Coupled-cluster method in Fock space. I. General formalism

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The problem of finding the spectrum of the Fock-space Hamiltonian $\hat{H}$ for a system of many fermions is analyzed. The quasiparticle formalism is employed, with "holes" and "particles" defined with respect to some N-particle determinantal wave function (the model vacuum). The basic idea behind the proposed approach is to perform a similarity transformation of Hamiltonian $\hat{H}$, such that the resulting effective Hamiltonian $\hat{G}$ is, unlike $\hat{H}$, a quasiparticle-number—conserving operator. It is shown that eigenvalues of $\hat{G}$, corresponding to small numbers of quasiparticles (0,1,2) can be easily calculated. This is equivalent to finding eigenvalues of $\hat{H}$ for certain states of N, $N\pm1$, and $N\pm2$ particles. The construction of the operator transforming $\hat{H}$ into $\hat{G}$ (the wave operator) stems from an analysis of the structure of the algebra of linear operators acting in a (finite-dimensional) Fock space. The exponential *Ansatz* for the wave operator is used, resulting in a generalization of the coupled-cluster (CC) method of Coester [Nucl. Phys. 7, 421 (1958)]. The generalized CC equations determining the wave operator, and equations determining the effective Hamiltonian $\hat{G}$, are presented in a diagrammatic form. An effort has been made to obtain a concise notation for expressing these equations in an algebraic form. Approximation schemes, necessary for practical applications of the proposed method, are also studied.

I. INTRODUCTION

The quantum many-body problem appears as a key issue in theoretical studies of electronic and nucleonic systems (finite and extended), and quantum fluids composed of helium isotopes. In this paper we propose a new approach to the nonrelativistic, time-independent problem of many fermions. Our considerations apply to a model known as the algebraic approximation.[1] In this model the Hamiltonian $\hat{\mathscr{H}}$ of a many-particle system is approximated by the projected Hamiltonian $\hat{H}=\hat{\mathscr{P}}\hat{\mathscr{H}}\hat{\mathscr{P}}$, where $\hat{\mathscr{P}}$ is an idempotent projector onto a certain finite-dimensional Hilbert space $\mathfrak{M}$. The construction of $\mathfrak{M}$ involves choosing a finite set of one-particle functions (spin orbitals); these functions are then used to generate a set of many-particle determinantal wave functions (configurations) which span $\mathfrak{M}$. The algebraic structure of the considered model becomes especially rich when $\mathfrak{M}$ is chosen to be a Fock space, i.e., it is spanned by all the possible configurations generated without fixing the number of particles in the system. In quantum chemistry, the use of the Fock-space Hamiltonian $\hat{H}$ was advocated by Kutzelnigg.[2] Our paper pursues this approach, albeit in a somewhat different fashion.

The exact solution to the many-particle problem in the algebraic approximation is provided by the full configuration-interaction (full CI) method in which diagonalization of matrix $\mathbf{H}$ (the matrix representation of operator $\hat{H}$ in the basis set of all configurations) is performed. This direct approach is seldom applied, because the dimensions of the matrices involved (these are diagonal blocks of $\mathbf{H}$, corresponding to symmetry properties of Hamiltonian $\hat{H}$) are usually very large. Among many methods devised for approximate calculations of eigenvalues of $\hat{H}$, the coupled-cluster (CC) method[3–5] occupies a special position since it is neither perturbative nor variational. In this approach, hereafter referred to as the single-reference CC method, some eigenfunction Ψ (usually representing a closed-shell ground state of the considered many-particle system), and the corresponding eigenvalue E of Hamiltonian $\hat{H}$ are determined by performing a similarity transformation

$$\hat{H}\rightarrow\hat{G}=\hat{\Omega}^{-1}\hat{H}\hat{\Omega}\ . \tag{1}$$

$\hat{\Omega}$ is here a wave operator such that $\Psi=\hat{\Omega}\Phi$ and Φ is some chosen determinantal wave function called the reference configuration. The CC method uses a characteristic prescription for constructing the wave operator: $\hat{\Omega}=\exp(\hat{T})$, and the CC operator $\hat{T}$ is expanded as a linear combination of so-called particle-hole operators. The important property of these operators is that they form an algebra that is nilpotent (and, incidentally, commutative). The linear parameters (the CC amplitudes) which appear in the definition of operator $\hat{T}$ can be calculated by solving a set of coupled nonlinear algebraic equations. These so-called CC equations are derived from the eigenvalue problem for the effective Hamiltonian $\hat{G}$:

$$\hat{G}\Phi=E\Phi\ . \tag{2}$$

The single-reference CC method is capable of providing the exact value of energy E, but this would require a numerical effort comparable to that of the full CI method. A very substantial reduction of the number of the CC equations can be achieved when a truncated expansion of operator $\hat{T}$ is used. This approximation proved to be

highly effective and, unlike a truncated CI treatment, it preserves the so-called size consistency (or size extensivity, see Ref. 5) of the calculated value of E.

Several generalizations of the single-reference CC method, devised to treat open-shell states of Hamiltonian $\hat{H}$, have been proposed.[6-10] Each of these methods, hereafter referred to as multireference CC methods, deals explicitly with several eigenstates of $\hat{H}$. The generalized CC method of the present paper is related, in some respects, to the methods of Mukherjee *et al.*[6] and Offerman *et al.*[7] Being essentially a single-reference approach, this method is formulated such that the entire spectrum of the Fock-space Hamiltonian $\hat{H}$ can be analyzed. There is no need for choosing a so-called model space in this approach, thus eliminating complications due to the classification of spin orbitals (the partition into core, valence, and virtual spin orbitals), and the occurrence of so-called unlinked terms when the model space is incomplete (see Ref. 10). We use the quasiparticle formalism in which the physical particles are formally replaced by quasiparticles: "holes" and "particles," defined with respect to the reference configuration Φ. This gives rise to an algebraic field-theoretical model, with Φ being the (model) vacuum, and the remaining configurations representing states with integer (greater than zero) number of quasiparticles. The Hamiltonian $\hat{H}$, being a particle-number—conserving operator, is not a quasiparticle-number—conserving operator when expressed in the quasiparticle formalism. This defect can be "corrected" with the help of a suitable "universal"[2] wave operator $\hat{\Omega}$, and in our generalization of the single-reference CC method condition (2) is supplemented by the requirement that the effective Hamiltonian $\hat{G}$ is a quasiparticle-number—conserving operator. The universal wave operator $\hat{\Omega}$ is constructed using the exponential Ansatz. Actually, we found that, although a "biexponential" form of $\hat{\Omega}$ is formally necessary in this case, we can achieve our goal with $\hat{\Omega}_{\rm ex}=\exp(\hat{\Theta})$. $\hat{\Theta}$ is here a generalized CC operator, and is expressed as a linear combination of so-called excitation operators. These operators form the largest nilpotent subalgebra contained in the algebra of all linear operators in the Fock space $\mathfrak{M}$. We also show that if the model vacuum Φ is fully symmetric with respect to the symmetry group of Hamiltonian $\hat{H}$, operators $\hat{\Theta}$ and $\hat{G}$ are symmetry adapted, i.e., they commute with all the symmetry operators of this group. This makes the spin-adapted version of the method possible.

