Variational Jastrow coupled-cluster theory of quantum many-body systems

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We study many-body correlations in the ground state of a general quantum system of bosons or fermions by including an additional Jastrow function in our recently proposed variational coupled-cluster method. Our approach combines the advantages of state-dependent correlations in the coupled-cluster theory and of the strong, short-ranged correlations of the Jastrow function. We apply a generalized linked-cluster expansion for the Jastrow wave function and provide a detailed analysis for practical evaluation of the Hamiltonian expectation value as an energy functional of the Jastrow function and the bare density-distribution functions introduced and calculated in our earlier publications; a simple, first-order energy functional is derived and detailed formulas for the higher-order contributions are provided. Our energy functional does not suffer the divergence as most coupled-cluster calculations often do when applying to Hamiltonians with hardcore potentials. We also discuss possible applications of our technique, including applications to strongly correlated fermion systems.

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I. INTRODUCTION

Most microscopic quantum many-body theories developed over the last five decades can perhaps be broadly divided into two categories, one in real space and the other in momentum (configurational) space. While a real-space many-body theory usually focuses on the interaction potential part of a Hamiltonian and evaluates the Hamiltonian expectation value in a first quantization form, a momentum-space theory often starts from the kinetic part of a Hamiltonian, is a basis of or closely related to many-body perturbation theories, and mostly deals with the Hamiltonian in a second quantization form [1,2]. A typical real-space approach to the ground state of a quantum many-body system is provided by the Jastrow wave function which is constructed by a state-independent two-body correlation function [3]. Systematic (perturbative) techniques based on the Jastrow wave function are now generally referred to as the method of correlated basis functions (CBFs) [4–6]. The CBF method has proved to be efficient in dealing with the strong, short-ranged correlations typified by those in quantum helium liquids [4]. On the other hand, momentum-space many-body theories, due to inclusion of the state-dependent correlations, are capable of producing accurate results for a wide range of quantum systems, such as boson gases [7], quantum antiferromagnets with the Néel order [8], finite nuclei [9], and electron systems such as the electron gas [10], atoms, and molecules [11]. A typical momentum theory is the coupled-cluster method (CCM) in which the wave functions are explicitly constructed by the state-dependent operators [12,13]. State-of-the-art calculations of the CCM with high accuracy have often been carried out in quantum chemistry [14], and recently in quantum spin lattices with the Néel order [15]. Systematic resummations of diagrams in a perturbation theory for boson systems have revealed interesting relations between the two approaches; for example, the hypernetted chain approximation in the CBF method, in fact, contains a consistent resummation of both infinite ring and infinite ladder diagrams of a momentum-space approach [16,17]. It appears that real-space and momentum-space approaches complement each other and unification of these two approaches may provide a quantitative description applicable to a wider range of quantum many-body systems [18], including, in particular, the strongly correlated fermion systems.

We recently extended the CCM to a variational formalism in which the bra and ket states are now Hermitian to one another [19–21], in contrast to the traditional CCM where they are not [22]. We introduced a Hermitian-conjugate pair of the important bare density-distribution functions for practical and systematical calculations; the traditional CCM was shown to correspond to a simple linear approximation in one set of the distribution functions of our variational coupled-cluster method (VCCM). The well-known momentum approaches such as the Bogoliubov theory of boson gas, Anderson's spin-wave theory (SWT), and BCS theory of superconductivity [23] can all be explicitly shown as special low-order approximations in both the ground- and excited-state wave functions of the VCCM. This has been demonstrated by a detailed application to quantum antiferromagnets with the Néel order. The approximations beyond the SWT improve results for the ground-state properties [20]; excitation states in addition to the magnon excitations of the SWT have also been obtained [21]. Furthermore, our calculations for the bare density-distribution functions can be carried out by diagrammatical techniques similar to those employed by the CBF methods. Hence, a bridge between the coupled-cluster theory and the Jastrow theory is built. We therefore believe it is a natural next step to combine the two methods for a unified description. This is our main purpose in this article. Krotscheck, Kümmel, and Zabolitzky made the first attempt in 1980 for fermion systems [18]. They employed the traditional CCM with only the ket state specified and the Jastrow function fixed beforehand; the Hamiltonian eigenequation was used to obtain the ground-state energy and equations for the ket-state coefficients. Here we take the advantage of the recent progress in the coupled-cluster theory and employ explicit ket and bra states of the VCCM and calculate the distribution functions in terms of these ket- and bra-state coefficients; the energy functional is derived in terms of the distribution functions and the Jastrow function.

We focus here on the formal development of our approach and organize this article as follows. In Sec. II we introduce our correlated wave functions and their distribution functions. The generalized linked-cluster expansion technique is employed for calculations of the generating functional in terms of the bare distribution functions. In Sec. III we evaluate the Hamiltonian expectation value using Jackson-Feenberg transformations; a first-order energy functional is derived and formulas for higher-order contributions are provided. We conclude in Sec. IV with a summary and discussion on the relations between our approach and other many-body theories, and on possible applications using our approach.

