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Coupled-cluster many-body theory in a correlated basis

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The correlated-basis-functions method of Feenberg and the coupled-cluster formalism of Coester and Kümmel are joined to form a new ground-state many-body method combining the advantages of both older methods and avoiding their disadvantages. From the point of view of the correlated-basis-functions method, coupled-cluster theory is used to sum the perturbation series partially to arbitrary order. From the point of view of the coupled-cluster method, correlated basis functions are used to take out the repulsive core of the two-body interaction in order to allow more efficient truncation schemes. It is found that powerful renormalizations are possible. Explicit equations are given for the two-body subsystems embodying generalized Bethe-Goldstone and random-phase equations summing, in the correlated basis, ladder and ring diagrams to arbitrary order.

I. INTRODUCTION

We describe in this paper the development of a combination of two quite different many-body techniques, the variational method[1,2] and the coupled-cluster [or exp(S)] theory[3-5] for the calculation of ground-state properties of interacting Fermi systems. Our goal is a quantitative description of extended systems like nuclear matter, neutron matter, or liquid ^{3}He, and in future work also finite systems like nuclei or droplets, interacting via realistic forces. For this purpose we generalize the coupled-cluster [or exp(S)] theory in such a way that it is able to deal with correlated, nonorthogonal wave functions. Thus, we will provide a link between two quite different many-body techniques: the variational method and perturbation theoretical approaches.

The variational method[1,2] approximates the ground-state wave function in the form

$$|\psi_0^-\rangle = F|\Phi_0^-\rangle , \tag{1.1}$$

where Φ_0^- is the wave function of the *noninteracting* system (a Slater determinant of plane-wave orbitals for the infinitely extended systems mainly under consideration here), and F is a *correlation operator*, which describes the dynamical correlations in the system.

The most widely studied *example* of the correlation operator F is the *Jastrow choice*

$$F = \prod_{1\le i<j\le A} f(r_{ij}) , \tag{1.2}$$

in which $f(r)$ is a real function, depending only on the distance $|\vec{r}_i - \vec{r}_j|$ of two interacting particles i and j. The major advantage of the simple choice (1.2) is that methods of classical statistical mechanics are relatively easily extended to the calculation of the energy expectation value

$$E = \langle\psi_0|H|\psi_0^-\rangle / \langle\psi_0^-|\psi_0^-\rangle . \tag{1.3}$$

Though the ansatz (1.2) has met with great success for the description of simple model systems,[6,7] its deficiencies are obvious from the very beginning: The lack of any state dependence in the Jastrow correlation function rules out its use for systems with strong noncentral components of the interaction. An evident way of overcoming this problem is the generalization of the Jastrow ansatz (1.2) to two- (three-...) body correlation operators

$$F = S\prod_{i<j} f(i,j) . \tag{1.4}$$

Here, $f(i,j)$ is a two-body *operator* acting on the states of the ith and the jth particle, and S is introduced to symmetrize the products of $f(i,j)$ operators, since the $f(i,j)$ do not, in general, commute. It is just this noncommuting feature of the correlation operators which causes the enormous complications coming with the generalization (1.4). Nevertheless, considerable success has been reported for various choices of state-dependent correlation operators (1.4).[8]

An alternate way of including state-dependent correlations in a systematic way is the method of correlated basis functions (CBF).[1] This method uses the correlation operator F to generate a set of normalized, but nonorthogonal, correlated wave functions

$$|\chi_{\vec{m}}\rangle = I_{\vec{m}\vec{m}}^{-1/2} F|\Phi_{\vec{m}}\rangle , \quad I_{\vec{m}\vec{m}} = \langle\Phi_{\vec{m}}|F^\dagger F|\Phi_{\vec{m}}\rangle , \tag{1.5}$$

from a complete orthonormal set of Slater determinants $|\Phi_{\vec{m}}\rangle$. The label $\vec{m} = (m_1 \ldots m_A)$ specifies (for homogeneous matter) the plane-wave orbitals entering $|\Phi_{\vec{m}}\rangle$, i.e.,

$$|\Phi_{\vec{m}}\rangle = (A!)^{-1/2} |m_1 \ldots m_A\rangle_a , \tag{1.6}$$

where the subscript a means "antisymmetrized." In fact, the CBF method is not restricted to the state-independent Jastrow choice (1.2): Throughout this paper no further assumption on the correlation operator F will be made than that it obeys the cluster-decomposition property

$$F_N(1,\ldots,N) \to F_p(i_1,\ldots,i_p) F_{N-p}(i_{p+1},\ldots,i_N) \tag{1.7}$$

if the subset $i_1,\ldots,i_p$ of particles is removed far from the rest.

Numerical applications of the CBF method have been reported by Clark, Ristig, and collaborators,[9-11] who calculated second-order perturbation-correction for the energy expectation value on the basis (1.5). One logical extension of the CBF method is the systematic extension of the perturbation series on the $|\psi_{\vec{m}}\rangle$ basis and the re-summation of certain classes of diagrams in order to establish a Brueckner-Bethe[12] (or a related) theory in the CBF framework. This project, which is the subject of the present work, is attractive for a number of reasons.

(i) We can use the state-independent Jastrow choice (1.2) for the correlation operator, for which high precision techniques are available for the calculation of the energy expectation value[2] (1.3) and of off-diagonal matrix elements $\langle \chi_{\vec{m}} | \chi_{\vec{n}} \rangle$ and $\langle \chi_{\vec{m}} | H | \chi_{\vec{n}} \rangle$.[13] In particular for the latter quantities, simple cluster-expansion techniques appear to be suspect even below the saturation density of nuclear matter.[14]

(ii) The theory provides a strong internal consistency test: The final result should within reasonable limits be independent of the Jastrow-correlation operator F. (In fact, if we were able to sum the full perturbation series, the results would be independent of F.) Thus the F dependence will be a measure for how accurately we have calculated the true ground state.

(iii) Brueckner-Bethe-Goldstone (BBG) theory is known to deal already fairly accurately with state-dependent interactions,[12,15,16] (at least in the nuclear-matter problem at not-too-high densities). Thus, the derivation of a "correlated" BBG theory appears to be a promising way of including state dependence in a variational theory. The Jastrow operator F will be used primarily for an approximate treatment of the strong repulsion of two particles at short distances, thereby unburdening the BBG theory from this task.

In the actual formulation of our project, we use the exp(S) formulation of many-body theory due to Coester and Kümmel,[3,5] from which the Bethe-Goldstone equation emerges as a special case.[17,18] The advantages of the exp(S) formulation over alternative approaches have been discussed elsewhere,[3,15] and we will find below that this formulation is also the most powerful one for our purposes.

The coupled-cluster method itself, without any reference to variational methods, has previously been applied quite successfully to interacting many-Fermion systems. It does incorporate state dependence and is able to deal with arbitrarily complex interactions without any formal problems. However, it is found that in most cases the solution of three-body Bethe-Faddeev equations cannot be circumvented[15,19,20] in this formalism if one wants to obtain quantitatively accurate results. Sometimes it is even necessary to consider four-body equations. Since one is forced to solve coupled, nonlinear equations in three or even more vector variables as opposed to the mere evaluation of integrals in variational methods, numerical execution is quite involved for the coupled-cluster scheme. The unsatisfying convergence of the theory is thought to be due in large part to the core-exclusion problem. If n particles come close to each other, overlap of *any* pair of strongly repulsive cores must be avoided which immediately leads to an n-body equation.

The present approach may therefore be considered from quite a different point of view. We perform a coupled-cluster calculation but help the convergence by using the correlation operator F to take care of the core exclusion. In other words, we are interested in a two-body version of the coupled-cluster theory where those effects previously treated via a three-body Bethe-Faddeev summation are now dealt with by the correlated basis functions.

Throughout this paper we restrict ourselves to the case of an infinite system, which allows us the most transparent formulation. There is, of course, no *a priori* reason which forbids the extension of our theory to finite systems,[3,20] thus forming a generalization of the CBF theory recently employed by Mead and Clark.[11,21]

The paper is organized as follows. In the next section, we describe briefly the present theoretical status of CBF theory and introduce the quantities needed for the further analysis. Section III presents the basic ideas of our approach together with the discussion of some alternatives. Sections IV and V lead us through the various stages of the cluster expansion of our coupled-cluster equations and the expression of the ground-state energy. These sections are rather technical in nature and may be skipped by the casual reader. We conclude in Sec. VI by discussing a possible sequence of approximation in the application of our theory as well as possibilities of further extensions.