The formulation of the CC method considering the entire spectrum of $\hat{H}$ is chosen here to illustrate the completeness of the underlying mathematical treatment, but is obviously impractical. We show, however, how by applying standard approximations (truncating the CC operator $\hat{\Theta}$) a tractable computational scheme emerges. In this approach energy E of the model vacuum, and energies of these states of $\hat{H}$ which (as eigenstates of $\hat{G}$) correspond to a small number of quasiparticles can be calculated. Even if we restrict our consideration to states with only 0, 1, and 2 quasiparticles (see the forthcoming paper,[11] hereafter referred to as paper II), this treatment provides an access to a fairly broad excitation spectrum of the system. This approach can be used to formulate a correlated band theory of crystals.[12]

The plan of the present paper is as follows. In Sec. II the construction of the Fock space is outlined. The quasiparticle formalism is introduced in Sec. III. Section IV contains an analysis of the algebraic structure of linear operators in the Fock space $\mathfrak{M}$, leading to the construction of the universal wave operator $\hat{\Omega}$. In Sec. V the structure of the effective Hamiltonian $\hat{G}$ is discussed, and generalized CC equations are defined. A diagrammatic form of these equations is studied in Sec. VI. A scheme of systematic approximations, necessary for practical applications of the method, is presented in Sec. VII. There are also three appendixes with some supplementary material.

II. FOCK SPACE

We consider a system of many fermions (e.g., electrons, nucleons, or ^{3}He atoms) embedded in an external, stationary field represented by a one-particle potential $\hat{u}$. The interparticle interactions are described by a two-particle potential $\hat{v}$ (three- and more-body forces can be taken into account, if necessary). The Hamiltonian for this system, for arbitrary numbers of particles, has the form

$$\hat{\mathscr{H}}=\bigoplus_{n=0}^{\infty}\hat{\mathscr{H}}_n\ , \tag{3}$$

where $\hat{\mathscr{H}}_n$ is the n-particle Hamiltonian

$$\hat{\mathscr{H}}_n=W+\sum_{i=1}^{n}\hat{h}(i)+\sum_{\substack{i,j=1\\(i<j)}}^{n}\hat{v}(i,j)\ , \tag{4}$$

$$\hat{h}=-\frac{1}{2m_0}\nabla^2+\hat{u}\ , \tag{5}$$

and m_0 is the particle mass. In Eq. (4), W is a constant term; in electronic systems, e.g., molecules, it represents the internuclear Coulombic repulsion.

In the algebraic approximation some finite (say, M-element) set of spin orbitals is chosen. This set, assumed to be linearly independent, spans an M-dimensional space $\aleph$. Let

$$\{\phi_i\}_{i=1}^{i=M} \tag{6}$$

be an orthonormal basis in $\aleph$. The set of annihilation operators, corresponding to set (6), can be constructed following the definition

$$\begin{aligned}\hat{a}_i\Psi(1,2,\ldots,n)&=n^{1/2}\int d\tau_n\phi_i^*(n)\Psi(1,2,\ldots,n)\\&=(\hat{a}_i\Psi)(1,2,\ldots,n-1)\ ,\end{aligned} \tag{7}$$

where we restrict the domain of $\hat{a}_i$ to antisymmetric Ψ's. The creation operators are defined as

$$\hat{a}^{\,i}=(\hat{a}_i)^{\dagger}\ . \tag{8}$$

The algebra generated by the set $\{\hat{a}_i,\hat{a}^{\,i}\}_{i=1}^{i=M}$ will be called here the Fermi-Dirac (FD) algebra, and denoted by $\mathscr{F}=\mathscr{F}(M)$. This algebra is characterized by the following anticommutation relations

$$\begin{aligned}&[\hat{a}_i,\hat{a}_j]_+=[\hat{a}^{\,i},\hat{a}^{\,j}]_+=0\ ,\\&[\hat{a}_i,\hat{a}^{\,j}]_+=\delta_i{}^j\ .\end{aligned} \tag{9}$$

Transformations of the annihilation and creation operators (jointly, they will be referred to as the fermion operators), induced by unitary transformations of the spin-orbital basis (6), are discussed in Appendix A.

The eigenstate Φ_0 of Hamiltonian $\hat{\mathscr{H}}$, corresponding to $n=0$ (physical vacuum), fulfills the equations

$$\hat{a}_i\Phi_0=0 , \tag{10}$$

for $i=1,2,\ldots,M$. Φ_0 and the set of creation operators $\{\hat{a}^i\}$ can be used to generate the Fock space $\mathfrak{M}=\mathfrak{M}(M)$

$$\mathfrak{M}=\bigoplus_{n=0}^{M}\mathfrak{M}_n , \tag{11}$$

where $\mathfrak{M}_0$ is spanned by Φ_0, $\mathfrak{M}_1$ is spanned by $\{\hat{a}^i\Phi_0\}$, $\mathfrak{M}_2$ is spanned by $\{\hat{a}^j\hat{a}^i\Phi_0,\ i<j\}$, etc. The functions spanning subspace $\mathfrak{M}_n$ can be expressed as Slater determinants built of n spin orbitals from basis (6); they are called configurations. It is easy to find that the dimension of $\mathfrak{M}_n$ is