II. DISTRIBUTION FUNCTIONS

As proposed earlier [20], we consider a general variational wave function by adding a Jastrow correlation operator on top of the Coester state $|\Psi^c\rangle$

$$|\Psi\rangle = e^{S^0/2}|\Psi^c\rangle \tag{1}$$

and we use the following notation:

$$\langle\tilde{\Psi}| = \langle\tilde{\Psi}^c|e^{S^0/2} \tag{2}$$

for the bra state. In Eqs. (1) and (2), the Hermitian operator S^0 is the Jastrow correlation operator, and is given in terms of field operators as [2]

$$S^0 = \frac{1}{2}\int dx_1 dx_2 \psi^\dagger(x_1)\psi^\dagger(x_2)u(x_1,x_2)\psi(x_2)\psi(x_1), \tag{3}$$

where field operators $\psi^\dagger(x)$ and $\psi(x)$ obey the usual boson or fermion commutation relations, $u(x_1,x_2)$ is a local, symmetric function $u(x_1,x_2)=u(x_2,x_1)$, and x are particle coordinates including spin degrees of freedom. We also require that $u(x_1,x_2)$ is bound and short-ranged in real space. We do not include in S^0 any single-body operator as it can be easily absorbed in the Coester states to be defined next. The boson or fermion symmetry is contained in the Coester states by definition. More specifically, the Coester ket state is given by, using the convenient notation invented by Arponen and Bishop [24],

$$|\Psi^c\rangle = e^S|\Phi\rangle, \quad S = \sum_I F_I C_I^\dagger, \tag{4}$$

where S is constructed by the so-called configurational creation operators $C_I^\dagger$ which are defined with respect to the model state $|\Phi\rangle$ with the nominal index I labeling multiparticle excitation states from the model state $|\Phi\rangle$, with F_I often referred to as the correlation coefficients. The Coester bra state $\langle\tilde{\Psi}^c|$ is given by the Hermitian conjugate of the ket state

$$\langle\tilde{\Psi}^c| = \langle\Phi|e^{\tilde{S}}, \quad \tilde{S} = \sum_I \tilde{F}_I C_I \tag{5}$$

in our VCCM. In the traditional CCM, however, the bra state is parametrized differently from the ket state and is written as [22]

$$\langle\tilde{\Psi}^c| = \langle\Phi|\tilde{S}'e^{-S}, \quad \tilde{S}' = 1 + \sum_I \tilde{F}'_I C_I, \tag{6}$$

where S is defined as in the ket state of Eq. (4) and $\tilde{F}'_I$ is the bra state coefficients which, in general, are not Hermitian conjugates of F_I. As discussed in the Appendix, the CCM states violate the condition for application of the generalized linked-cluster expansion due to the linear construction of the bra state. We therefore will not discuss the CCM further and focus only on the VCCM basis of Eqs. (4) and (5). Clearly, the natural variational parameters are $(F,\tilde{F},u)$ in the VCCM basis, where we have used the notations $F=\{F_I\}$, $\tilde{F}=\{\tilde{F}_I\}$, and $u=u(x_1,x_2)$. In principle, if these Coester states are exact [namely, all configurations are included in the summations over all I indices in Eqs. (4) and (5)], the parameter u is redundant. However, as we always need to make a finite truncation approximation in the summations over I indices in any practical application and it is well known that the Coester states in a finite truncation approximation are not efficient in dealing with the strong, short-ranged correlations, the two-body Jastrow function $u(x_1,x_2)$ is a useful, important variational parameter in a real application. We hence always assume that the summations in Eqs. (4) and (5) are within the subset of a truncation approximation. One of such truncations is the so-called SUBm approximation in which we retain up to m-body creation operators only.

Our basic strategy for calculations is to evaluate the generating functional W of Eqs. (1) and (2),

$$W = \ln\langle\tilde{\Psi}|\Psi\rangle = W^c + W^u, \tag{7}$$

where W^c is the generating function for the pure Coester states without the Jastrow operator

$$W^c = \ln\langle\tilde{\Psi}^c|\Psi^c\rangle \tag{8}$$

and W^u is the remainder containing the u function

$$W^u = \ln\langle e^{S^0}\rangle^c, \quad \langle e^{S^0}\rangle^c = \frac{\langle\tilde{\Psi}^c|e^{S^0}|\Psi^c\rangle}{\langle\tilde{\Psi}^c|\Psi^c\rangle}. \tag{9}$$

The general strategy for calculating $W^c=W^c(F,\tilde{F})$ was discussed in our earlier papers and detailed calculations were demonstrated in the spin-lattice application [19,20]. Briefly, we first introduce the Hermitian-conjugate pair of the bare density-distribution functions

$$\tilde{g}_I^c = \langle C_I^\dagger\rangle^c = \frac{\partial W^c}{\partial F_I}, \quad g_I^c = \langle C_I\rangle^c = \frac{\partial W^c}{\partial \tilde{F}_I}, \tag{10}$$

where the expectation values $\langle\cdots\rangle^c$ are calculated using the Coester states of Eqs. (4) and (5); any physical quantity is expressed in terms of these distribution functions; these distribution functions are then calculated either by the algebraic technique [19] or by the diagrammatic technique [20]. In particular, in the diagrammatic approach, many techniques employed by the CBF method are also applicable here. For example, the coefficients $\tilde{F}_I$ can be replaced in every diagram of W^c expansion by the bare distribution functions $\tilde{g}_I^c$ after resummations of infinite ring diagrams. In general, the en-

ergy expectation value can be expressed as a functional polynomial in F and $\tilde{g}^c$ as $E^c=E^c(F,\tilde{g}^c)$; and the variational equations can then be derived by the functional derivatives in $E^c(F,\tilde{g}^c)$ [25].