II. A SHORT REVIEW OF CBF THEORY

In this section we wish to introduce briefly the classic ingredients of the CBF perturbation-correction formulas and also our correlated coupled-cluster theory. In the correlated (in general nonorthogonal) basis (1.5) we have to calculate[2] the following:

(i) diagonal-matrix elements of the Hamiltonian

$$H_{\vec{m}\vec{m}} = \langle \chi_{\vec{m}} | H | \chi_{\vec{m}} \rangle \tag{2.1}$$

and differences thereof;

(ii) off-diagonal-matrix elements of the unit operator

$$N_{\vec{m}\vec{n}} = \langle \chi_{\vec{m}} | \chi_{\vec{n}} \rangle, \quad J_{\vec{m}\vec{n}} = N_{\vec{m}\vec{n}}(1 - \delta_{\vec{m}\vec{n}}); \tag{2.2}$$

(iii) off-diagonal-matrix elements of the Hamiltonian

$$H_{\vec{m}\vec{n}} = \langle \chi_{\vec{m}} | H | \chi_{\vec{n}} \rangle; \tag{2.3}$$

these occur in fact only in the combination

$$H'_{\vec{m}\vec{n}} = (H_{\vec{m}\vec{n}} - H_{\vec{0}\vec{0}} N_{\vec{m}\vec{n}})(1 - \delta_{\vec{m}\vec{n}}). \tag{2.4}$$

In order to avoid large-scale cancellations between the two constituents of $H'_{\vec{m}\vec{n}}$, it is also convenient to introduce[13]

$$W_{\vec{m}\vec{n}} = H_{\vec{m}\vec{n}} - \tfrac{1}{2}(H_{\vec{m}\vec{m}} + H_{\vec{n}\vec{n}}) N_{\vec{m}\vec{n}} \tag{2.5}$$

and to represent $H'_{\vec{m}\vec{n}}$ as

$$H'_{\vec{m}\vec{n}} = [W_{\vec{m}\vec{n}} + \tfrac{1}{2}(H_{\vec{m}\vec{m}} + H_{\vec{n}\vec{n}} - 2H_{\vec{0}\vec{0}}) N_{\vec{m}\vec{n}}](1 - \delta_{\vec{m}\vec{n}}). \tag{2.6}$$

The latter representation has the advantage that both terms are of the correct order in the particle number. Moreover, $W_{\vec{m}\vec{n}}$, $N_{\vec{m}\vec{n}}$, and $(H_{\vec{m}\vec{m}} + H_{\vec{n}\vec{n}} - 2H_{\vec{0}\vec{0}})$ are conveniently represented as matrix elements of a (nonlocal) effective interaction, a normalization function, and differences of single-particle energies.

With the ingredients defined above, the first terms in the CBF perturbation expansion read[11]

$$\begin{aligned} E = H_{\vec{0}\vec{0}} &- \sum_{\vec{m}} \frac{H'_{\vec{0}\vec{m}} H'_{\vec{m}\vec{0}}}{H_{\vec{m}\vec{m}} - H_{\vec{0}\vec{0}}} + \sum_{\vec{m}\vec{n}} \frac{H'_{\vec{0}\vec{m}} H'_{\vec{m}\vec{n}} H'_{\vec{n}\vec{0}}}{(H_{\vec{m}\vec{m}} - H_{\vec{0}\vec{0}})(H_{\vec{n}\vec{n}} - H_{\vec{0}\vec{0}})} \\ &+ \Bigg(\sum_{\vec{m}\vec{n}\vec{p}} \frac{H'_{\vec{0}\vec{m}} H'_{\vec{m}\vec{n}} H'_{\vec{n}\vec{p}} H'_{\vec{p}\vec{0}}}{(H_{\vec{m}\vec{m}} - H_{\vec{0}\vec{0}})(H_{\vec{n}\vec{n}} - H_{\vec{0}\vec{0}})(H_{\vec{p}\vec{p}} - H_{\vec{0}\vec{0}})} + \sum_{\vec{m}\vec{n}} \frac{H'_{\vec{0}\vec{m}} H'_{\vec{m}\vec{0}} H'_{\vec{0}\vec{n}} H'_{\vec{n}\vec{0}}}{(H_{\vec{m}\vec{m}} - H_{\vec{0}\vec{0}})^2 (H_{\vec{n}\vec{n}} - H_{\vec{0}\vec{0}})} \\ &- \sum_{\vec{m}\vec{n}} \frac{J_{\vec{0}\vec{m}} H'_{\vec{m}\vec{0}} H'_{\vec{0}\vec{n}} H'_{\vec{n}\vec{0}}}{(H_{\vec{m}\vec{m}} - H_{\vec{0}\vec{0}})(H_{\vec{n}\vec{n}} - H_{\vec{0}\vec{0}})} - \sum_{\vec{m}\vec{n}} \frac{H'_{\vec{0}\vec{m}} J_{\vec{m}\vec{0}} H'_{\vec{0}\vec{n}} H'_{\vec{n}\vec{0}}}{(H_{\vec{m}\vec{m}} - H_{\vec{0}\vec{0}})(H_{\vec{n}\vec{n}} - H_{\vec{0}\vec{0}})} \Bigg) + \cdots . \end{aligned} \tag{2.7}$$

As a next step in the application of the CBF perturbation-correction formula (2.7) we have to restrict the set of states $|\Phi_{\vec{m}}\rangle$ over which the sums of (2.7) are to run. An obvious and useful classification is to count the number d of orbitals in which the states $|\Phi_{\vec{m}}\rangle$, $|\Phi_{\vec{n}}\rangle$ differ from each other (one of these states may be identified with the ground state $|\Phi_{\vec{0}}\rangle$). For convenience, we shall suppose that the orbitals in which $\vec{m}$ and $\vec{n}$ differ have been shuffled to the beginning of the sequence, i.e., $m_i \neq n_j$ $(i,j \leq d)$, $m_i = n_i$ $(i > d)$. The simplest case for the infinitely extended systems under consideration here is $d=2$ (or $d=0$).

For our further considerations it turns out to be convenient to introduce d-body operators $\mathfrak{N}^{(d)}[\vec{m}]$; $\mathfrak{W}^{(d)}[\vec{m}]$ which act on the d orbitals in which $\vec{m}$ and $\vec{n}$ differ, i.e.,

$$\begin{aligned} J_{\vec{m}\vec{n}} &= \langle m_1 \cdots m_d | \mathfrak{N}^{(d)}[\vec{m}] | n_1 \cdots n_d \rangle_a \\ &= N_{m_1 \cdots m_d, n_1 \cdots n_d}[\vec{m}] \\ W_{\vec{m}\vec{n}} &= \langle m_1 \cdots m_d | \mathfrak{W}^{(d)}[\vec{m}] | n_1 \cdots n_d \rangle_a \\ &= W_{m_1 \cdots m_d, n_1 \cdots n_d}[\vec{m}], \end{aligned} \tag{2.8}$$

for two states $|\Phi_{\vec{m}}\rangle$ and $|\Phi_{\vec{n}}\rangle$ which differ in the first d orbitals. If the states $\vec{m}$ and $\vec{n}$ differ only by few orbitals from the ground state $|\Phi_{\vec{0}}\rangle$ we have

$$\begin{aligned} \mathfrak{W}^{(d)}[\vec{m}] &= \mathfrak{W}^{(d)}[\vec{0}] + O(A^{-1}), \\ \mathfrak{N}^{(d)}[\vec{m}] &= \mathfrak{N}^{(d)}[\vec{0}] + O(A^{-1}). \end{aligned} \tag{2.9}$$

For a state-independent Jastrow F, the operators $\mathfrak{W}^{(d)}$ and $\mathfrak{N}^{(d)}$ have been constructed in Ref. 13 for $d=2$. The extension of these considerations to higher d values is thereafter quite obvious and does not require a repetition of the tedious calculations presented in Ref. 13, the properties of these operators may be verified in low orders by straight-forward cluster expansion techniques.

For $d=2$ and $d=3$, $\mathfrak{W}$ and $\mathfrak{N}$ are proper d-body operators in the sense that they vanish if one of the particles is removed far from the others. This property (which reflects just the cluster property of the correlation operator F) is no longer maintained for $d \geq 4$.[22,23] We have, for example

$$\begin{aligned} \mathfrak{N}^{(4)}(1,2,3,4) = [&\mathfrak{N}^{(2)}(12)\mathfrak{N}^{(2)}(34) + \mathfrak{N}^{(2)}(13)\mathfrak{N}^{(2)}(24) \\ &+ \mathfrak{N}^{(2)}(14)\mathfrak{N}^{(2)}(23)] + \mathfrak{N}_c^{(4)}(1,2,3,4), \end{aligned} \tag{2.10}$$

where $\mathfrak{N}_c^{(4)}$ stands for the "connected" part of the $\mathfrak{N}^{(4)}$ operator. The corresponding decompositions

of $\mathfrak{W}^{(4)}$ and the $\mathfrak{W}$ and $\mathfrak{N}$ operators for $d>4$ are obvious. Decompositions of this structure are repeatedly found in cluster expansion theories.[2]

It is just these unlinked terms in the off-diagonal-matrix elements that generate some of the obstacles to the further development of the CBF theory. If we include, e.g., $d=4$ combinations in the second-order CBF correction, we obtain unlinked contributions with an unphysical dependence on the particle number A. These contributions are canceled by $d=2$ contributions to the fourth-order correction [the last two contributions explicitly given in (2.7)] and further sixth-order terms of similar structure. A systematic further development of the CBF-perturbation series must include higher-order terms in the perturbation series and simultaneously include contributions with larger d in the lower-order terms.