$$\begin{bmatrix} M \\ n \end{bmatrix}=\frac{M!}{n!(M-n)!} . \tag{12}$$

Hence, the dimension of the Fock space (11) is

$$\sum_{n=0}^{M}\begin{bmatrix} M \\ n \end{bmatrix}=2^M . \tag{13}$$

Operators belonging to the FD algebra $\mathscr{F}$ are all linear operators acting in $\mathfrak{M}$. As a vector space, $\mathscr{F}$ is spanned by the set

$$\{\hat{X}^\dagger\hat{Y}\} , \tag{14}$$

where operators $\hat{X}$ and $\hat{Y}$ are represented by products ("strings") of annihilation operators, e.g.,

$$\hat{X}=\hat{a}_i\hat{a}_j\cdots , \tag{15a}$$

with $i<j<\cdots$. The number of annihilation operators in string $\hat{X}$ will be denoted by x; for $x=0$ we assume

$$\hat{X}=1 . \tag{15b}$$

An operator string of the form $\hat{X}^\dagger\hat{Y}$, where $\hat{X}$ and $\hat{Y}$ are defined in Eqs. (15), is called the normal product of fermion operators. There are exactly 2^M different strings (15) [see Eq. (13)], hence the dimension of the vector space $\mathscr{F}$ is $(2^M)^2=2^{2M}$. We conclude that the FD algebra $\mathscr{F}$ is identical with the algebra of all linear operators acting in $\mathfrak{M}$ (the so-called endomorphisms of $\mathfrak{M}$).

Any linear operator in the Fock space $\mathfrak{M}$ can be written as a linear combination of operators from basis (14). In particular, the projection of Hamiltonian (3) on $\mathfrak{M}$ has a simple form

$$\hat{H}=W+h_i{}^j\hat{a}^i\hat{a}_j+\tfrac{1}{4}v_{ij}{}^{kl}\hat{a}^j\hat{a}^i\hat{a}_k\hat{a}_l , \tag{16}$$

where the Einstein convention is used to indicate unrestricted summations over repeated upper and lower indices; this convention will be used whenever possible throughout this paper. The parameters appearing in Eq. (16) are so-called one-particle integrals

$$h_i{}^j=\langle\phi_i\,|\,\hat{h}\phi_j\rangle , \tag{17a}$$

and (antisymmetrized) two-particle integrals

$$v_{ij}{}^{kl}=\langle\phi_i(1)\phi_j(2)\,|\,v(1,2)\phi_k(1)\phi_l(2)\rangle - \langle\phi_i(1)\phi_j(2)\,|\,v(1,2)\phi_l(1)\phi_k(2)\rangle . \tag{17b}$$

In Eqs. (17), because of the orthonormality of basis (6), one can shift indices between the lower (covariant) and upper (contravariant) position:

$$h_i{}^j=h^{i,j}=h^i{}_j=h_{i,j} \tag{18a}$$

$$v_{ij}{}^{kl}=v^{ij,kl}=v^{ij}{}_{kl}=v_{ij,kl} . \tag{18b}$$

Since operators $\hat{h}$ and $\hat{v}$ are assumed to be Hermitian, it follows that

$$h_i{}^j=(h^j{}_i)^* , \tag{19a}$$

$$v_{ij}{}^{kl}=(v^{kl}{}_{ij})^* . \tag{19b}$$

According to definition (17b) parameters $v_{ij}{}^{kl}$ are antisymmetric with respect to (separate) permutations of their lower and upper indices.

An important linear operator in the Fock space is the particle-number operator

$$\hat{N}=\hat{a}^i\hat{a}_i \tag{20}$$

corresponding to the structure revealed in Eq. (11):

$$\hat{N}\chi=n\chi \tag{21}$$

for $\chi\in\mathfrak{M}_n$. The commutation relation

$$[\hat{H},\hat{N}]_-=0 \tag{22}$$

indicates that Hamiltonian $\hat{H}$ is a particle-number $\hat{N}$ conserving operator.

III. QUASIPARTICLE FORMALISM

In the algebraic approximation it is usually assumed that the one-particle space $\mathfrak{K}$ is invariant with respect to the symmetry group of Hamiltonian $\hat{\mathscr{H}}$ of Eq. (3). In this case Hamiltonian $\hat{H}$ of Eq. (16) is also invariant with respect to this symmetry group. We would like to put aside the question of what is the optimal choice of $\mathfrak{K}$ for a given M. We notice, however, that probably only a very small fraction of 2^M eigenfunctions of $\hat{H}$ can provide acceptable approximations for some eigenfunctions of $\hat{\mathscr{H}}$. Suppose that $\mathfrak{K}$ has been chosen such that a certain N-particle eigenfunction of $\hat{H}$, Ψ, can be regarded as a good approximation to an eigenfunction of $\hat{\mathscr{H}}$. We shall assume that Ψ is nondegenerate and corresponds to the lowest eigenvalue of $\hat{H}$ in subspace $\mathfrak{M}_N$ (although these assumptions are not essential to our further considerations). If $\mathfrak{K}$ is suitably chosen one can expect that also some other eigenfunctions of $\hat{\mathscr{H}}$ describing a few lowest excited N-particle states, as well as certain $(N-1)$- and $(N+1)$-particle states, can be fairly represented by appropriate eigenfunctions of $\hat{H}$.

Let us consider an N-particle determinantal wave functions Φ, expressed in terms of spin orbitals from $\mathfrak{K}$. Φ is chosen to be an approximation to Ψ, although we need not

assume that Φ is optimal, e.g., as Hartree-Fock-Roothaan (HFR) (Ref. 13) wave function, maximum-overlap configuration (see Ref. 14, and references therein), etc. From the formal point of view it is sufficient to require

$$\langle \Phi \mid \Psi \rangle \neq 0 \ . \tag{23}$$

The choice of Φ determines the partition

$$\aleph = \aleph_{\rm h} \oplus \aleph_{\rm p} \ , \tag{24}$$

where $\aleph_{\rm h}$ is spanned by the spin orbitals occupied in Φ. We shall assume that the basis set (6) is chosen such that

$$\{\phi_\rho\}_{\rho=1}^{\rho=N} \tag{25a}$$

spans subspace $\aleph_{\rm h}$, and

$$\{\phi_r\}_{r=N+1}^{r=M} \tag{25b}$$

spans $\aleph_{\rm p}$. Due to requirements of the spin symmetry M and N must be even. From now on indices $\rho,\sigma,\ldots$ are used to enumerate the spin orbitals occupied in Φ, indices $r,s,\ldots$ are used for unoccupied spin orbitals, and indices $i,j,\ldots$ are used for both types of spin orbitals.