In terms of the distribution functions as discussed above, we now consider evaluating $\langle e^{S^0}\rangle^c$ of Eq. (9). After cluster expansion of the Jastrow part of the wave functions, we apply the generalized linked-cluster theorem discussed in the Appendix in a similar fashion as the traditional Jastrow theory [2,26] to obtain

$$W^u = \ln\langle e^{S^0}\rangle^c = \sum_{n=2} \frac{1}{n!}\int dx_1 \cdots dx_n [Z_n \rho_n^c]_L, \tag{11}$$

where $Z_n(Y)$ are the n-body Yvon-Mayer functions of the bound function $Y_{12}=e^{u(x_1,x_2)}-1$, ρ_n^c is the n-body density distribution functions of the Coester states, and the notations $[\cdots]_L$ denote that only the linked components of the products are included. In deriving Eq. (11) in the Appendix, we have assumed that the Coester states satisfy the cluster-decomposition properties (i.e., the higher-order ρ_n^c are given by a sum of products of the lower-order ones plus a nondecomposable core). While this is true in a SUB2 approximation in our spin lattice application and the SUB2 approximation for the Bose gas and BCS superconductors [20,27], we are not able to provide a general proof for a general SUBm approximation (or even the SUB2 approximation for a general fermion system) without the details of truncation approximations employed in the Coester states in a real application. Hence by using Eq. (11), we have assumed its validity for the truncation approximations of the Coester states employed. In the following discussion this assumption is understood and we will examine this property in real applications. The following analysis for calculating ρ_n^c in terms of F_I and $\tilde{g}_I^c$ shows such examination causing no major difficulty.

As all the Yvon-Mayer diagrams in Z_2 and Z_3 are linked, we simply have

$$[Z_2\rho_2^c]_L = Y_{12}\rho_2^c, \quad \rho_2^c(x_1,x_2) = \langle \psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2)\psi(x_1)\rangle^c \tag{12}$$

for the two-body cluster contribution and

$$[Z_3\rho_3^c]_L = (Y_{12}Y_{23} + Y_{23}Y_{31} + Y_{31}Y_{12} + Y_{12}Y_{23}Y_{31})\rho_3^c \tag{13}$$

for the three-body cluster contributions with ρ_3^c as the three-body distribution function in the Coester states. From the four-body function $Z_4(Y)$ and onward, however, there are unlinked Yvon-Mayer diagrams which are to be included in the product $[Z_n\rho_n^c]_L$ only after multiplying with the terms of ρ_n^c to form the linked components, and details of which will depend on applications with a truncation approximation in the Coester states. There is clearly a trade-off between the order of the linked-cluster expansion and the order of the truncation approximation of the Coester states. We hope to get experience in real applications in the future. Importantly, these density-distribution functions can be calculated in terms of F and $\tilde{g}^c$; by using the linearity theorem of the VCCM [21], we can show that all ρ_n^c functions contain only up to linear terms in $\tilde{g}^c$ and finite-order terms in F. As a demonstration, we consider the two-body function ρ_2^c

$$\rho_2^c(x_1,x_2) = \langle A_2\rangle^c = \frac{1}{\langle\tilde{\Psi}^c|\Psi^c\rangle}\langle\tilde{\Psi}^c|A_2 e^S|\Phi\rangle = \frac{1}{\langle\tilde{\Psi}^c|\Psi^c\rangle}\langle\tilde{\Psi}^c|e^S\bar{A}_2|\Phi\rangle, \tag{14}$$

where $A_2=\psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2)\psi(x_1)$ and $\bar{A}_2=e^{-S}A_2e^S$. Using the nested commutation series [12,19], it is easy to show that evaluation of $\bar{A}_2|\Phi\rangle$ in general leaves only a constant and creation operators acting on $|\Phi\rangle$, namely,

$$\bar{A}_2|\Phi\rangle = [X_{2,0}(F;x_1,x_2) + \sum_I X_{2,I}(F;x_1,x_2)C_I^\dagger]|\Phi\rangle, \tag{15}$$

where $X_{2,0}$ and $X_{2,I}$ are two-body functions containing up to fourth-order terms in F. Therefore, using the definition of Eq. (10)

$$\rho_2^c(x_1,x_2) = X_{2,0}(F;x_1,x_2) + \sum_I X_{2,I}(F;x_1,x_2)\tilde{g}_I^c. \tag{16}$$