III. CORRELATED COUPLED-CLUSTER THEORY

There are basically three ways to arrive at a Bethe-Goldstone equation or a related theory in an uncorrelated basis. The first, most straightforward and historically original way is to analyze the Rayleigh-Schrodinger perturbation expansion and perform re-summations of infinite classes of selected diagrams.[24] The CBF analog to this would be a further analysis of the expansion (2.7) with the same aim—a project of prohibitive complexity owing to the appearance of the unlinked structures (2.10).

Alternatively, the ground-state wave function can be written in the exp(S)form[3-5]

$$|\psi_{\vec{0}}\rangle = e^{S}|\Phi_{\vec{0}}\rangle, \tag{3.1}$$

where

$$S=\sum_{n\geq 2} S^{(n)} \tag{3.2}$$

is a sum of n particle-hole (p-h) operators.

The $S^{(n)}$ may be determined either by a variational procedure[25,26]

$$\frac{\delta}{\delta S^{(n)\dagger}} \frac{\langle\Phi_{\vec{0}}|e^{S^\dagger}He^{S}|\Phi_{\vec{0}}\rangle}{\langle\Phi_{\vec{0}}|e^{S^\dagger}e^{S}|\Phi_{\vec{0}}\rangle}=0 \tag{3.3}$$

or by writing the Schrödinger equation in the form

$$e^{-S}He^{S}|\Phi_{\vec{0}}\rangle = E|\Phi_{\vec{0}}\rangle, \tag{3.4}$$

and observing that for all n p-h states $|\Phi_{\vec{m}}\rangle$

$$\langle\Phi_{\vec{m}}|e^{-S}He^{S}|\Phi_{\vec{0}}\rangle=0 \quad (\vec{m}\neq\vec{0}) \tag{3.5}$$

[exp(S) Method].

The method of Eqs. (3.5) has been shown to be formally equivalent to Eqs. (3.3), but more advantageous in practical applications since in each step only a finite number of diagrams is generated. For a thorough discussion of this point see Kümmel and Lührman.[3,26,27]

Both approaches, the variational method (3.3) or the coupled-cluster method (3.5) are readily extended to correlated wave functions. Instead of (3.1), write the *exact* ground-state wave function in the form

$$|\psi\rangle = Fe^{S}|\Phi_{\vec{0}}\rangle, \tag{3.6}$$

where F is, as in (1.1), a correlation operator which provides an *approximate* description of the short-ranged dynamical correlations in the system. Employing such a correlation operator, we can unburden S from providing a gross description of the short ranged two- , three- , and four-body correlations and leave for it only the task of describing in more detail those strongly state-dependent effects which are hard to model with a correlation operator F.

Again, we can determine S either by the variational prescription

$$\frac{\delta}{\delta S^{(n)\dagger}} \frac{\langle\Phi_{\vec{0}}|e^{S^\dagger}F^\dagger HFe^{S}|\Phi_{\vec{0}}\rangle}{\langle\Phi_{\vec{0}}|e^{S^\dagger}F^\dagger Fe^{S}|\Phi_{\vec{0}}\rangle}=0 \tag{3.7}$$

or through the Schrödinger equation

$$HFe^{S}|\Phi_{\vec{0}}\rangle = EFe^{S}|\Phi_{\vec{0}}\rangle, \tag{3.8}$$

where F is always determined beforehand. Multiplication of (3.8) with $e^{-S}F^\dagger$ and projection on complete sets of np-nh states $|\Phi_{\vec{m}}\rangle$ leads us, after the elimination of the ground-state energy through

$$E=\frac{\langle\Phi_{\vec{0}}|e^{-S}F^\dagger HFe^{S}|\Phi_{\vec{0}}\rangle}{\langle\Phi_{\vec{0}}|e^{-S}F^\dagger Fe^{S}|\Phi_{\vec{0}}\rangle} \tag{3.9}$$

and proper normalization, to a set of *correlated coupled-cluster equations*

$$\frac{\langle\Phi_{\vec{m}}|e^{-S}F^\dagger HFe^{S}|\Phi_{\vec{0}}\rangle}{\langle\Phi_{\vec{0}}|e^{-S}F^\dagger Fe^{S}|\Phi_{\vec{0}}\rangle} = \frac{\langle\Phi_{\vec{0}}|e^{-S}F^\dagger HFe^{S}|\Phi_{\vec{0}}\rangle\langle\Phi_{\vec{m}}|e^{-S}F^\dagger Fe^{S}|\Phi_{\vec{0}}\rangle}{\langle\Phi_{0}|e^{-S}F^\dagger Fe^{S}|\Phi_{0}\rangle^{2}}. \tag{3.10}$$

It is again straightforward to verify the identity of (3.10) with the variational problem (3.7). The latter leads however to *linear superposition* of Eqs. (3.10), coupled through coefficients which contain $S^\dagger$ alone. For this reason we choose to start with Eqs. (3.9) and (3.10), a decision which will be justified by the comparatively simple form of the final equations which we will derive below.

We conclude this section by comparing our way of including state-dependent correlations in a variational theory with the pure variational approach, which tries to find better and better cor-

relation operators F. There are three problems with the latter method.

(i) With the inclusion of more complicated interactions, also more complicated correlation operators have to be invented. In our theory, we need only to know how a certain operator ($\vec{\sigma}_1\cdot\vec{\sigma}_2$; S_{12}, $\vec{L}\cdot\vec{S}$, etc.) appearing in the Hamiltonian acts on a given F. For the pure Jastrow F, the action of $\vec{\sigma}_1\cdot\vec{\sigma}_2$, $\vec{\tau}_1\cdot\vec{\tau}_2$ and S_{12} on F is almost trivial,[13] and the inclusion of $\vec{L}\cdot\vec{S}$ or L^2 components in the interaction does not cause undue complications.[28]

(ii) One of the main difficulties in the pure variational approach is the fact that different f operators do not commute. This problem has been overcome within the purely variational approach by Owen's restricted product wave functions[29,30] and by Smith's commuting, noncentral correlation operators.[31] This difficulty does also not appear in our theory: the $S^{(n)}$ do commute.

(iii) The next step in the development of the variational method is the summation of "chain diagrams" and "parallel connections".[2] While the summation of chain diagrams is currently under control for two-body operators no more complicated than the tensor operator,[8,32] success for parallel connections has been reported only for special choices of f.[29-31] Such problems do not occur in our theory: no parallel connections appear, and chain diagrams, which can be summed trivially by a suitable renormalization of S^2, do not appear either in the final version of our equations.

IV. THE GROUND-STATE ENERGY

Some considerations are in order before we proceed to establish cluster expansions for our ground-state energy expression (3.9) and our coupled-cluster equation (3.10). Clearly, our theory has the aim of providing a many-body method which achieves accuracy comparable to present techniques, but with simpler tools. Thus, in this stage of the theory we do not aim at the derivation of an analog of the Bethe-Faddeev equations on the correlated basis, since in such degree of elaboration the coupled-cluster theory is already capable of giving a fairly realistic description of nuclear many-body systems[15,16] *without* an additional correlation operator F. To be definite, we restrict ourselves to

$$S=S^{(2)}=\frac{1}{(2!)^2}\sum_{\rho_1\rho_2\nu_1\nu_2} S_{\rho_1\rho_2(\nu_1\nu_2)_a}a^\dagger_{\rho_1}a^\dagger_{\rho_2}a_{\nu_2}a_{\nu_1}. \quad (4.1)$$

(Quite generally, we will label particle states by ρ_1,ρ_2 and hole states by $\nu_1,\nu_2,\ldots$.) The *ansatz* (4.1) would not be sufficient in the usual exp(S) theory if strongly repulsive cores were present in the two-body interaction.[3,17] In the present case, however, the exp(S) has to deal only with the "effective interactions" $\mathcal{W}$ and $\mathfrak{N}$, which will be very smooth. Therefore, Eq. (4.1), which has been shown to lead to extremely accurate results in various model studies[33,34] as well as in the electron fluid problem,[35] is quite promising here.

A second approximation is made consistent with (4.1): We shall include only those many-body matrix elements of the Hamiltonian and the unit operator, which may be written in terms of the effective two-body operator $\mathcal{W}^{(2)}(1,2)$ and $\mathfrak{N}^{(2)}(1,2)$ and products thereof. Two types of higher-order contributions occur beyond these.

(i) Off-diagonal matrix elements of linked three-, four- body operators $\mathcal{W}^{(d)}(1\cdots d)$, $\mathfrak{N}^{(d)}(1\cdots d)$ $(d>2)$. Inclusion of these sets of many-body contributions will not cause any qualitative change in the cluster expansions to be developed below.