The notion of quasiparticles is introduced via transformation: $\hat{a}_i \rightarrow \hat{b}_i$, where the new fermion operators

$$\{\hat{b}_i, \hat{b}^{\,i}\}_{i=1}^{i=M} \tag{26}$$

must fulfill the same anticommutation relations (9) as the old ones. The most general linear transformation of this kind is the Bogoliubov-Valatin transformation.[15] Here we employ a special case of this transformation, namely the particle-hole transformation:

$$\hat{b}_\rho = \hat{a}^{\,\rho} \tag{27a}$$

for $\rho = 1,2,\ldots,N$; and

$$\hat{b}_r = \hat{a}_r \tag{27b}$$

for $r = N+1, N+2, \ldots, M$. Now, the operators $\hat{b}_\rho$ and $\hat{b}_r$ describe the annihilation of the quasiparticle "holes" and "particles," respectively. Our reference configuration Φ satisfies the equations

$$\hat{b}_i \Phi = 0 \ , \tag{28}$$

for $i = 1,2,\ldots,M$. [Compare Eq. (10) for the physical vacuum Φ_0.] Thus, Φ serves as the vacuum state in the quasiparticle formalism, and is referred to as the model vacuum. (Kutzelnigg[2] calls Φ the physical vacuum; the name "Fermi vacuum" is also sometimes used.)

With the help of the model vacuum Φ and the set of creation operators $\{b^i\}$ a new structure of the Fock space can be introduced:

$$\mathfrak{M} = \bigoplus_{n=0}^{M} \tilde{\mathfrak{M}}_n \ , \tag{29}$$

where $\tilde{\mathfrak{M}}_0$ is spanned by Φ, $\tilde{\mathfrak{M}}_1$ is spanned by $\{\Phi^i = \hat{b}^{\,i}\Phi\}$, $\tilde{\mathfrak{M}}_2$ is spanned by $\{\Phi^{ij} = \hat{b}^{\,j}\hat{b}^{\,i}\Phi,\ i<j\}$, etc. Further partitioning of subspaces $\tilde{\mathfrak{M}}_n$ is possible when a distinction between "holes" and "particles" is made:

$$\tilde{\mathfrak{M}}_1 = \tilde{\mathfrak{M}}_{\rm h} \oplus \tilde{\mathfrak{M}}_{\rm p} \ , \tag{30a}$$

where $\tilde{\mathfrak{M}}_{\rm h} \subset \mathfrak{M}_{N-1}$ is spanned by $\{\Phi^\rho\}$, and $\tilde{\mathfrak{M}}_{\rm p} \subset \mathfrak{M}_{N+1}$ is spanned by $\{\Phi^r\}$;

$$\tilde{\mathfrak{M}}_2 = \tilde{\mathfrak{M}}_{\rm hh} \oplus \tilde{\mathfrak{M}}_{\rm hp} \oplus \tilde{\mathfrak{M}}_{\rm pp} \ , \tag{30b}$$

where $\tilde{\mathfrak{M}}_{\rm hh} \subset \mathfrak{M}_{N-2}$ is spanned by $\{\Phi^{\rho\sigma},\ \sigma<\rho\}$, $\tilde{\mathfrak{M}}_{\rm hp} \subset \mathfrak{M}_N$ is spanned by $\{\Phi^{\rho r}\}$, $\tilde{\mathfrak{M}}_{\rm pp} \subset \mathfrak{M}_{N+2}$ is spanned by $\{\Phi^{rs},\ r<s\}$, etc.

Operators $\hat{H}$ and $\hat{N}$ defined in Sec. II [see Eqs. (16) and (20), respectively] have to be expressed using the new fermion operators (26). This can be done simply by inserting Eqs. (27) into appropriate expressions. Some additional effort is necessary to put the fermion operator strings in these expressions into the normal product form with respect to new fermion operators. This can be done conveniently by using the time-independent Wick's theorem.[16] Hamiltonian $\hat{H}$ in the quasiparticle representation becomes

$$\begin{aligned}\hat{H} = \eta &+ \eta_i{}^j \hat{b}^{\,i}\hat{b}_j + \tfrac{1}{2}\eta^{ij}\hat{b}_i\hat{b}_j + \tfrac{1}{2}\eta_{ij}\hat{b}^{\,j}\hat{b}^{\,i} + \tfrac{1}{4}\eta_{ij}{}^{kl}\hat{b}^{\,j}\hat{b}^{\,i}\hat{b}_k\hat{b}_l \\ &+ \tfrac{1}{6}\eta_i{}^{jkl}\hat{b}^{\,i}\hat{b}_j\hat{b}_k\hat{b}_l + \tfrac{1}{6}\eta_{ijk}{}^{l}\hat{b}^{\,k}\hat{b}^{\,j}\hat{b}^{\,i}\hat{b}_l \\ &+ \tfrac{1}{24}\eta^{ijkl}\hat{b}_i\hat{b}_j\hat{b}_k\hat{b}_l + \tfrac{1}{24}\eta_{ijkl}\hat{b}^{\,l}\hat{b}^{\,k}\hat{b}^{\,j}\hat{b}^{\,i} \ .\end{aligned} \tag{31}$$