In similar fashion, we derive

$$\rho_n^c = X_{n,0} + \sum_I X_{n,I}\tilde{g}_I^c \tag{17}$$

for the n-body density-distribution function of the Coester states. Therefore, the linked-cluster contribution of Eq. (11) is written as

$$W^u = \frac{1}{2}\int dx_1dx_2Z_2[X_{2,0} + \sum_I X_{2,I}\tilde{g}_I^c] + \frac{1}{6}\int dx_1dx_2dx_3Z_3\left[X_{3,0} + \sum_I X_{3,I}\tilde{g}_I^c\right] + \cdots. \tag{18}$$

Before we consider the density-distribution functions of the Jastrow-Coester states of Eqs. (1) and (2), we need to define biased distribution functions as

$$\tilde{g}_I \equiv \frac{1}{\langle\tilde{\Psi}|\Psi\rangle}\langle\tilde{\Psi}^c|e^{S^0}C_I^\dagger|\Psi^c\rangle, \quad g_I \equiv \frac{1}{\langle\tilde{\Psi}|\Psi\rangle}\langle\tilde{\Psi}^c|C_Ie^{S^0}|\Psi^c\rangle. \tag{19}$$

They are so called because they are not defined usually as $\langle C_I^\dagger\rangle$, and clearly $\tilde{g}_I\neq\langle C_I^\dagger\rangle$ due to the fact that $C_I^\dagger$ and $S^0/2$ do not commute in general. These biased distribution functions can be calculated by the functional derivatives of the generating functional of Eq. (7) as

$$\tilde{g}_I = \frac{\partial W}{\partial F_I} = \tilde{g}_I^c + \frac{\partial W^u}{\partial F_I}, \tag{20}$$

where the functional derivative $\partial W^u/\partial F_I$ can be calculated using Eq. (18).

Using the fact that $S^0/2$ commutes with density operator $\psi^\dagger(x)\psi(x)$, the single-particle density function $\rho_1(x)=\langle\psi^\dagger(x)\psi(x)\rangle$ can then be calculated as

$$\rho_1(x) = \frac{1}{\langle\tilde{\Psi}|\Psi\rangle}\langle\tilde{\Psi}^c|e^{S^0}\psi^\dagger(x)\psi(x)e^S|\Phi\rangle$$
$$= \rho_1^c(x) + \sum_I X_{1,I}(F;x)\frac{\partial W^u}{\partial F_I}, \tag{21}$$

where we have used Eq. (17) and where $\rho_1^c(x)$ is the one-body density-distribution function of the Coester states. The two-body density-distribution function of states of Eqs. (1) and (2) can be calculated in a similar fashion as ρ_1 shown above. We take a more efficient calculation by the functional derivative as $\rho_2(x_1,x_2)=2\partial W/\partial u(x_1,x_2)$ which involves only the Yvon-Mayor functions Z_n and it is easy to derive as

$$\rho_2(x_1,x_2) = e^{u(x_1,x_2)}\rho_2^c(x_1,x_2) + \frac{1}{3}\int dx_1'dx_2'dx_3'\frac{\partial Z_3(x_1',x_2',x_3')}{\partial u(x_1,x_2)}\rho_3^c(x_1',x_2',x_3') + \cdots. \tag{22}$$

We can see immediately that the short-ranged correlation function $u(x_1,x_2)$ will play an important role for applications to the strongly correlated systems, where the pure Coester states are known to be inefficient.

III. EVALUATION OF HAMILTONIAN EXPECTATION VALUE

In evaluating a general Hamiltonian expectation value, we first notice that the kinetic part of a Hamiltonian in general does not commute with the Jastrow operator $S^0/2$ in our states of Eqs. (1) and (2). In real space, however, the kinetic operator contains only second-order derivatives in particle coordinates. We want to take this advantage by expressing our states in real space for the first part of the calculations. As can be shown, the wave functions of the Jastrow-Coester states of Eqs. (1) and (2) in real space are given by a product

$$\Psi = \Psi^u\Psi^c, \quad \tilde{\Psi} = \tilde{\Psi}^c\Psi^u, \tag{23}$$

where $\Psi^u=e^{U/2}=\exp[\Sigma_{i<j}u(x_i,x_j)/2]$ is the familiar Jastrow wave function and $\Psi^c(x_1,\ldots,x_N)$ and $\tilde{\Psi}^c(x_1,\ldots,x_N)$ are real-space wave functions of the corresponding Coester ket and bra states, respectively. In general, we do not need to know the explicit functional forms of Ψ^c and $\tilde{\Psi}^c$ as our calculations involving them are always carried out in a second quantization form as we show below. It is interesting nevertheless to know that in a low-order SUB2 approximation, many-body function Ψ^c is known explicitly as independent pair functions for boson gas [28] or BCS superconductors [29].