(ii) Differences of $\mathfrak{N}^{(d)}[\vec{\tilde{m}}]$ or $\mathcal{W}^{(d)}[\vec{\tilde{m}}]$ for different reference sets of plane-wave orbitals $\vec{\tilde{m}}$, e.g.,

$$\mathfrak{N}^{(2)}[\vec{\tilde{m}}]-\mathfrak{N}^{(2)}[\vec{\tilde{n}}]=O(A^{-1}), \quad (4.2)$$

which enter our expansion through the cancellation of unlinked diagrams. These may be written as matrix elements of r-body operators, which are off-diagonal in $d(<r)$ states and diagonal in $(r-d)$ states. The omission of this type of contribution (to the energy or the coupled-cluster equations) corresponds also to our concept of including only effective two-body operators. It allows us, moreover, to omit the *explicit* specification of the reference state by the argument $[\vec{\tilde{m}}]$. More detailed studies which have to involve the specification of the correlation operator F will lead to a feedback of our theory to the starting point (viz., the cluster-expansion and re-summation techniques for correlated matrix elements) through a renormalization of the so-called "exchange line".[2]

Some manipulations on the ground-state energy (3.9) are needed before we go on to derive an expansion in terms of powers of S. We define for any integer power k

$$S^k_{\vec{\tilde{m}}\vec{\tilde{n}}}=\langle\Phi_{\vec{\tilde{m}}}|S^k|\Phi_{\vec{\tilde{n}}}\rangle \quad (4.3)$$

and, for ease of writing the following manipulations, a set of operators $\hat{S}^k$ through their matrix elements

$$(\hat{S}^k)_{\vec{\tilde{m}}\vec{\tilde{n}}}=(I_{\vec{\tilde{m}}\vec{\tilde{m}}}/I_{\vec{\tilde{n}}\vec{\tilde{n}}})^{1/2}S^k_{\vec{\tilde{m}}\vec{\tilde{n}}}, \quad (4.4)$$

and rewrite (3.9) in the form (note that $\langle\Phi_{\vec{\tilde{0}}}|e^{-S}=\langle\Phi_{\vec{\tilde{0}}}|$)

$$E=\frac{\sum_{\vec{\tilde{m}}}\langle\Phi_{\vec{\tilde{0}}}|F^\dagger HF|\Phi_{\vec{\tilde{m}}}\rangle(e^{\hat{S}})_{\vec{\tilde{m}}\vec{\tilde{0}}}}{\sum_{\vec{\tilde{m}}}\langle\Phi_{\vec{\tilde{0}}}|F^\dagger F|\Phi_{\vec{\tilde{m}}}\rangle(e^{\hat{S}})_{\vec{\tilde{m}}\vec{\tilde{0}}}}$$

$$=H_{\vec{\tilde{0}}\vec{\tilde{0}}}+\frac{\sum'_{\vec{\tilde{m}}}H'_{\vec{\tilde{0}}\vec{\tilde{m}}}(e^{\hat{S}})_{\vec{\tilde{m}}\vec{\tilde{0}}}}{1+\sum'_{\vec{\tilde{m}}}J_{\vec{\tilde{0}}\vec{\tilde{m}}}(e^{\hat{S}})_{\vec{\tilde{m}}\vec{\tilde{0}}}} \quad (4.5)$$

in which the prime on the summation symbols mean that the summations are to be carried out over all A particle Slater determinants $|\Phi_{\vec{m}}\rangle$ *different* from the ground-state determinant $|\Phi_{\vec{0}}\rangle$. We discover in (4.5) again the effective perturbation $H'_{\vec{m}\vec{n}}$ [see Eq. (2.4)] entering the CBF perturbation correction formula (2.7). We will demonstrate, however, that the expression (4.4) is well behaved in the large A limit, since the disconnected portions (2.10), etc., will be canceled by corresponding denominator diagrams.

An expansion in powers of S is now readily derived using the power-series expansion method

$$E = H_{\vec{0}\vec{0}} + \sum_{\vec{m}}{}' H'_{\vec{0}\vec{m}} \hat{S}_{\vec{m}\vec{0}} + \frac{1}{2!}\Big[\sum_{\vec{m}}{}' H'_{\vec{0}\vec{m}} (\hat{S}^2)_{\vec{m}\vec{0}} - \Big(\sum_{\vec{m}}{}' H'_{\vec{0}\vec{m}} \hat{S}_{\vec{m}\vec{0}}\Big)\Big(\sum_{\vec{m}}{}' N_{\vec{0}\vec{m}} \hat{S}_{\vec{m}\vec{0}}\Big)\Big] = H_{\vec{0}\vec{0}} + (\delta E)_1 + (\delta E)_2 + \cdots \tag{4.6}$$

[$(\delta E)_n$ denotes the contribution to the energy containing n S factors].

With the ansatz (4.1) for S all matrix elements $H'_{\vec{0}\vec{m}}$ and $J_{\vec{0}\vec{m}}$ explicitly appearing in (4.6) are taken between the ground state and a two-particle–two-hole state, except the term $\sum'_{\vec{m}} H'_{\vec{0}\vec{m}} (\hat{S}^2)_{\vec{m}\vec{0}}$, which contains 4p-4h matrix elements.

According to our decompositions (2.6) and the definitions (2.10), we write in the 4p-4h case, labeling the particle states with $\rho_1 \cdots \rho_j$ and the hole states with $\nu_1 \cdots \nu_j$,

$$H'_{\vec{0}\vec{m}} = \langle \nu_1 \cdots \nu_4 | \mathcal{W}^{(4)}(1 \cdots 4) | \rho_1 \cdots \rho_4 \rangle_a + \tfrac{1}{2}(H_{\vec{m}\vec{m}} - H_{\vec{0}\vec{0}}) \langle \nu_1 \cdots \nu_4 | \mathfrak{N}^{(4)}(1 \cdots 4) | \rho_i \cdots \rho_4 \rangle_a . \tag{4.7}$$

The difference $H_{mm} - H_{00}$ is expanded in leading order in differences of single-particle energies

$$H_{\vec{m}\vec{m}} - H_{\vec{0}\vec{0}} = \sum_{i=1}^{4} [\epsilon(\rho_i) - \epsilon(\nu_i)] + O(A^{-1}) . \tag{4.8}$$

Following our strategy of retaining only (products of) two-body operators we are left with the *unlinked* contributions [see (2.10)] to $\mathcal{W}^{(4)}$ and $\mathfrak{N}^{(4)}$. These may, after some reordering and combination with the second contribution to $(\delta E)_2$, be written in the form

$$(\delta E)_2 = \tfrac{1}{4} \sum_{\rho_1\rho_2\nu_1\nu_2} \langle \nu_1\nu_2 | \mathcal{U}^{(2)} | \rho_1\rho_2 \rangle_a \tfrac{1}{8} \sum_{\rho_3\rho_4\nu_3\nu_4} \langle \nu_3\nu_4 | \mathfrak{N}^{(2)} | \rho_3\rho_4 \rangle_a \times [(\hat{S}^2)_{\rho_1\rho_2\rho_3\rho_4, (\nu_1\nu_2\nu_3\nu_4)_a} - \hat{S}_{\rho_1\rho_2, (\nu_1\nu_2)_a} \hat{S}_{\rho_3\rho_4, (\nu_3\nu_4)_a}] . \tag{4.9}$$

[Note that we also neglect here differences of the type (4.2).] In (4.8) we have defined for any np-nh state $|\Phi_{\vec{m}}\rangle = a^\dagger_{\rho_1} \cdots a^\dagger_{\rho_n} a_{\nu_n} \cdots a_{\nu_1} |\Phi_{\vec{0}}\rangle$

$$(S^k)_{\rho_1 \cdots \rho_n, \nu_1 \cdots \nu_n} \equiv (S^k)_{\vec{m}\vec{0}} \tag{4.10}$$

and the effective interaction

$$V_{\alpha\beta,\gamma\delta} \equiv \langle \alpha\beta | \mathcal{U}^{(2)} | \gamma\delta \rangle = W_{\alpha\beta,\gamma\delta} + \tfrac{1}{2}(\pm\epsilon_\alpha \pm \epsilon_\beta \pm \epsilon_\gamma \pm \epsilon_\delta) N_{\alpha\beta,\gamma\delta} , \tag{4.11}$$

where $\alpha, \beta, \gamma, \delta$ can be particle or hole states, the + sign applying for the particle states and the − sign for the hole states.

We are now ready to introduce a renormalized counterpart of the S operator, which includes all powers of S and all nonorthogonality corrections entering our expansion (4.5) through $\mathfrak{N}^{(2)}(12)$ or through ratios of normalization integrals $I_{\vec{m}\vec{m}}/I_{\vec{0}\vec{0}}$:

$$\langle \rho\rho' | \mathcal{S} | \nu\nu' \rangle_a \equiv \mathcal{S}_{\rho\rho'(\nu\nu')_a} = \hat{S}_{\rho\rho'(\nu\nu')_a} + \tfrac{1}{8} \sum_{\rho_1\rho_2\rho_1\rho_2} N_{\nu_1\nu_2(\rho_1\rho_2)_a} [(\hat{S}^2)_{\rho\rho'\rho_1\rho_2, (\nu\nu'\nu_1\nu_2)_a} - \hat{S}_{\rho\rho', (\nu\nu')_a} \hat{S}_{\rho_1\rho_2(\nu_1\nu_2)_a}] + \cdots . \tag{4.12}$$

Finally, this allows us to write the energy in the form

$$E = H_{\vec{0}\vec{0}} + \tfrac{1}{4} \sum_{\rho\rho'\nu\nu'} V_{\nu\nu'(\rho\rho')_a} \mathcal{S}_{\rho\rho'(\nu\nu')_a} . \tag{4.13}$$

Carrying our expansion (4.5) to higher orders in S would lead to higher-order contributions to the $\mathcal{S}$ operator and includes vast classes of nonorthogonality corrections. (Note that $\mathcal{S}$ is identical with S in the limit $F \to 1$.)