The linear parameters appearing on the right-hand side (rhs) of the above equations can be expressed through the one- and two-particle integrals (17) as follows:

$$\eta = W + \tfrac{1}{2}(h_\rho{}^\rho + f_\rho{}^\rho) \ , \tag{32a}$$

where we introduce new parameters

$$f_i{}^j = h_i{}^j + v_{\sigma i}{}^{\sigma j} \ ; \tag{32b}$$

$$\eta_i{}^j = \begin{cases} \eta_\rho{}^\sigma = -f_\sigma{}^\rho \ , \\ \eta_r{}^s = f_r{}^s \ ; \end{cases} \tag{32c}$$

$$\eta_{ij} = (\eta^{ij})^* = \eta_{\rho r} = f_r{}^\rho \ , \tag{32d}$$

for $i<j$;

$$\eta_{ij}{}^{kl} = \begin{cases} \eta_{\rho\sigma}{}^{\tau\upsilon} = v_{\tau\upsilon}{}^{\rho\sigma} \\ \eta_{\rho r}{}^{\sigma s} = -v_{\sigma r}{}^{\rho s} \\ \eta_{rs}{}^{tu} = v_{rs}{}^{tu} \ , \end{cases} \tag{32e}$$

for $i<j$, $k<l$;

$$\eta_{ijk}{}^{l} = (\eta_l{}^{ijk})^* = \begin{cases} \eta_{\rho\sigma r}{}^{\tau} = -v_{\tau r}{}^{\rho\sigma} \\ \eta_{\rho rs}{}^{t} = v_{rs}{}^{\rho t} , \end{cases} \tag{32f}$$

for $i<j<k$;

$$\eta_{ijkl} = (\eta^{ijkl})^* = \eta_{\rho\sigma rs} = -v_{rs}{}^{\rho\sigma} \tag{32g}$$

for $i<j<k<l$. Parameters η_{ij}, $\eta_{ij}{}^{kl}$, etc., are assumed to be antisymmetric with respect to permutations of the

lower (and upper) indices. Since this property is not automatically satisfied by the rhs's of Eqs. (32d)—(32g), one has to put, for instance,

$$\eta_{r\rho}=-f_{\rho}{}^{r}\ , \tag{32h}$$

etc. Parameters not defined in Eqs. (32) are identically equal to zero. The scalar parameter of Eq. (32a) is equal to the mean value of Hamiltonian $\hat{H}$ in the state described by Φ:

$$\eta=\langle\Phi\,|\,\hat{H}\,|\,\Phi\rangle\ . \tag{33}$$

Parameters of Eq. (32b) define the so-called HFR operator $\hat{f}$ which can be conveniently expressed using the fermion operators of Sec. II:

$$\hat{f}=f_i{}^j\hat{a}^i\hat{a}_j\ . \tag{34}$$

In the quasiparticle representation involving the fermion operators (27) the particle-number operator can be written in the form

$$\hat{N}=N+\hat{Q}\ , \tag{35}$$

where N is the number of particles in state Φ and $\hat{Q}$ is what we call the pseudocharge operator

$$\hat{Q}=-\hat{b}^{\rho}\hat{b}_{\rho}+\hat{b}^{r}\hat{b}_{r}\ . \tag{36}$$

Configurations spanning the Fock space $\mathfrak{M}$ [see Eqs. (29) and (30)] are eigenfunctions of $\hat{Q}$:

$$\hat{Q}\Phi=0 \tag{37a}$$

$$\hat{Q}\Phi^{\rho}=-\Phi^{\rho}\ , \tag{37b}$$

$$\hat{Q}\Phi^{r}=\Phi^{r}\ , \tag{37c}$$

etc. It is easy to observe that each "hole" contributes (-1) and each "particle" $(+1)$ to the total pseudocharge. This quantity may be interpreted as the quantum number distinguishing between "holes" and "particles," see Eqs. (37b) and (37c). The pseudocharge cannot be identified with the charge of the physical particles, because Eqs. (37b) and (37c) are true also for systems of neutral particles (neutrons or ^{3}He). The commutation relation (22) is equivalent to

$$[\hat{H},\hat{Q}]_-=0\ , \tag{38}$$

which can be interpreted as the pseudocharge symmetry of Hamiltonian $\hat{H}$. We shall treat it on the same footing as other symmetries of $\hat{H}$. If the Bogoliubov-Valatin[15] transformation of a general kind is used to define fermion operators (26), the corresponding (generalized) configurations are no longer eigenfunctions of the pseudocharge operator $\hat{Q}=\hat{N}-N$. Hence, the Bogoliubov quasiparticles correspond to indefinite pseudocharge.

It will be useful to introduce the quasiparticle-number operator

$$\hat{N}_q=\hat{b}^i\hat{b}_i\ . \tag{39}$$

It is easy to check that Hamiltonian $\hat{H}$ is not quasiparticle-number conserving,

$$[\hat{H},\hat{N}_q]_-\neq 0\ . \tag{40}$$

Moreover, the model vacuum Φ is not an eigenfunction of $\hat{H}$. Φ is hence "unstable," and its time evolution would create an admixture of states (configurations) with one, two, etc., "hole"-"particle" pairs. In Sec. IV we shall construct the universal wave operator $\hat{\Omega}$ transforming $\hat{H}$ into the effective Hamiltonian $\hat{G}$ [see formula (1)] fulfilling

$$[\hat{G},\hat{N}_q]_-=0\ . \tag{41}$$

It can be shown that the above condition implies also Eq. (2), where now E replaces η of Eqs. (32a) and (33), as the true energy of the model vacuum Φ.

IV. CONSTRUCTION OF UNIVERSAL WAVE OPERATOR

In this section we will discuss the structure of the FD algebra $\mathcal{F}$. This analysis is helpful in constructing the universal wave operator $\hat{\Omega}$. The set of generators of $\mathcal{F}$ is chosen in the form (26) where definition (27) applies. The vector-space structure of $\mathcal{F}$ is determined by basis (14), where operators $\hat{X}$ and $\hat{Y}$ are defined as in Eqs. (15), with $\{\hat{a}_i\}$ replaced by $\{\hat{b}_i\}$. It is useful to consider strings $\hat{X}$ as composed of operators $\hat{b}_i$ taken in an arbitrary order. The corresponding strings of indices will be denoted by X, with the special case of an ordered set of indices [see Eq. (15a)] denoted by $\overline{X}$. Again, we use symbol x for the number of operators $\hat{b}_i$ in string $\hat{X}$. The basis of the vector space $\mathcal{F}$ can now be written in the form

$$\{\hat{X}^{\dagger}\hat{Y}:\ X=\overline{X},\ Y=\overline{Y}\}_{x,y=0}^{x,y=M}\ . \tag{42}$$