Evaluating the kinetic energy involving the Jastrow function is helped by the Jackson-Feenberg transformation [2]. In particular, it can be shown that

$$\int dX\tilde{\Psi}\nabla_i^2\Psi = \int dX\left[\tilde{\Psi}^c e^U\nabla_i^2\Psi^c + \frac{1}{4}\tilde{\Psi}^c e^U(\nabla_i^2U)\Psi^c - \frac{1}{4}e^U\nabla_i^2(\tilde{\Psi}^c\Psi^c)\right] \tag{24}$$

and another equivalent expression

$$\int dX\tilde{\Psi}\nabla_i^2\Psi = \int dX\tilde{\Psi}^c e^U\left[\nabla_i^2 + \frac{1}{4}(\nabla_i^2U) + \frac{1}{2}(\nabla_iU)\cdot\nabla_i\right]\Psi^c, \tag{25}$$

where $dX=dx_1dx_2\cdots dx_N$. Both the above transformations involve one- and two-body density-distribution functions only, and the Jastrow factor e^U appears on the left of the derivatives. The biased distribution functions defined in Eq. (19) are then applicable. The expectation value of a general Hamiltonian with an external field (and/or chemical potential) $A(x)$ and a pair-interaction potential $v(x_i,x_j)$ is calculated as, using Eq. (24),

$$E_1 = \int dx\left[-\frac{\hbar^2}{2m}\rho_1'(x) + \hat{A}_{\text{eff}}(x)\rho_1(x)\right] + \frac{1}{2}\int dx_1dx_2v_{\text{eff}}(x_1,x_2)\rho_2, \tag{26}$$

where ρ_1 and ρ_2 are the one- and two-body density-distribution functions, $\hat{A}_{\text{eff}}(x)=A(x)-\frac{\hbar^2}{8m}(\nabla^c)^2$ is the effective external field operator with operator ∇^c defined as applying to the Coester states only; $v_{\text{eff}}=v(x_1,x_2)-\frac{\hbar^2}{8m}(\nabla_1^2+\nabla_2^2)u(x_1,x_2)$ is the effective potential, and ρ_1' is the one-body density function derived from the first term of Eq. (24) and is written in the second quantization form as

$$\rho_1'(x) = \frac{1}{\langle\tilde{\Psi}|\Psi\rangle}\langle\tilde{\Psi}^c|e^{S^0}T_1|\Psi^c\rangle, \quad T_1(x) = \psi^\dagger(x)\nabla^2\psi(x). \tag{27}$$

The other equivalent expression for the energy functional is obtained by using Eq. (25),

$$E_2 = \int dx\left[-\frac{\hbar^2}{2m}\rho_1'(x) + A(x)\rho_1(x)\right] + \frac{1}{2}\int dx_1dx_2\left[v_{\text{eff}}(x_1,x_2)\rho_2 - \frac{\hbar^2}{4m}\rho_2'(u)\right], \tag{28}$$

where $\rho_2'(u)$ is the two-body density functions derived from the third integral of Eq. (25),

$$\rho_2'(u) = \frac{1}{\langle\tilde{\Psi}|\Psi\rangle}\langle\tilde{\Psi}^c|e^{S^0}T_2(u)|\Psi^c\rangle, \tag{29}$$

with the two-body operator $T_2(u)$ given by

$$T_2(u) = \psi^\dagger(x_1)\psi^\dagger(x_2)[\nabla_1u(x_1,x_2)\cdot\nabla_1 + \nabla_2u(x_1,x_2)\cdot\nabla_2]\psi(x_2)\psi(x_1). \tag{30}$$

The difference between the two energy functionals derived above is that in E_1 of Eq. (26) we need to take care of the

operator ∇^c which applies only to the Coester states and in E_2 of Eq. (28) we need to calculate the two-body density function $\rho_2'(u)$. We hope to get experience in real applications as to which form is more practical. The density-distribution functions ρ_1 and ρ_2 were calculated earlier by Eqs. (21) and (22). Calculations of ρ_1' and ρ_2' follow the similar fashion. We hence obtain

$$\rho_n' = \rho_n'^c(x) + \sum_I X_{n,I}'(F;x)\frac{\partial W^u}{\partial F_I}, \quad n = 1,2, \tag{31}$$

where $\rho_n'^c = \langle T_n \rangle^c$ and $X_{n,I}'$ are obtained in the similar fashion as before in Eq. (17).

Equations (31) together with density distributions of Eq. (21) and (22) are all we need for calculating the two equivalent energy functionals of Eqs. (26) and (28). Denoting the three terms from the first term of ρ_1', ρ_1, and ρ_2 as ϵ, and the higher-order remainders as ΔE_l with $l=1,2$ for the two energy functionals, we rewrite the energy functionals of Eqs. (26) and (28) as

$$E_l(F,\tilde{g}^c,u) = \epsilon(F,\tilde{g}^c,u) + \Delta E_l(F,\tilde{g}^c,u), \quad l = 1,2, \tag{32}$$

where the same $\epsilon(F,\tilde{g}^c,u)$ is given by

$$\epsilon = K_1^c + \int dx A(x)\rho_1^c(x) + \frac{1}{2}\int dx_1 dx_2 v_{\text{eff}}(x_1,x_2)e^{u(x_1,x_2)}\rho_2^c(x_1,x_2), \tag{33}$$