In order to appreciate the generality of (4.13) it is worth studying the expansion (4.12) in some detail. For this purpose it is convenient to use the Goldstone-type graphical notation of conventional exp(S) theory,[3] with the additional specification that we represent $\mathfrak{N}^{(2)}$ by a dashed, horizontal line. Some further analysis is required for the combination of normalization integrals and S oper-

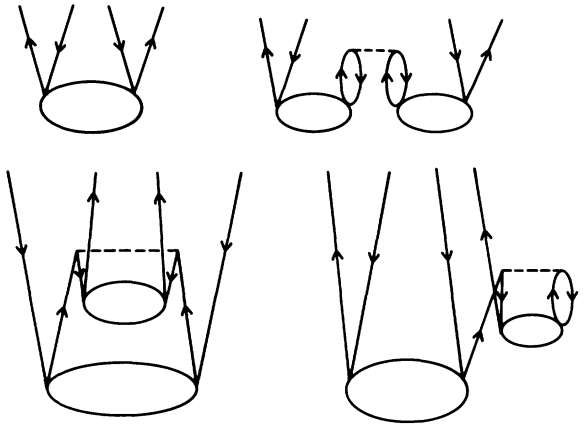

FIG. 1. Some typical diagrams contributing to the expansion of S in terms of $S^{(2)}$. Note that the bare $S^{(2)}$ (first diagram) is always multiplied with a factor $[I(\rho\rho';\nu\nu')/I_{00}]^{1/2}$.

ators in the curly bracket in Eq. (4.12): The ratio of two normalization integrals factorizes in leading order in the particle number into a product of functions depending only on one of the particle states, i.e., we have for the normalization integral of any np-nh state $|\Phi_{\vec{m}}\rangle$

$$I_{\vec{m}\vec{m}}/I_{\vec{0}\vec{0}} \equiv I(\rho_1 \cdots \rho_n;\nu_1 \cdots \nu_n)/I_{00} = \prod_{i=1}^{n} \frac{z(\rho_i)}{z(\nu_i)} + O(A^{-1}). \tag{4.14}$$

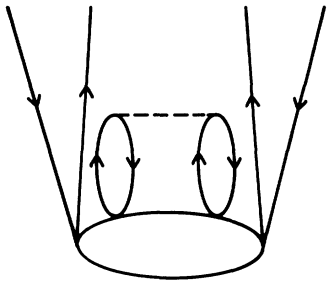

FIG. 2. Example of an $S^{(4)}$ contribution to $\mathcal{S}$.

The fact that the factorization holds only up to the order A^{-1} in the particle number has the consequence

$$(\hat{S}^2)_{\rho_1\cdots\rho_4,(\nu_1\cdots\nu_4)_a} = A_\nu(\hat{S}_{\rho_1\rho_2,\nu_1\nu_2}\hat{S}_{\rho_3\rho_4,\nu_3\nu_4})[1+O(A^{-1})], \tag{4.15}$$

where A_ν is the antisymmetrization operator acting on the hole labels ν_i. This incomplete cancellation causes another (diagonal) nonorthogonality correction in (4.12). Rewriting (4.12) in terms of $\hat{S}$-matrix elements and retaining only the terms of leading order in the particle number, we arrive at

$$\mathcal{S}_{\rho\rho'(\nu\nu')_a} = \hat{S}_{\rho\rho'(\nu\nu')_a} + \tfrac{1}{8}\sum_{\rho_1\rho_2\nu_1\nu_2} N_{\nu_1\nu_2(\rho_1\rho_2)_a}[A_\nu(\hat{S}_{\rho\rho'\nu\nu'}\hat{S}_{\rho_1\rho_2,\nu_1\nu_2}) - \hat{S}_{\rho\rho'(\nu\nu')_a}\hat{S}_{\rho_1\rho_2(\nu_1\nu_2)_a}]$$
$$+ \tfrac{1}{8}\sum_{\rho_1\rho_2\nu_1\nu_2} N_{\nu_1\nu_2(\rho_1\rho_2)_a}\hat{S}_{\rho\rho'(\nu\nu')_a}\hat{S}_{\rho_1\rho_2(\nu_1\nu_2)_a}\left[\left(\frac{I(\rho\rho'\rho_1\rho_2;\nu\nu'\nu_1\nu_2)I_{00}}{I(\rho\rho';\nu\nu')I(\rho_1\rho_2;\nu_1\nu_2)}\right)^{1/2} - 1\right]. \tag{4.16}$$

We are now ready to construct the diagrammatical expansion of $\mathcal{S}$ in terms of $S^{(2)}$ and $\mathfrak{N}^{(2)}$. Some typical diagrams are shown in Fig. 1, from which the general construction principle of $\mathcal{S}$ becomes quite obvious: $\mathcal{S}$ is represented by the sum of all diagrams which can be constructed from $S^{(2)}$ and $\mathfrak{N}^{(2)}$ in such a way that the external lines enter only $S^{(2)}$; only internal lines may enter $\mathfrak{N}^{(2)}$. Furthermore, no two $\mathfrak{N}^{(2)}$ operators may be connected directly by a particle or a hole line. The diagonal correction terms [the last explicitly given contribution to the expansion (4.16)] may be represented in a similar way by introducing a new graphical element; further specifications are, however, not necessary at this point.

The definition of $\mathcal{S}$ is now readily extended to the inclusion of $S^{(d)}$ and $\mathfrak{N}^{(d)}$ for $d>2$: We define $\mathcal{S}$ to be the sum of *all* diagrams formed according to the rules given above which contribute to the energy through the effective two-body interaction $\mathfrak{W}^{(2)}$. An example of an $S^{(4)}$ term contributing to $\mathcal{S}$ is shown in Fig. 2. The introduction of the operator $\mathcal{S}$ is, at this point, of course, of only aesthetic appeal as long as we are bound to derive an algorithm for calculating $\mathcal{S}$ from a given $S^{(2)}$. We will find, however, that the same quantity can be introduced to re-sum our correlated coupled-cluster Eqs. (3.10) and eliminate the "bare" S entirely from our theory.

V. COUPLED-CLUSTER EQUATIONS

We proceed now to an expansion of the coupled-cluster equations (3.10) in powers of S. Since we aim only at the determination of $S^{(2)}$, it is sufficient to choose $|\Phi_{\vec{m}}\rangle$ to be (any) 2p-2h state. This simplifies, in turn, our considerations due to

$$(e^{-S})_{\vec{m}\vec{0}} = \delta_{\vec{m}\vec{0}} - S_{\vec{m}\vec{0}}. \tag{5.1}$$

Rewriting Eq. (3.10) in terms of the correlated-state quantities $H_{\vec{m}\vec{n}}$, $N_{\vec{m}\vec{n}}$ and making use of the expression (3.9) and (4.5) for the energy we obtain

$$\frac{\sum_{\vec{n}}(H_{\vec{m}\vec{n}}-H_{\vec{0}\vec{0}}N_{\vec{m}\vec{n}})(e^{\hat{S}})_{\vec{n}\vec{0}}}{1+\sum_{\vec{n}}{}'J_{\vec{0}\vec{n}}(e^{\hat{S}})_{\vec{n}\vec{0}}}=\frac{\sum_{\vec{n}}(H_{\vec{0}\vec{n}}-H_{\vec{0}\vec{0}}N_{\vec{0}\vec{n}})(e^{\hat{S}})_{\vec{0}\vec{n}}\sum_{\vec{n}}N_{\vec{m}\vec{n}}(e^{\hat{S}})_{\vec{n}\vec{0}}}{(1+\sum_{\vec{n}}{}'J_{\vec{0}\vec{n}}(e^{\hat{S}})_{\vec{n}\vec{0}})^2}\,, \tag{5.2}$$

which is just the (properly normalized) Schrödinger equation for the wave function (3.6), projected onto the correlated 2p-2h wave functions $|\chi_{\vec{m}}\rangle$ defined in (1.5). The first three terms in the expansion of (5.2) in powers of S are

$$O=H'_{\vec{m}\vec{0}}+\sum_{\vec{n}}(H_{\vec{m}\vec{n}}-H_{\vec{0}\vec{0}}N_{\vec{m}\vec{n}}-H'_{\vec{m}\vec{0}}J_{\vec{0}\vec{n}}-J_{\vec{m}\vec{0}}H'_{\vec{0}\vec{n}})\hat{S}_{\vec{n}\vec{0}}$$

$$+\frac{1}{2!}\Big(\sum_{n}(H_{\vec{m}\vec{n}}-H_{\vec{0}\vec{0}}N_{\vec{m}\vec{n}}-H'_{\vec{m}\vec{n}}J_{\vec{0}\vec{n}}-J_{\vec{m}\vec{0}}H'_{\vec{0}\vec{n}})(\hat{S}^2)_{\vec{n}\vec{0}}-\sum_{\vec{n}\vec{n}'}[2(H_{\vec{m}\vec{n}}-H_{\vec{0}\vec{0}}N_{\vec{m}\vec{n}})J_{\vec{0}\vec{n}'}+2H'_{\vec{0}\vec{n}}N_{\vec{m}\vec{n}'}-H'_{\vec{m}\vec{0}}J_{\vec{0}\vec{n}}J_{\vec{0}\vec{n}'}]\hat{S}_{\vec{n}\vec{0}}\hat{S}_{\vec{n}'\vec{0}}\Big)+\cdots\,. \tag{5.3}$$