The basis of the Fock space $\mathfrak{M}$, composed of configurations [see Eqs. (29) and (30)], reads

$$\{\Phi^X:\ X=\overline{X}\}_{x=0}^{x=M}\ , \tag{43}$$

where

$$\tilde{\mathfrak{M}}_x\ni\Phi^X=\hat{X}^{\dagger}\Phi\ . \tag{44}$$

For any $\hat{X}$, one can express its "length" x as

$$x=x_{\mathrm{h}}+x_{\mathrm{p}}\ , \tag{45}$$

where x_{h} (x_{p}) is the number of "hole" ("particle") annihilation operators in $\hat{X}$. Equation (37) for the pseudocharge operator of Eq. (36) can now be written in a compact form

$$\hat{Q}\Phi^X=(x_{\mathrm{p}}-x_{\mathrm{h}})\Phi^X\ . \tag{46}$$

The orthonormality of basis (43) can be used to define the generalized Kronecker delta

$$\delta_X{}^Y=\langle\Phi^X\,|\,\Phi^Y\rangle \tag{47}$$

which, due to definition (44), is antisymmetric with respect to permutations of lower (and upper) indices. The generalized Kronecker delta can be expressed through the usual one, e.g.,

$$\delta_{ij}{}^{kl}=\delta_i{}^k\delta_j{}^l-\delta_i{}^l\delta_j{}^k\ , \tag{48}$$

etc.

The notation introduced above proves to be very convenient in the discussion of algebraic properties of the FD algebra $\mathscr{F}$. Any linear operator $\hat{\Lambda}$ in $\mathfrak{M}$ can now be expressed as

$$\hat{\Lambda}=\sum_X \sum_Y \lambda_X{}^Y \hat{X}^\dagger \hat{Y} , \tag{49}$$

where $\sum_X$ symbolizes a constrained summation over all the strings of indices X and of length x, with $0 \le x \le M$. The constraint is that if a string X appears in the summation, all the strings which can be obtained from X by permutations of indices are excluded. The ordering of indices in X and Y appearing in Eq. (49) can be arbitrary because we assume that parameters $\lambda_X{}^Y$ are antisymmetric with respect to permutations of set X (and set Y). Operator $\hat{\Lambda}$ can also be expressed by applying a generalized Einstein summation convention

$$\hat{\Lambda}=(x!y!)^{-1}\lambda_X{}^Y \hat{X}^\dagger \hat{Y} , \tag{50}$$

where now the unconstrained summation over all the strings X and Y is performed. The above form is used in Eqs. (31), (36), and (39), and will be applied when convenient. We define also the matrix representation $\mathbf{\Lambda}$ of operator $\hat{\Lambda}$:

$$\mathbf{\Lambda}=\{\Lambda_X{}^Y:\ X=\bar{X},\ Y=\bar{Y}\}_{x,y=0}^{x,y=M} , \tag{51}$$

where

$$\Lambda_X{}^Y=\langle \Phi^X | \hat{\Lambda} \Phi^Y \rangle . \tag{52}$$

Again, matrix elements (52) can be regarded as being antisymmetric with respect to permutations of indices in X and Y. In Appendix B some useful formulas for linear operators expressed in the form (49) are derived.

Now we focus our considerations on the algebraic structure of the FD algebra $\mathscr{F}$. The following partition of $\mathscr{F}$ as a vector space is introduced:

$$\mathscr{F}=\mathscr{F}^\uparrow \oplus \mathscr{F}^0 \oplus \mathscr{F}^\downarrow , \tag{53}$$

where subspace $\mathscr{F}^\uparrow$ is spanned by

$$\{\hat{X}^\dagger \hat{Y}:\ X=\bar{X},\ Y=\bar{Y};\ x>y\} , \tag{54a}$$

subspace $\mathscr{F}^0$ is spanned by

$$\{\hat{X}^\dagger \hat{Y}:\ X=\bar{X},\ Y=\bar{Y};\ x=y\} , \tag{54b}$$

and subspace $\mathscr{F}^\downarrow$ by

$$\{\hat{X}^\dagger \hat{Y}:\ X=\bar{X},\ Y=\bar{Y};\ x<y\} . \tag{54c}$$

From result (B9) of Appendix B one can infer that each subspace in Eq. (53) is closed with respect to multiplication of operators. Therefore, $\mathscr{F}^\uparrow$, $\mathscr{F}^0$, and $\mathscr{F}^\downarrow$ are subalgebras of the FD algebra $\mathscr{F}$. It can also be easily found that $\mathscr{F}^\uparrow$ and $\mathscr{F}^\downarrow$ are nilpotent algebras, i.e., for any operator $\hat{\Lambda} \in \mathscr{F}^\uparrow$ ($\mathscr{F}^\downarrow$) there is a positive integer $n<\infty$ such that

$$\hat{\Lambda}^n=0 . \tag{55}$$

It is easy to find that condition (55) if fulfilled for $n \ge M$.

Algebras $\mathscr{F}^\uparrow$ and $\mathscr{F}^\downarrow$ are Hermitian "images" of each other,

$$(\mathscr{F}^\uparrow)^\dagger=\mathscr{F}^\downarrow , \tag{56}$$

where the left-hand side (lhs) of the above equation corresponds to taking the Hermitian conjugate of all the operators belonging to $\mathscr{F}^\uparrow$; $\mathscr{F}^0$ is the Hermitian "image" of itself. We shall refer to operators of set (54a) as excitation operators, and to algebra $\mathscr{F}^\uparrow$ as excitation algebra. Operators of set (54c) will be called deexcitation operators, and $\mathscr{F}^\downarrow$ will be called deexcitation algebra. It should be stressed that partition (53) depends in general on the choice of the generators (fermion operators). Specifically, unitary transformations of fermion operators (see Appendix A) do not change the algebras $\mathscr{F}^\uparrow$, $\mathscr{F}^0$, and $\mathscr{F}^\downarrow$, but transformations (27) (or more general Bogoliubov-Valatin[15] transformations) necessarily do. An important example is provided by the Hamiltonian operator. When the original fermion operators are used (see Sec. II), $\hat{H} \in \mathscr{F}^0$ [see Eq. (16)]; after transformation (27) $\hat{H}$ contains some terms from $\mathscr{F}^\uparrow$ and $\mathscr{F}^\downarrow$, as can be seen in Eq. (31).