with $K_1^c = -(\hbar^2/2m)\langle T_1 \rangle^c$ for the kinetic energy of the VCCM states. We notice that this first-order energy functional ϵ is nothing but the energy functional of the VCCM after replacing the bare potential v by the new potential $V = v_{\text{eff}}e^u$, namely,

$$\epsilon(F,\tilde{g}^c,u) = E^c(F,\tilde{g}^c)\big|_{v\to V},$$

$$V(v,u) = \left[v(x_1,x_2) - \frac{\hbar^2}{8m}(\nabla_1^2 + \nabla_2^2)u(x_1,x_2) \right] e^{u(x_1,x_2)}, \tag{34}$$

where $E^c(F,\tilde{g}^c)$ is the energy functional of the pure VCCM states. This is convenient indeed as no new calculations are needed after the VCCM calculations have been done. We notice also that ϵ of Eq. (33) or (34) involves only the first-order approximation in the cluster expansion of the Jastrow function, and it does not specify the approximations such as the SUBm truncation in the Coester states which will be needed for any practical calculations of the density functions ρ_1^c and ρ_2^c in Eq. (33).

IV. SUMMARY AND DISCUSSION

In summary, we have calculated the Hamiltonian expectation value of a general quantum many-body system as energy functionals of the Coester-state coefficients $\{F_I\}$, bare distribution functions $\{\tilde{g}_I^c\}$ of the Coester states, and the Jastrow correlation function $u(x_1,x_2)$. Two equivalent energy functionals are derived by Eqs. (26) and (28). A simple, first-order energy functional of Eq. (34) from both expressions is derived as the usual VCCM energy functional but with a new potential $V(v,u) = v_{\text{eff}}e^u$. The formulas for practical calculations of the higher-order terms are also provided in details for calculations. It is easy to see that, due to the short-ranged Jastrow factor, our energy functionals do not suffer the divergence as most coupled-cluster calculations often do when potential $v(x_1,x_2)$ approaches hardcore potentials. It will be a straightforward extension of an earlier work of Fantoni *et al.* [28], which corresponds to the VCCM SUB2 calculations for soft-core potentials, and will be interesting to demonstrate the convergence for the ground-state energy even in the hard-core limit. We wish to report this result soon.

Similar wave functions to Eqs. (23) were employed by Owen for a study of the spin-dependent correlations in nuclear matter [30]. In particular, Ψ^c was approximated by the product of an independent pair function (spin dependent) and the Slater determinant; and in the cluster expansion, the Jastrow function and the independent pair function are treated together. This differs from our approach. Our calculations involving the Coester states are always in a second quantization form and are applicable to the higher-order truncation approximations. There are a few earlier works [31,32] extending the traditional Jastrow wave function to include state-dependent correlation functions. The obvious difficulty in these approaches lies in the fact that these state-dependent operators do not commute with one another and this problem was also discussed in detail by Krotscheck [33]. As pointed out in Ref. [18], the advantage of combining the state-independent Jastrow function and the state-dependent Coester states as given by Eqs. (1) and (2) over the traditional approaches is that all state-dependent operators in the Coester states commute with one another. We believe this advantage of our approach may increase the accuracy for numerical results. Clearly, our approach presented here provides an alternative method for calculating the state-dependent many-body correlations in nuclear problems.

We are also encouraged by the numerical results of computer simulations [34] using the wave function similar to Eq. (23). In particular, the Coester-state part of total wave functions are represented by a linear approximation in real space for finite systems. Numerical results clearly demonstrate significant improvements for the ground-state energy of finite helium-4 clusters over the pure Jastrow wave function when including (linear-approximated) Coester states in the SUB2 and SUB3 levels. Again, it will be interesting to apply our analytical approach presented here to such systems, particularly for the large clusters and extended systems where the linear approximation in the Coester states in Ref. [34] will not be appropriate.

On the technical aspect, it is interesting to compare our energy functional $E(F,\tilde{g}^c,u)$ with the counterpart in the traditional Jastrow theory $E(a,u)$, where a is the one-body function. Clearly, the missing state-dependent correlations in $E(a,u)$ are now included in our $E(F,\tilde{g}^c,u)$ in terms of F and $\tilde{g}^c$. However, a typical calculation of the Jastrow theory practiced today mostly includes resummation of all cluster terms of the linked cluster expansion by the hypernetted chain (HNC) approximation for bosons or Fermi-HNC approximation for fermions [5,6], and one optimization route for the

boson system is provided by the pair-phonon analysis (PPA) of Campbell and Feenberg [35]. This is possible as the reference states are the product of the single-particle wave functions. In our cluster expansion calculations, the reference state is the Coester states which already contain rich multiparticle correlations including, in particular, the correct long-ranged correlations such as in the SUB2 approximation. The introduction of the Jastrow function is to provide a correct description of the strong, short-ranged correlations and we expect such a scheme may provide reasonable results even if we include a first few cluster terms. It will also be interesting to investigate the relations between our approach and the PPA of Campbell and Feenberg.

