is set to zero. In the previous section, we have already obtained whole spectrums of eigenvalues and eigenfunctionals of the parent Hamiltonian $\tilde{H}_0$. Therefore, the Rayleigh-Schrödinger perturbation procedure [1] can be readily adopted for improving the Gaussian approximation. However, in order to carry out the calculation, it is necessary to have a general rule for combination of Grassmann operations which is similar to Wick's theorem of the Green function approach. In the following, we show that another perturbative approach in the time independent formulation, namely Goldstone's expansion [27], becomes an extremely useful tool in the present approach. Since final results from Goldstone's expansion are same as from the Rayleigh-Schrödinger scheme order by order, we follow the Goldstone's approach to obtain the expressions for the Rayleigh-Schrödinger perturbation.

Goldstone's expansion is as follows. If $H = H_0 + H_1$, $H_0|\Phi_0\rangle = E_0|\Phi_0\rangle$ and $H|\Psi_0\rangle = (E_0 + \Delta E)|\Psi_0\rangle$, then

$$|\Psi_0\rangle = \sum_n{}' \left(\frac{1}{E_0 - H_0}H_1\right)^n |\Phi_0\rangle_L, \tag{20}$$

$$\Delta E = \sum_n{}' \langle\Phi_0|H_1 \left(\frac{1}{E_0 - H_0}H_1\right)^n |\Phi_0\rangle_C, \tag{21}$$

where $|\Psi_0\rangle$ is normalized as $\langle\Phi_0|\Psi_0\rangle = 1$. The prime in summation represents exclusion of terms with zero denominators and subscripts L and C represent *linked* and *connected* diagrams respectively. The *connected* has the same meaning as in other many-particle theories. However, the *linked* diagrams in the Goldstone's usage are such that even when some diagrams have unconnected parts, if unconnected parts all have external lines, then, the diagrams are treated *linked*.

Let's expand the exact ground state wavefunctional Ψ in terms of the renormalized interaction, $H - \tilde{H}_0$. It gives $\Psi = \sum_n \Psi_n$, where $\Psi_0 = \Psi_G = e^{G_{ij}u_i^* u_j}$. Then, the nth order wavefunctional is given by

$$\Psi_n = \sum{}' \left(\frac{1}{E_0 - \tilde{H}_0}\left(H - \tilde{H}_0\right)\right)_L^n e^{G_{ij}u_i^* u_j}, \tag{22}$$

where $\int D[u^*u]\bar{\Psi}_G\Psi = \int D[u^*u]\bar{\Psi}_G\Psi_G$ is satisfied.

In order to represent explicitly the Grassmann wavefunctional, we use the following useful relations. When capital (small) letters are defined for states above(below) the Fermi see, that is, $A, B, \cdots > k_F$ and $a, b, \cdots < k_F$, we arrive at simple commuting relations as follows,

$$\begin{aligned}
\tilde{a}_A^\dagger \Psi_G &= \Psi_G \sqrt{2}\tilde{u}_A^*, \\
\tilde{a}_A \Psi_G &= \Psi_G \frac{1}{\sqrt{2}}\frac{\partial}{\partial \tilde{u}_A^*}, \\
\tilde{a}_a^\dagger \Psi_G &= \Psi_G \frac{1}{\sqrt{2}}\frac{\partial}{\partial \tilde{u}_a}, \\
\tilde{a}_a \Psi_G &= \Psi_G \sqrt{2}\tilde{u}_a.
\end{aligned} \tag{23}$$

These commuting relations will be shown to reduce calculational efforts substantially in the FJR. We further define $\bar{i}$ and i for notational simplicity as

$$\begin{aligned}
\tilde{a}_i^\dagger \Psi_G &= \Psi_G \bar{i}, \\
\tilde{a}_i \Psi_G &= \Psi_G i,
\end{aligned} \tag{24}$$

where explicit forms of $\bar{i}$ and i in the right-hand side are defined through equation (23) according to their position in the Fermi see. Then, we obtain

$$\begin{aligned}
\Psi_n = \sum{}' & e^{G_{ij}u_i^* u_j} \\
& \times \left(\frac{1}{E_0 - \tilde{H}_0}\left(\tilde{V}_{ijkl}\left(\bar{i}\bar{j}kl\right) - \tilde{\Sigma}_{ij}\left(\bar{i}j\right)\right)\right)_L^n.
\end{aligned} \tag{25}$$