The Fock space can be expressed as

$$\mathfrak{M}=\mathfrak{M}(\text{even}) \oplus \mathfrak{M}(\text{odd}) , \tag{57}$$

where $\mathfrak{M}$(even) contains states of even numbers of (quasi)particles, and $\mathfrak{M}$(odd) contains states of odd numbers of (quasi)particles. It can be shown that transformation (27) does not change the partition (57). Hence, we can observe that the Hamiltonian $\hat{H}$ of Eq. (31) does not mix the subspaces $\mathfrak{M}$(even) and $\mathfrak{M}$(odd). This is a general property of operators built of strings of even numbers of fermion operators. One can write

$$\mathscr{F}=\mathscr{F}(\text{even}) \oplus \mathscr{F}(\text{odd}) , \tag{58}$$

where $\mathscr{F}$(even) is the subspace of $\mathscr{F}$ spanned by

$$\{\hat{X}^\dagger \hat{Y}:\ X=\bar{X},\ Y=\bar{Y};\ x+y=\text{even}\} . \tag{59}$$

Again, it is easy to check that $\mathscr{F}$(even) is also a subalgebra of $\mathscr{F}$. In a complete analogy to Eq. (53)

$$\mathscr{F}(\text{even})=\mathscr{F}^\uparrow(\text{even}) \oplus \mathscr{F}^0 \oplus \mathscr{F}^\downarrow(\text{even}) , \tag{60}$$

where $\mathscr{F}^\uparrow$(even) and $\mathscr{F}^\downarrow$(even) are subalgebras of $\mathscr{F}^\uparrow$ and $\mathscr{F}^\downarrow$, respectively. The algebras $\mathscr{F}^\uparrow$(even) and $\mathscr{F}^\downarrow$(even) are nilpotent, the condition (55) is now fulfilled for $n \ge \frac{1}{2}M$. Since our wave operator $\hat{\Omega}$ is not supposed to mix $\mathfrak{M}$(even) and $\mathfrak{M}$(odd), we restrict our further considerations to $\mathscr{F}$(even).

Consider two operators

$$\mathscr{F}^\uparrow(\text{even}) \ni \hat{C}=\sum_X \sum_{\substack{Y \\ (y<x)}} c_X{}^Y \hat{X}^\dagger \hat{Y} , \tag{61}$$

and

$$\mathscr{F}^\downarrow(\text{even}) \ni \hat{D}=\sum_X \sum_{\substack{Y \\ (y>x)}} d_X{}^Y \hat{X}^\dagger \hat{Y} . \tag{62}$$

It can be shown (see Appendix B 5) that

$$\hat{C}\Phi^W=\sum_{\substack{V\\(v>w)}}\Phi^V C_V{}^W\,, \tag{63}$$

$$\hat{D}\Phi^W=\sum_{\substack{V\\(v<w)}}\Phi^V D_V{}^W\,, \tag{64}$$

where linear coefficients $C_V{}^W$ ($D_V{}^W$) correspond to the matrix representation of $\hat{C}$ ($\hat{D}$) [see Eqs. (51) and (52)], and can be expressed as linear combinations of parameters $c_V{}^W$ ($d_V{}^W$) [see Eq. (B30) of Appendix B].

It is important for our purposes that operators

$$\hat{\Theta}=\ln(1+\hat{C}) \tag{65}$$

and

$$\hat{\Xi}=\ln(1+\hat{D}) \tag{66}$$

exist. This is because there is only a finite number of terms in expansions

$$\hat{\Theta}=\sum_{n=1} n^{-1}(-1)^{n-1}\hat{C}^n \tag{67}$$

and

$$\hat{\Xi}=\sum_{n=1} n^{-1}(-1)^{n-1}\hat{D}^n\,, \tag{68}$$

due to the nilpotency of $\hat{C}$ and $\hat{D}$ [see condition (55)]. We have also

$$1+\hat{C}=\exp(\hat{\Theta})=\sum_{n=0}(n!)^{-1}\hat{\Theta}^n \tag{69}$$

and

$$1+\hat{D}=\exp(\hat{\Xi})=\sum_{n=0}(n!)^{-1}\hat{\Xi}^n\,, \tag{70}$$

and it is seen that the inverses of the above operators exist:

$$(1+\hat{C})^{-1}=\exp(-\hat{\Theta})\,, \tag{71}$$

$$(1+\hat{D})^{-1}=\exp(-\hat{\Xi})\,, \tag{72}$$

for any choices of the linear coefficients in Eqs. (61) and (62).

After these preparations the problem of constructing the universal wave operator $\hat{\Omega}$ can be studied. Consider a mapping of the set of all 2^M configurations [basis (43)] onto the set $\{\Psi^X\}$ of all 2^M eigenfunctions of Hamiltonians $\hat{H}$. This mapping may be described by a certain unitary operator $\hat{A}$:

$$\Psi^X=\hat{A}\Phi^X\,. \tag{73}$$

$\hat{A}$ is by no means unique, because arbitrary mappings $X\rightarrow\Psi^X$ can be considered. Therefore, we can impose some conditions on $\hat{A}$.

(i) $\hat{A}\in\mathscr{F}$ (even).

(ii) Φ^X contains a symmetry component corresponding to the (pure) symmetry of Ψ^X. It means that Φ^X and Ψ^X are not orthogonal by symmetry.

(iii) It is assumed that

$$\hat{A}\Phi=\Psi\,, \tag{74}$$

where Ψ corresponds to the ground state of the N-particle system.