Next, we separate out all those terms, where diagonal-matrix elements $H_{\vec{m}\vec{n}}-H_{\vec{0}\vec{0}}$ and $N_{\vec{m}\vec{m}}=1$ occur:

$$0=H'_{\vec{m}\vec{0}}+(H_{\vec{m}\vec{m}}-H_{\vec{0}\vec{0}})\hat{S}_{\vec{m}\vec{0}}+\sum_{\vec{n}}(H'_{\vec{m}\vec{n}}-H'_{\vec{m}\vec{0}}J_{\vec{0}\vec{n}}-J_{\vec{m}\vec{0}}H'_{\vec{0}\vec{n}})\hat{S}_{\vec{n}\vec{0}}-\sum_{\vec{n}}[H_{\vec{0}\vec{n}}+J_{\vec{0}\vec{n}}(H_{\vec{m}\vec{m}}-H_{\vec{0}\vec{0}})]\hat{S}_{\vec{n}\vec{0}}\hat{S}_{\vec{m}\vec{0}}$$

$$+\frac{1}{2!}\sum_{\vec{n}}(H'_{\vec{m}\vec{n}}-H'_{\vec{m}\vec{0}}J_{\vec{0}\vec{n}}-J_{\vec{m}\vec{0}}H'_{\vec{0}\vec{n}})(\hat{S}^2)_{\vec{n}\vec{0}}-\sum_{\vec{n},\vec{n}'}(2H'_{\vec{m}\vec{n}}J_{\vec{0}\vec{n}'}+2H'_{\vec{0}\vec{n}}J_{\vec{m}\vec{n}'}-H'_{\vec{m}\vec{0}}J_{\vec{0}\vec{n}}J_{\vec{0}\vec{n}'})\hat{S}_{\vec{n}\vec{0}}\hat{S}_{\vec{n}'\vec{0}}+\cdots\,. \tag{5.4}$$

It is worth noting here that the second-order CBF correction for the energy is obtained by retaining only the first two terms of the expansion (5.4). The further analysis of our expansion (5.4) goes along very much the same lines as the one for the expansion of the ground-state energy (4.5). It is, however, quite tedious and purely technical so that we pass over the details and demonstrate the procedure only for the simplest examples, the terms which are linear in S. For the higher terms, we will give only the general calculational recipe below.

By construction, the states $|\Phi_{\vec{m}}>$ and $|\Phi_{\vec{n}}\rangle$ are 2p-2h states. To be definite, we write

$$\begin{aligned}|\Phi_{\vec{m}}\rangle&=a^{\dagger}_{\rho}a^{\dagger}_{\rho'}a_{\nu'}a_{\nu}|\Phi_{\vec{0}}\rangle\,,\\ |\Phi_{\vec{n}}\rangle&=a^{\dagger}_{\rho_1}a^{\dagger}_{\rho'_1}a_{\nu'_1}a_{\nu_1}|\Phi_{\vec{0}}\rangle\,.\end{aligned} \tag{5.5}$$

Matrix elements of effective two-body operators of the type specified in Sec. IV. arise when $|\Phi_{\vec{m}}\rangle$ and $|\Phi_{\vec{n}}\rangle$ differ by two or four orbitals. States differing by two orbitals may be generated by coincidence of (i) the particle orbitals in $|\Phi_{\vec{m}}\rangle$ with the particle orbitals in $|\Phi_{\vec{n}}\rangle$, (ii) the hole orbitals in $|\Phi_{\vec{m}}\rangle$ with the hole orbitals in $|\Phi_{\vec{n}}\rangle$, or (iii) a particle-hole pair in $|\Phi_{\vec{m}}\rangle$ with a particle-hole pair in $|\Phi_{\vec{n}}\rangle$. In the $d=4$ contribution we take all terms which can be written as matrix elements of unlinked products of two-body operators. Spelling out explicitly the distinct two-body operators, we arrive at

$$\begin{aligned}\sum_{\vec{n}\neq\vec{m}}(W_{\vec{m}\vec{n}}-N_{\vec{m}\vec{0}}W_{\vec{0}\vec{n}})\hat{S}_{\vec{n}\vec{0}}&=\tfrac{1}{2}\sum_{\rho_1\rho'_1}[V_{\rho\rho'(\rho_1\rho'_1)_a}-(\epsilon_{\nu}+\epsilon_{\nu'})N_{\rho\rho(\rho_1\rho'_1)_a}]\hat{S}_{\rho_1\rho'_1(\nu\nu')_a}\\&+\tfrac{1}{2}\sum_{\nu_1\nu'_1}\hat{S}_{\rho\rho(\nu_1\nu'_1)_a}[V_{\nu'_1\nu'_1(\nu\nu')_a}+(\epsilon_{\rho}+\epsilon_{\rho'})N_{\nu'_1\nu'_1(\nu\nu)_a}]\\&+\sum_{\rho_1\nu_1}\{\hat{S}_{\rho_1\rho(\nu_1\nu)_a}[N_{\rho\nu_1(\rho_1\nu)_a}+(\epsilon_{\rho'}-\epsilon_{\nu'})N_{\rho\nu_1(\rho_1\nu)_a}]+\mathrm{exch}(\rho\rho')(\nu\nu')\}\\&+\Big(\frac{1}{2!}\Big)^2\sum_{\rho_1\rho'_1\nu_1\nu'_1}[N_{\rho\rho'(\rho_1\rho'_1)_a}N_{\nu_1\nu'_1(\nu\nu')_a}+V_{\nu_1\nu'_1(\nu\nu')_a}N_{\rho\rho'(\rho_1\rho'_1)_a}\\&\qquad+4(V_{\rho\nu_1(\rho_1\nu)_a}N_{\rho'\nu'_1(\rho'_1\nu')_a}-V_{\rho\nu_1(\rho_1\nu')_a}N_{\rho'\nu'_1(\rho'_1\nu)_a}-V_{\rho'\nu_1(\rho_1\nu)_a}N_{\rho\nu'_1(\rho'_1\nu')_a})\\&\qquad+V_{\rho'\nu_1(\rho_1\nu')_a}N_{\rho\nu'_1(\rho'_1\nu')_a}]\hat{S}_{\rho_1\rho'_1(\nu_1\nu'_1)_a}\,,\end{aligned} \tag{5.6}$$

where exch $(\rho\rho')(\nu\nu')$ represents a sum of similar terms with ρ interchanged with ρ', and/or ν with ν'. An inspection and classification of the distinct contributions is again most efficiently performed using a graphical language. We have to supplement the graphical elements introduced above by the effective two-body interaction $\mathcal{U}^{(2)}$ (depicted as a wavy line) and the CBF—single-particle (or hole) energies depicted as a dot on a particle or hole line. Some typical diagrams are shown in Fig. 3. The

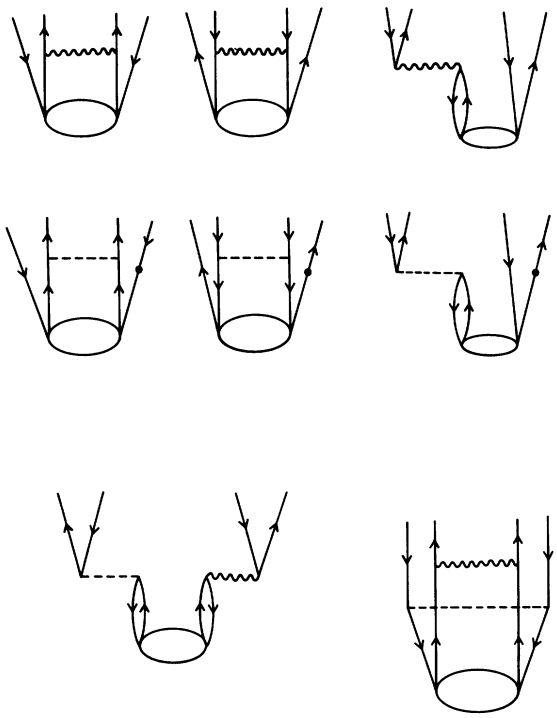

FIG. 3. Some typical diagrams contributing to the correlated coupled-cluster equations for S.

first three diagrams are well known from the conventional exp(S) theory with the bare interaction replaced by the tamed effective interaction $v^{(2)}$. They generate [upon solving the exp(S) equations] particle ladders, hole ladders, and ring diagrams. The next three diagrams show non-orthogonality corrections which are generated from the first diagram by replacing the effective interaction by an $\mathfrak{N}$ line, and substituting a single-particle (or hole) energy on one of the outgoing (or incoming) particle (hole) lines directly attached to $S^{(2)}$. Finally we show some diagram arising from the $d=4$ portions of Eq. (5.6) which represent ladder and ring diagrams containing an interaction line *and* a normalization correction.