The right-hand side above consists of combinations of Grassmann variables and Grassmann derivatives. We can easily see that if there is no u_i (u_i^*) on the right-hand side of $\frac{\partial}{\partial u_i}$ ($\frac{\partial}{\partial u_i^*}$), it should be zero. *Contraction* is defined as a Grassmann derivative result which is expressed by

$$\overbrace{\bar{i}j} = \frac{\partial}{\partial u_i}u_j\Theta(k_F - i) = \delta_{ij}\Theta(k_F - i), \tag{26}$$

$$\overbrace{i\bar{j}} = \frac{\partial}{\partial u_i^*}u_j^*\Theta(i - k_F) = \delta_{ij}\Theta(i - k_F). \tag{27}$$

Self-contractions of bare interaction, $\tilde{V}_{ijkl}(\bar{i}\bar{j}kl)$ are canceled out by $\tilde{\Sigma}_{ij}(\bar{i}j)$ because

$$\begin{aligned}
\tilde{\Sigma}_{ij}\left(\bar{i}j\right) &= \left(\bar{V}_{kijl} - \bar{V}_{ikjl}\right)\left(U\Omega U^\dagger\right)_{lk}\left(\bar{i}j\right) \\
&= 2\left(\bar{V}_{kijl} - \bar{V}_{ikjl}\right)\delta_{lk}\left(\Theta(k_F - l) - \Theta(l - k_F)\right)\left(\bar{i}j\right).
\end{aligned}$$

Therefore, the interaction term can be simply expressed as

$$\tilde{V}_{ijkl}\left(\bar{i}\bar{j}kl\right) - \tilde{\Sigma}_{ij}\left(\bar{i}j\right) \equiv \tilde{V}_{ijkl}\left(\bar{i}\bar{j}kl\right)', \tag{28}$$

where the prime means that contractions should be performed with elements outside $(\bar{i}\bar{j}kl)$. With this prime notation, the wavefunctional is expressed as

$$\begin{aligned}
\Psi_n = & \left[e^{G_{ij}u_i^* u_j}\sum{}' \frac{-\tilde{V}_{i_1 j_1 k_1 l_1}}{\delta E_1}\frac{-\tilde{V}_{i_2 j_2 k_2 l_2}}{\delta E_2}\cdots\frac{-\tilde{V}_{i_n j_n k_n l_n}}{\delta E_n}\right] \\
& \times \left[\left(\left(\bar{i}_1\bar{j}_1 k_1 l_1\right)'\left(\bar{i}_2\bar{j}_2 k_2 l_2\right)'\cdots\left(\bar{i}_n\bar{j}_n k_n l_n\right)'\right)_L\right],
\end{aligned} \tag{29}$$

where $\delta E_\mu \equiv \sum_{a=\mu}^n(\tilde{\epsilon}_{i_a} + \tilde{\epsilon}_{j_a} - \tilde{\epsilon}_{k_a} - \tilde{\epsilon}_{l_a})$ means excitation energy. Each index in the second square bracket in equation (29) could be a Grassmann variable or a Grassmann derivative. Therefore, in order to be non-zero, all derivatives should be contracted out with corresponding variables and finally remaining elements should be Grassmann variables only. They are summarized as follows: (i) The following steps are repeated for each $m = [0, 2n - 1]$. (ii) A possible set of m pairs of bar and non-bar indices is selected. Self-contractions are forbidden and isolated parts fully connected by contractions are also excluded. (iii) Each contraction has the value given by equation (26) or equation (27). If odd numbers of permutations are performed for contraction, (-1) is multiplied. Remaining indices without contraction are converted by $\bar{i} \to \sqrt{2}u_i^*\Theta(i - k_F)$ and $i \to \sqrt{2}u_i\Theta(k_F - i)$. (iv) All other possible m contractions are performed. Then, Ψ_n is calculated by multiplying the first square bracket term of equation (29) to each contraction term and finally by summing out all indices.