We are also applying our Jastrow coupled-cluster method to the spin-lattice problems which, in fact, motivated this approach in the first place. In particular, we believe that the Jastrow-types of correlations (i.e., $S^0 \rightarrow \Sigma_{ij} f_{ij} s_i^z s_j^z$ with s^z as the z component of the angular momentum operator) are important in the low-dimensional systems as discussed earlier [20,21], and the one-dimensional antiferromagnetic Heisenberg model is in fact a strongly correlated system for which the SWT fails. Our long term projects also include investigation of helium-3 quantum liquids which still represent a challenge to the existing many-body theories [36].

APPENDIX: Δ REPRESENTATION AND GENERALIZED LINKED-CLUSTER EXPANSION

It is straightforward to show that the states of Eqs. (1) and (2) correspond to the following real space wave functions:

$$\Psi(x_1, \ldots, x_N) = \Psi^u \Psi^c, \quad \tilde{\Psi}(x_1, \ldots, x_N) = \tilde{\Psi}^c \Psi^u, \quad \text{(A1)}$$

where $\Psi^u = e^{U/2} = \exp[\Sigma_{i<j} u(x_i, x_j)/2]$ is the familiar Jastrow wave function and $\Psi^c(x_1, \ldots, x_N)$ and $\tilde{\Psi}^c(x_1, \ldots, x_N)$ are the corresponding Coester state functions in real space. The Coester wave functions Ψ^c and $\tilde{\Psi}^c$ obey proper symmetry; namely, they are antisymmetric for fermions and symmetric for bosons under the exchange of any pair $x_i \rightleftharpoons x_j$. We do not need to know their explicit functional forms as our later calculations are always carried out in a second quantization form of momentum space.

We follow a similar analysis for the evaluation of Eq. (11) as in the traditional Jastrow theory [2,16]. After the usual cluster expansion of the Jastrow wave function in terms of Yvon-Mayor functions $Z_n(Y)$ with the bound function $Y_{12} = e^{u(x_1,x_2)} - 1$,

$$e^U = 1 + \sum_{i<j} Z_2(x_i, x_j) + \sum_{i<j<k} Z_3(x_i, x_j, x_k) + \cdots, \quad \text{(A2)}$$

the expectation in Eq. (11) is written as

$$\langle e^{S^0} \rangle^c = 1 + \frac{1}{I_c} \sum_{n=2} \frac{N!}{(N-n)!\, n!} \times \int dx_1 \cdots dx_N \tilde{\Psi}^c Z_n(x_1, \ldots, x_n) \Psi^c = 1 + \sum_{n=2} \frac{1}{n!} \int dx_1 \cdots dx_n Z_n \rho_n^c, \quad \text{(A3)}$$

where $I_c = \langle \Psi^c | \Psi^c \rangle$ is the normalization integral, the first few Z_n are given by

$$Z_2 = Y_{12}, \quad Z_3 = Y_{12} Y_{23} + Y_{23} Y_{31} + Y_{31} Y_{12} + Y_{12} Y_{23} Y_{31}, \quad \text{(A4)}$$

etc., and ρ_n^c is the n-body density-distribution functions

$$\rho_n^c = \langle \psi^\dagger(x_1) \cdots \psi^\dagger(x_n) \psi(x_n) \cdots \psi(x_1) \rangle^c. \quad \text{(A5)}$$

Evaluation of ρ_n^c of the Coester states in terms of the bare distribution function $\tilde{g}^c$ were discussed in details by Eqs. (14)–(17) of Sec. II. Here we need to consider their cluster properties in order to apply the linked-cluster theorem. For this purpose, we introduce the so-called Δ representation discussed as follows. We consider evaluation of n-body distribution functions in the state $|\Psi^d\rangle$ with the following cluster decomposition property: any higher-order ρ_n^d can be written as products of the lower order ρ_m^d with $m = 1, 2, \ldots, n-1$, plus a nondecomposable core Δ_n. Let us demonstrate this property in details. We start with the one-body density-distribution matrix, also the one-body core matrix by definition,

$$\rho_1^d(x; x') = \langle \psi^\dagger(x) \psi(x') \rangle^d = \Delta_1(x; x'), \quad \text{(A6)}$$

where we have used the usual notation $\langle \cdots \rangle^d$ for the expectation value in state $|\Psi^d\rangle$. The two-body distribution (diagonal) function $\rho_2^d = \langle \psi^\dagger(x_1) \psi^\dagger(x_2) \psi(x_2) \psi(x_1) \rangle^d$ is then given by, using this decomposition property,

$$\rho_2^d = \Delta_1(x_1; x_1) \Delta_1(x_2; x_2) - \Delta_1(x_1; x_2) \Delta_1(x_2; x_1) + \Delta_2(x_1, x_2; x_1, x_2), \quad \text{(A7)}$$

where the first two terms are as given before for the fermions (for bosons, all terms have positive sign) and Δ_2 is the two-body nondecomposable core tensor. We can also write Eq. (A7) in a symbolic notation as