We discover already the diagrammatical construction scheme according to which further diagrams contributing to our expansion (5.4) are generated.

The expansion (5.4) of the coupled-cluster equations is represented graphically by the sum of all diagrams which have the following:

(i) Two hole lines entering and two particle lines exiting at the top of each diagram,

(ii) an arbitrary number of $\hat{S}$ elements,

(iii) an arbitrary number of $\mathfrak{N}^{(2)}$ elements,

(iv) one effective interaction operator *or* one single-particle (or hole) energy, and obey the rules [(v) and (vi)],

(v) the $\hat{S}$ elements have only incoming hole lines and outgoing particle lines,

(vi) no $\mathfrak{N}^{(2)}$ line and no $v^{(2)}$ or ϵ element may be connected directly to another $\mathfrak{N}$ element.

The further explicit construction of higher-order contributions to Eq. (5.4) serve essentially to confirm the rules (i) to (vi). [We have in fact worked out all of the terms of the expansion (5.4) which are quadratic in S.] It suffices to sketch the general way the calculation goes. First, we classify the distinct off-diagonal quantities $H'_{\vec{m}\vec{n}}$, $J_{\vec{m}\vec{n}}$ according to the number of plane-wave orbitals in which the states $|\Phi_{\vec{m}}\rangle$ and $|\Phi_{\vec{n}}\rangle$ (one of which will casually be identified with the ground state $|\Phi_{\vec{0}}\rangle$) differ. Products of more than one off-diagonal quantity are sorted in such a way that all terms with the same *sum* of d values are kept together. Due to our choice (6.1) for S, the maximum d value for an nth-order contribution in S will be $d_{\max}=2n+2$. Next, we retain only those portions of the d-body operators, which factorize into products of two body ($v^{(2)}$ or $\mathfrak{N}^{(2)}$) operators. Upon cancellation of all unlinked diagrams we arrive at our final linked expression for a certain nth-order contribution to our equations (5.4). It is not necessary to present all diagrams which we have obtained explicitly; progress is as usual accelerated by studying the *structure* of the expansion and certain *subclasses* of diagrams.

First, we study all diagrams of second order (in S) which contain one N element and have a *common factor* $\epsilon_\rho+\epsilon_{\rho'}-\epsilon_\nu-\epsilon_{\nu'}$. It turns out that (removing the stated common factor) these are identical with the corresponding diagrams appear-

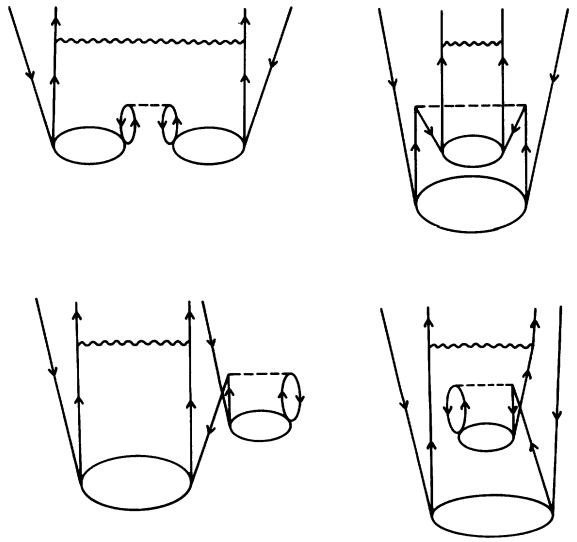

FIG. 4. Diagrams contributing to the correlated coupled-cluster equations which are re-summed through the introduction of the renormalized operator $\mathcal{S}$.

ing in the second-order term of our "dressed" 2p-2h operator $\mathcal{S}$ [Eq. (4.16)]. Identical subseries arise also from diagrams forming extensions of the "particle-ladder", "hole-ladder", etc., diagrams shown in Fig. 3 (see Fig. 4). In fact, in all other cases we have studied, we found the building up of the series (4.16). [This statement may, of course, also be obtained directly from our construction rules (i) to (vi); as already mentioned, further explicit elaboration of the series (5.4) has served merely to confirm these rules.] Consequently, we may re-sum all 2p-h subdiagrams formed from $\hat{S}$ and $\mathfrak{N}$ objects according to the rules of Sec. IV., into the renormalized 2p-2h operator $\mathcal{S}$. Here, we mean by a 2p-h subdiagram a structure, which can be separated from any graph occurring in the expansion (5.4) by cutting two particle and two hole lines. Since (according to our graphical rules), this re-summation can be performed in any place where a bare $\hat{S}$ element appears, we can re-sum vast classes of nonorthogonality corrections by simply replacing everywhere $\hat{S}$ by $\mathcal{S}$ and omitting the diagrams summed in the latter object. By this re-summation procedure we can eliminate $\hat{S}$ entirely from our equations in favor of $\mathcal{S}$, and achieve a considerable simplification of the equations. The rules according to which graphical contributions to our (new) coupled-cluster equations in terms of $\mathcal{U}^{(2)}$, $\mathfrak{N}^{(2)}$, ϵ_α, and $\mathcal{S}$ are constructed are identical with the rules (i)–(vi) given above, with the additional provision (vii) no 2p-h subdiagrams occur in which all external lines enter an $\mathcal{S}$ operator, with the trivial exception of the single $\mathcal{S}$ operator.

The fact that we are able to eliminate these vast classes of nonorthogonality corrections at no extra expense by a simple redefinition $S \to \mathcal{S}$ seems surprising at the first glance. This circumstance may be understood in terms of a transformation of our original nonorthogonal basis (1.5) into another one, which avoids the appearance of the above-mentioned diagrams from the beginning. It is also partly attributable to our choice of working not only with the energy expression (4.4), but also with the Schrödinger equation in the form (5.2). The reader is reminded of the situation in the simple Jastrow variational theory for the energy expectation value: As long as one computes only the energy expectation value $H_{\mathfrak{JJ}}$, one has to specify the Jastrow correlation function and solve for the distribution functions. Upon deriving Euler-Lagrange equations for $f(r)$, one is able to eliminate $f(r)$ entirely from the theory in favor of distribution functions, which are, in terms of $f(r)$, highly re-summed quantities.[36,37]

Next, we study *factorizable* diagrams containing the effective interaction $\mathcal{U}^{(2)}$, noting that all factorizable diagrams containing the normalization function $\mathfrak{N}^{(2)}$ have already been included in $\mathcal{S}$. The former diagrams can appear on *external* lines (Fig. 5) and contribute there to a renormalization of the single particle (and hole) energies through

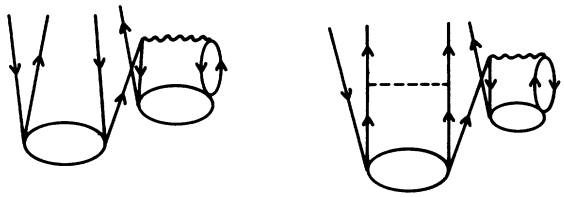

FIG. 5. Factorizable particle- (hole-) line diagrams contributing to the renormalization of the single-particle (hole) energies.

$$e_\rho = \epsilon_\rho + \tfrac{1}{2}\sum_{\rho'\nu\nu'} \mathcal{S}_{\rho\rho'(\nu\nu')_a} V_{\nu\nu'(\rho\rho')_a}\,,$$
$$e_\nu = \epsilon_\nu - \tfrac{1}{2}\sum_{\nu'\rho\rho} V_{\nu\nu'(\rho\rho')_a} \mathcal{S}_{\rho\rho'(\nu\nu')_a}\,. \tag{5.7}$$

Moreover, factorizable particle- and hole-line insertions can also appear on *internal* lines. (See the first diagram of Fig. 6). Such an insertion may be combined with the *energy numerator* part of an associated diagram and a corresponding interaction line (see, for example, the second diagram of Fig. 6) to generate (partially) renormalized energy numerators. [Recall that CBF single-particle energies also enter our effective interaction $\mathcal{U}$; see Eq. (4.9).] This renormalization is, however, not as complete as for the single-particle spectrum in (5.7) according to rule (vi) factorizable insertions can be applied only on *incoming* particle lines and *outgoing* hole lines.

We have thereby arrived at the final form of our equations, defining a self-consistent effective interaction $V^{sc}_{\alpha\beta,\gamma\delta}$ by adding to $V_{\alpha\beta,\gamma\delta}$ all factorizable energy numerator corrections.