The corresponding nth order energy $\mathcal{E}_n$ ($\Delta E = \sum_n \mathcal{E}_n$) is calculated as

$$\begin{aligned}
\mathcal{E}_n &= \frac{\int D[u^*u]\bar{\Psi}_G\left(H - \tilde{H}_0\right)\Psi_n}{\int D[u^*u]\bar{\Psi}_G\Psi_G} \\
&= \sum{}' \tilde{V}_{i_1 j_1 k_1 l_1}\frac{-\tilde{V}_{i_2 j_2 k_2 l_2}}{\delta E_2}\cdots\frac{-\tilde{V}_{i_n j_n k_n l_n}}{\delta E_n} \\
&\quad \times \left(\left(\bar{i}_1\bar{j}_1 k_1 l_1\right)'\left(\bar{i}_2\bar{j}_2 k_2 l_2\right)'\cdots\left(\bar{i}_n\bar{j}_n k_n l_n\right)'\right)_C,
\end{aligned} \tag{30}$$

where subscript C means that we should perform fully connected contractions.

As well as energy values, Gaussian expectation values of any operators like $\mathcal{O}(\tilde{a}_i^\dagger, \tilde{a}_j, \cdots)$ are also simply expressed in the FJR as follows,

$$\begin{aligned}\langle\mathcal{O}\rangle &= \frac{\int D[u^*u] e^{G_{ij}u_i^*u_j}\mathcal{O}\left(\tilde{a}_i^\dagger, \tilde{a}_j, \cdots\right) e^{G_{ij}u_i^*u_j}}{\int D[u^*u] e^{2G_{ij}u_i^*u_j}} \\ &= \frac{\int D[u^*u] e^{2G_{ij}u_i^*u_j}\mathcal{O}\left(\bar{i}, j, \cdots\right)}{\int D[u^*u] e^{2G_{ij}u_i^*u_j}} \\ &= \mathcal{O}\left(\bar{i}, j, \cdots\right)|_{u^*, u=0}, \end{aligned} \tag{31}$$

where G should be the variational solution, equation (12), and the notational abbreviations, equations (16) and (24) are also used. The third line of equation (31) is equivalent to the full contractions allowing unconnected ones.

As examples, we calculate the first order wavefunctional Ψ_1 and the second order energy $\mathcal{E}_2$. If we use capital (small) letters above(below) the Fermi see in the correction parts, they are represented as

$$\Psi_1 = -4e^{G_{ij}u_i^*u_j}\sum_{A,B,a,b}\frac{\tilde{V}_{ABab}}{\tilde{\epsilon}_A+\tilde{\epsilon}_B-\tilde{\epsilon}_a-\tilde{\epsilon}_b}\tilde{u}_A^*\tilde{u}_B^*\tilde{u}_a\tilde{u}_b, \tag{32}$$

$$\mathcal{E}_1 = 0, \tag{33}$$

$$\mathcal{E}_2 = -2\frac{\tilde{V}_{abAB}\left(\tilde{V}_{ABab}-\tilde{V}_{BAab}\right)}{\tilde{\epsilon}_A+\tilde{\epsilon}_B-\tilde{\epsilon}_a-\tilde{\epsilon}_b}. \tag{34}$$

Here, we note that $\mathcal{E}_1$ is always zero and Ψ_1 has no terms like $\tilde{u}_A^*\tilde{u}_a$ because self-contraction is forbidden.

In the case of electron gas, the quantum numbers are usual wavevector k and spin σ and the interaction has a form,

$$\begin{aligned}V_{ijkl} &\to V_{k_1\sigma_1,k_2\sigma_2,k_3\sigma_3,k_4\sigma_4} \\ &= \frac{1}{2}v(|k_4-k_1|)\delta_{k_1+k_2,k_3+k_4}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}. \end{aligned} \tag{35}$$

For a homogeneous case, the Gaussian variational solution G of equation (12) is already diagonalized by $k\sigma$ representation. Therefore, we can use the Grassmann variables $u_{k\sigma}^*, u_{k\sigma}$ as basis states instead of $\tilde{u}_{k\sigma}^*, \tilde{u}_{k\sigma}$. The energy component of parent Hamiltonian $\tilde{H}_0$ is calculated as $\tilde{\epsilon}_{k\sigma} = (h+\Sigma)_{k\sigma,k\sigma} = \epsilon_k^0 - \sum_q v(q)n_{k+q\sigma}$ where ϵ_k^0 is the free electron energy band and $n_{k\sigma}$ is the Fermi distribution function at zero temperature. Thus, we finally have