$$\rho_2^d = \Delta_1 * \Delta_1 + \Delta_2. \quad \text{(A8)}$$

In a similar way, the three-body density-distribution function is then given by

$$\rho_3^d = \Delta_1 * \Delta_1 * \Delta_1 + \Delta_1 * \Delta_2 + \Delta_3, \quad \text{(A9)}$$

where Δ_3 is the nondecomposable core tensor. All terms from the product $\Delta_1 * \Delta_1 * \Delta_1$ of Eq. (A9) were given in details as diagrams in the references quoted earlier. Similar to these diagrams, the new contributions in products $\Delta_1 * \Delta_2$ also include both unlinked terms such as $\Delta_1(x_1; x_1) \Delta_1(x_2, x_3; x_2, x_3)$, and linked terms such as $\Delta_1(x_1; x_3) \Delta_2(x_2, x_3; x_2, x_1)$. The rules for sign and for the symbolic product $(*)$ can also be defined in a similar fashion as before and we will discuss them in details somewhere else. Clearly, such decomposition can be carried to higher order.

Using the cluster decomposition property as discussed above, we have the key ingredient for the linked-cluster expansion; namely, all contributions in the product $Z_n \rho_n^d$ can be represented by clusters of diagrams. If we denote the linked diagrams as Γ_A, Γ_B, etc., a contribution in similar cluster expansion as Eq. (A3) for the state $|\Psi^d\rangle$ can then be written as

$$\Gamma = (\Gamma_A)^{\nu_A}(\Gamma_B)^{\nu_B}\cdots, \quad A \neq B, \tag{A10}$$

with coefficients

$$N(A,B,\ldots) = \frac{n!}{(n_A!)^{\nu_A}(n_B!)^{\nu_B}\cdots}, \tag{A11}$$

giving by the number of distributing the linked part along the n points of the diagram. We therefore have

$$\sum_{\Gamma_n}\frac{1}{n!}\Gamma_n = \sum_{A,B,\ldots}\frac{1}{n!}N(A,B,\ldots)(\Gamma_A)^{\nu_A}(\Gamma_B)^{\nu_B}\cdots$$
$$= \exp(\Gamma_A/n_A\,! + \Gamma_B/n_B\,! + \cdots). \tag{A12}$$

Hence we have the following generalized linked-cluster expansion for the state $|\Psi^d\rangle$,

$$\ln\langle e^{S^0}\rangle^d = \sum_{n=2}\frac{1}{n!}\int dx_1\cdots dx_n[Z_n\rho_n^d]_L, \tag{A13}$$

where the notation $[Z_n\rho_n^d]_L$ denotes the contributions to $Z_n\rho_n^d$ by the linked diagrams only. Since all terms in Z_2 and Z_3 are linked, the first two terms in Eq. (A13) are independent of the diagram structures of ρ_2^d and ρ_3^d and we write

$$\ln\langle e^{S^0}\rangle^d = \frac{1}{2}\int dx_1dx_2Z_2\rho_2^d + \frac{1}{6}\int dx_1dx_2dx_3Z_3\rho_3^d$$
$$+ \sum_{n=4}\frac{1}{n!}\int dx_1\cdots dx_n[Z_n\rho_n^d]_L. \tag{A14}$$

From $n=4$ and onward, we need to know the diagram details of ρ_n^d for calculating their contributions.

In order to apply the generalized linked-cluster expansion of Eq. (A14) to our Coester states, we need to prove that the Coester states satisfy the cluster decomposition property as discussed above. In our earlier VCCM calculation for spin lattices, we have shown indeed the Coester states satisfy such property in a SUB2 approximation employed, where arbitrary order distribution functions can be calculated by the simple functional derivative $\partial\tilde{g}_{i'j'}/\partial F_{ij} = \tilde{g}_{ij'}\tilde{g}_{i'j}$ and these bare distribution functions correspond to the density-distribution matrices (similar analysis also applied to the SUB2 state for the Bose gas and the BCS superconductors) [20,27]. We also notice that a similar so-called SUBm truncation approximation in the Δ representation can be defined as the approximation retaining up to m core distribution tensors only (i.e., $\Delta_n=0$ for $n>m$). It is intuitive to relate the real-space cluster parametrization by the core distribution tensor $\{\Delta_n\}$ in the Δ representation and momentum-space parametrization by $\{F_I,\tilde{g}_I\}$ in the Coester states; the Coester representation provides a practical way to calculate these core tensors. We will not intend to provide a general proof that the Coester states in any truncation approximation will satisfy the cluster decomposition property. We will adopt a practical strategy to apply the linked-cluster expansion formula of Eq. (A14) to the Coester states in real applications and to examine the cluster property in the particular truncation approximation employed. We believe this will not cause a major difficulty as we use the relations between the full distribution functions ρ_n^c and the bare distribution functions $\tilde{g}_I^c$ as given by Eqs. (17).

We would also like to point out that the traditional CCM states certainly fail the cluster decomposition property due to the linear construction of the bra state of Eq. (6). This can be easily seen as any expectation in the CCM is always linear in the bra state coefficients, contradictory to the cluster decomposition property. Therefore, the generalized linked-cluster expansion of Eq. (A14) cannot be applied to the CCM states.

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