For further reference, we display explicitly the final form of our equations, including all terms

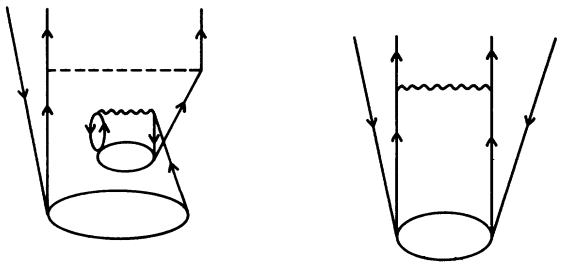

FIG. 6. Renormalization of the *energy numerator* of the effective interaction. The first diagram contributes to the renormalization of the second one, which does already contain the energy numerator parts due to the bare CBF-single-particle energies [see Eq. (4.11)].

linear in $\mathcal{S}$:

$$
\begin{aligned}
0 = {} & V_{\rho\rho'(\nu\nu')_a} + (e_\rho + e_{\rho'} - e_\nu - e_{\nu'})\mathcal{S}_{\rho\rho'(\nu\nu')_a} \\
& + \tfrac{1}{2}\sum_{\rho_1\rho_1'} [V^{sc}_{\rho\rho'(\rho_1\rho_1')_a} - (e_\nu + e_{\nu'})N_{\rho\rho'(\rho_1\rho_1')_a}]\mathcal{S}_{\rho_1\rho_1'(\nu\nu')_a} \\
& + \tfrac{1}{2}\sum_{\nu_1\nu_1'} \mathcal{S}_{\rho\rho'(\nu_1\nu_1')_a}[V^{sc}_{\nu_1\nu_1'(\nu\nu')_a} + (e_\rho + e_{\rho'})N_{\nu_1\nu_1'(\nu\nu')_a}] \\
& + \sum_{\rho\nu_1}\{[V^{sc}_{\rho\nu_1(\rho_1\nu)_a} + (e_{\rho'} - e_{\nu'})N_{\rho\nu_1(\rho_1\nu)_a}]\mathcal{S}_{\rho_1\rho'(\nu'\nu_1)_a} + \mathrm{exch}(\rho,\rho')(\nu,\nu')\} \\
& + \tfrac{1}{4}\sum_{\rho_1\rho'\nu_1\nu_1'} [V^{sc}_{\rho\rho'(\rho_1\rho_1')_a}\mathcal{S}_{\rho_1\rho_1'(\nu_1\nu_1')_a}N_{\nu_1\nu_1'(\nu\nu')_a} + N_{\rho\rho'(\rho_1\rho_1')_a}\mathcal{S}_{\rho_1\rho_1'(\nu_1\nu_1')_a}V^{sc}_{\nu_1\nu_1'(\nu\nu')_a}] \\
& + \sum_{\rho_1\rho_1'\nu_1\nu_1'} [V^{sc}_{\rho\nu_1(\rho_1\nu)_a}N_{\rho'\nu_1'(\rho_1'\nu')_a}\mathcal{S}_{\rho_1\rho_1'(\nu_1\nu_1')_a} + \mathrm{exch}(\rho,\rho'),(\nu,\nu')] + O(\mathcal{S}^2). \qquad (5.8)
\end{aligned}
$$

Clearly, our theory contains first of all terms of the conventional exp(S) equations for $S^{(2)}$, but with the bare interaction replaced by V^{sc}, and the bare kinetic energies replaced by the CBF single-particle energies ϵ_α. (In contradistinction to the conventional theory, no diagonal-matrix elements of V^{sc} appear, since the diagonal portions of the interaction are already absorbed in ϵ_α.) Beyond these conventional terms we have an infinite series of nonorthogonality corrections involving the explicit occurence of $\mathfrak{N}^{(2)}$, whose treatment calls for a suitable truncation scheme. We shall discuss this point in the next section.

VI. DISCUSSION AND COMPARISON WITH OTHER THEORIES

By construction, our theory still admits manifold possibilities for further re-summation of nonorthogonality corrections. These further elaborations would, however, be somehow in contradiction to the original aim of our work. Owing to the application of a Jastrow correlation operator we expect that the tamed effective interaction $v^{(2)}$ will turn out to be weak enough that rather simple approximations to our equations are sufficient for an accurate description of the many-body system. We have already mentioned the simplest approximation, retaining only the first two terms of the expansion (5.8):

$$
\mathcal{S}^{CBF}_{\rho\rho'(\nu\nu')_a} = -\frac{V_{\rho\rho'(\nu\nu')_a}}{e_\rho + e_{\rho'} - e_\nu - e_{\nu'}} \qquad (6.1)
$$

which generates through Eq. (4.11) the second-order CBF correction. Next, the CBF analog of the Bethe-Goldstone (BG) equation is obtained by retaining only particle-ladder diagrams, i.e., truncating the expansion (5.8) after the third term:

$$
\mathcal{S}^{BG}_{\rho\rho'(\nu\nu')_a} = -\frac{1}{e_\rho + e_{\rho'} - e_\nu - e_{\nu'}}\left(V_{\rho\rho'(\nu\nu')_a} + \sum_{\rho_1\rho_1'} [V^{sc}_{\rho\rho'(\rho_1\rho_1')_a} - (e_\nu + e_{\nu'})N_{\rho\rho'(\rho_1\rho_1')_a}]\mathcal{S}^{BG}_{\rho_1\rho_1'(\nu\nu')_a}\right). \qquad (6.2)
$$

An especially promising feature of our theory is that we also are able to include ring diagrams without having to be concerned with the inclusion of $S^{(3)}$, while in the conventional exp(S) theory $S^{(3)}$ must be invoked to cancel the short-ranged repulsive part of the bare two-body interaction. One may expect that these ring diagrams play an important role in the calculation of transport coefficients. This is also the point at which the infinite series of chain diagrams re-enter our theory; whereas, when considering only the energy expectation value, ring diagrams have to be summed explicitly for any correlation operator, these diagrams enter our theory through iteration of the equations.

In short, we may characterize the relation between our theory and the conventional exp(S) theory as follows: By the introduction of an explicit correlation operator F we can replace the strong, bare two-particle interaction by a weak, effective interaction $v^{(2)}$. This will first of all result in a better convergence of the augumented truncation schemes for the equations determining $\mathcal{S}$. Moreover, we are no longer bound to truncation schemes which take care of the core repulsion of the bare interaction step by step. The summation of the above-mentioned ring diagrams is just one example; the use of self-consistent particle energies provides another one.[38] Quite generally, we can generate, through suitable truncation and iteration of our equations, the CBF analogs of all special classes of Goldstone diagrams which may be of

interest in traditional many-body theory. Therefore, our theory may also be understood as the construction of an explicit mapping of the bare particle description into a "quasiparticle" description of a many-body system. In this quasiparticle picture, we are in principle able to generalize all the well-known descriptions of a system of weakly interacting particles, without burdening (as in a purely variational approach) the correlation operator F with the incorporation of complicated state-dependent effects.

How does our theory compare to other, purely variational methods which do incorporate state-dependent components into the wave function via the correlation operator F? These methods suffer predominantly from the noncommuting features of two general two-body $f(i,j)$ employed in (1.4). Our choice of the correlation operator (note that we could simply redefine $\mathrm{Fe}^S \to F$) obviates this problem from the outset, since all S operators commute. Further simplification is reached by choosing an appropriate form for the ground-state energy: Using expression (3.9) rather than the representation as an expectation value (3.7), we eliminate all "operator-chain" diagrams from the energy expression, since these can enter only via chains of S^* and S elements. The final resummation of S into its "renormalized" counterpart $\mathcal{S}$ eliminates ultimately all chain diagrams of S and $\mathfrak{N}$ operators with the exception of their generators.

The method proposed here is somewhat related to Owen's independent-pair ansatz for the correlation operator F,[29]

$$F = \prod_{i<j} f_c(r_{ij}) \sum_{i<j} (1 + U_{ij}) = \prod_{i<j} f_c(r_{ij})(1 + U + \tfrac{1}{2}U^2 + \cdots) \qquad (6.3)$$

with

$$U = \sum_{i<j} U_{ij},$$

where the sum runs over all pairs having no particle in common. Owen's basic idea is closely related to ours: Use the complete Jastrow product form for the purely radial correlations, and treat more complicated correlations by means of the independent-pair form, which is far more tractable than (1.4). The complete correlation operator of the present work may be written, if we use the two-body Jastrow choice for F,

$$\mathrm{Fe}^{S^{(2)}} = \prod_{i<j} f_c(r_{ij})(1 + S^{(2)} + \tfrac{1}{2}S^{(2)2} + \cdots) \qquad (6.4)$$

clearly establishing the correspondence to Owen's scheme. The conceptual difference is that in our approach we arrive at an independent-pair type of wave function through the definition of the *two-body* correlation operator $S^{(2)}$, whereas in Owen's theory this wave function is generated through the definition of the *many-body* correlation operator F. Using the energy expression (3.9) and in particular the correlated Schrödinger equation (3.10) instead of a variational determination of S simplifies our present approach so much that use of the *completely general* form for $S^{(2)}$ used above becomes feasible, whereas only restricted forms have been treated in the variational method.

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