$$\begin{aligned}\Psi_1 = &-2e^{G_{k\sigma,k'\sigma'}u_{k\sigma}^*u_{k'\sigma'}} \\ &\times\sum_{kk'q\sigma\sigma'}\frac{v(q)}{\tilde{\epsilon}_{k'+q}+\tilde{\epsilon}_{k-q}-\tilde{\epsilon}_k-\tilde{\epsilon}_{k'}}u_{k'+q\sigma}^*u_{k-q\sigma'}^*u_{k\sigma'}u_{k'\sigma}, \end{aligned} \tag{36}$$

$$\begin{aligned}\mathcal{E}_2 = &-\sum_{kk'q}\frac{v(q)^2n_kn_{k'}(1-n_{k'+q})(1-n_{k-q})}{\tilde{\epsilon}_{k'+q}+\tilde{\epsilon}_{k-q}-\tilde{\epsilon}_k-\tilde{\epsilon}_{k'}} \\ &+\sum_{kk'q}\frac{v(q)v(q')n_{k+q+q'}(1-n_{k+q'})n_k(1-n_{k+q})}{\tilde{\epsilon}_{k+q}+\tilde{\epsilon}_{k+q'}-\tilde{\epsilon}_k-\tilde{\epsilon}_{k+q+q'}}. \end{aligned} \tag{37}$$

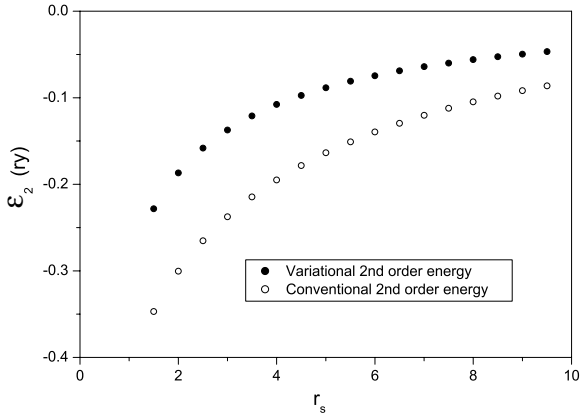

Fig. 1. The second order energy correction (Eq. (36)) per particle for the electron gas with the Yukawa-type interaction. ($\alpha = 1.1$, $\gamma = 1.1$ and $\lambda = 0.1$); filled circles are from the present variational perturbation and open circles from the conventional perturbation.

The first order wavefunctional has a very simple form and higher order ones are also expected to have such simple forms in this variational FJR. We find that the above second order ground state energy is same as the zero temperature limit of the variational perturbation theory [25] previously obtained from a functional integral representation, because Gaussian approximations of both representations employed same variational basis. For a numerical energy value, we modeled an electron gas with a bare kinetic energy $\epsilon_k^0 = \frac{\hbar^2k^2}{2m_e\alpha}$ and a Yukawa-type interaction $v(q) = 4\pi\gamma e^2/V(q^2+(\frac{\lambda}{a_0})^2)$ where m_e and e are the bare electron mass and the charge, and V and a_0 are the system volume and the Bohr's radius respectively. α, γ, and λ are parameters to modulate the mass, charge and interaction range. In Figure 1, we plot the second order contribution to the ground state energy as a function of r_s, which is the average distance ratio between electrons defined by $V = \frac{4}{3}\pi(r_sa_0)^3N$. We find the second order contribution is much reduced in the present variationl procedure than the conventional one which usually gives exceedingly negative result. We are emphasizing that the present formulation should provide a more rapidly convergent ground state energy than in a conventional perturbation result order by order, which is because higher orders are already contained in basis states by the variational calculation. Therefore, each perturbative correction term is expected to have smaller absolute value than corresponding conventional perturbative result as in Figure 1. More rapid convergence will result in a closer value to the true energy.

5 Summary

We have presented a Rayleigh-Schrödinger-Goldstone perturbation formalism using the Floreanini-Jackiw representation on fermion systems. With the aid of Goldstone's expansion, formal expressions for the ground state wavefunctional and the corresponding energy are obtained in

terms of a renormalized interaction. An important aspect of the present result is that the excited state wavefunctionals have the same simple structure as in the Bose systems, thus allowing straightforward perturbation calculations for higher order terms for many Fermion systems. It is also shown that it can be conveniently used for both standard perturbation and variational perturbation schemes. Useful commuting relations between creation and annihilation operators with the Gaussian wavefunctional have been found. As examples, we have calculated the first order wavefunctional and the second order ground state energy of electron gas with Yukawa-type interaction.

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