Other conditions for $\hat{A}$ will be considered later. Now we propose that $\hat{A}$ can be expressed in the form

$$\hat{A}=\hat{\Omega}\hat{B}\,, \tag{75}$$

where $\hat{\Omega}$ is our universal wave operator and $\hat{B}$ is a nonsingular operator belonging to subalgebra $\mathscr{F}^0$. Operator $\hat{\Omega}$ is defined as

$$\hat{\Omega}=(1+\hat{C})(1+\hat{D})\,, \tag{76}$$

and operators $\hat{C}$ and $\hat{D}$ were introduced in Eqs. (61) and (62), respectively. We show that if Eq. (75) holds, this representation is unique, i.e., there is only one choice of operators $\hat{B}$, $\hat{C}$, and $\hat{D}$. Assume that

$$(1+\hat{C})(1+\hat{D})\hat{B}=(1+\hat{C}')(1+\hat{D}')\hat{B}'\,, \tag{77}$$

where operators $\hat{B}'$, $\hat{C}'$, and $\hat{D}'$, can be different from $\hat{B}$, $\hat{C}$, and $\hat{D}$, respectively. Equation (77) can be transformed [see Eqs. (71) and (72)] into

$$\hat{C}''=(1+\hat{D})\hat{B}''(1+\hat{D}')^{-1}-1\,, \tag{78}$$

where

$$\mathscr{F}^\dagger(\text{even})\ni\hat{C}''=[(1+\hat{C})^{-1}(1+\hat{C}')-1]\,, \tag{79}$$

and

$$\mathscr{F}^0\ni\hat{B}''=\hat{B}(\hat{B}')^{-1}\,. \tag{80}$$

It is seen that the rhs of Eq. (78) does not contain any contribution from $\mathscr{F}^\dagger$(even), and hence $\hat{C}''=0$. Further arguments lead to the conclusion that $\hat{B}'=\hat{B}$, $\hat{C}'=\hat{C}$, and $\hat{D}'=\hat{D}$, thus proving that Eq. (75) provides the unique representation of $\hat{A}$. The question remains, however, whether this representation is sufficiently general, i.e., whether operator $\hat{\Omega}$ of the form (76) exists for any unitary $\hat{A}$ fulfilling conditions (i)—(iii).

Consider the (full) CI expansions

$$\Psi^Y=\hat{A}\Phi^Y=\sum_{\substack{X\\(x>y)}}\Phi^X A_X{}^Y+\sum_{\substack{X\\(x=y)}}\Phi^X A_X{}^Y+\sum_{\substack{X\\(x<y)}}\Phi^X A_X{}^Y\,, \tag{81}$$

for the eigenfunctions of $\hat{H}$, where the matrix representation of operator $\hat{A}$ [see Eqs. (51) and (52)] is used. Equations for operator $\hat{B}$ are also to be considered:

$$\hat{B}\Phi^Y=\sum_{\substack{X\\(x=y)}}\Phi^X B_X{}^Y\,. \tag{82}$$

According to our previous assumptions matrix $\mathbf{B}$ is nonsingular; hence its inverse [see Eq. (A2)]

$$\tilde{\mathbf{B}}:=\mathbf{B}^{-1} \tag{83}$$

exists. Now we shall attempt to express the matrix elements $B_X{}^Y$, $C_X{}^Y$, and $D_X{}^Y$ appearing in Eqs. (82), (63), and (64), respectively, in terms of the CI amplitudes $A_X{}^Y$ of Eq. (81). One finds that

$$\begin{aligned}\Psi^Y&=(1+\hat{C})(1+\hat{D})\hat{B}\Phi^Y=(1+\hat{C})(1+\hat{D})\sum_{\substack{X\\(x=y)}}\Phi^X B_X{}^Y\\&=(1+\hat{C})\sum_{\substack{X\\(x=y)}}\left[\Phi^X B_X{}^Y+\sum_{\substack{W\\(w<y)}}\Phi^W D_W{}^X B_X{}^Y\right]\\&=\sum_{\substack{X\\(x=y)}}\left[\Phi^X B_X{}^Y+\sum_{\substack{W\\(w>y)}}\Phi^W C_W{}^X B_X{}^Y+\sum_{\substack{W\\(w<y)}}\Phi^W D_W{}^X B_X{}^Y+\sum_{\substack{W\\(w<y)}}\sum_{\substack{V\\(v>w)}}\Phi^V C_V{}^W D_W{}^X B_X{}^Y\right].\end{aligned} \tag{84}$$

By comparing with Eq. (81) one finds the following relations: For $x=y$,

$$A_X{}^Y=B_X{}^Y+\sum_{\substack{W\\(w=y)}}\sum_{\substack{V\\(v<y)}}C_X{}^V D_V{}^W B_W{}^Y ; \tag{85a}$$

for $x>y$,

$$A_X{}^Y=\sum_{\substack{W\\(w=y)}}C_X{}^W B_W{}^Y+\sum_{\substack{W\\(w=y)}}\sum_{\substack{V\\(v<y)}}C_X{}^V D_V{}^W B_W{}^Y ; \tag{85b}$$

for $x<y$,

$$A_X{}^Y=\sum_{\substack{W\\(w=y)}}D_X{}^W B_W{}^Y+\sum_{\substack{W\\(w=y)}}\sum_{\substack{V\\(v<x)}}C_X{}^V D_V{}^W B_W{}^Y . \tag{85c}$$

It is seen that the number of unknowns (parameters $B_X{}^Y$, $C_X{}^Y$, and $D_X{}^Y$) equals the number of CI coefficients $A_X{}^Y$. A simpler form of these equations follows when equation $\hat{\Omega}=\hat{A}\hat{B}^{-1}$ is used as the starting point instead of Eq. (75). Now the elements of matrix $\tilde{\mathbf{B}}$ replace elements $B_X{}^Y$ as unknowns. The resulting equations are the following: For $x=y$,

$$\sum_{\substack{Z\\(z=y)}}A_X{}^Z\tilde{B}_Z{}^Y=\delta_X{}^Y+\sum_{\substack{V\\(v<y)}}C_X{}^V D_V{}^Y ; \tag{86a}$$

for $x>y$,

$$\sum_{\substack{Z\\(z=y)}}A_X{}^Z\tilde{B}_Z{}^Y=C_X{}^Y+\sum_{\substack{V\\(v<y)}}C_X{}^V D_V{}^Y ; \tag{86b}$$

for $x<y$,

$$\sum_{\substack{Z\\(z=y)}}A_X{}^Z\tilde{B}_Z{}^Y=D_X{}^Y+\sum_{\substack{V\\(v<x)}}C_X{}^V D_V{}^Y . \tag{86c}$$

Solutions of Eqs. (86) are equivalent to the solutions of Eqs. (85) only when matrix $\tilde{\mathbf{B}}$ is nonsingular. We can observe that among states $\{\Psi^Y\}$ there are states for which "deexcitation" coefficients $A_X{}^Y$ $(x<y)$ are zero. Important examples of such states are state Ψ, and states Ψ^i. When pseudocharge [see Eq. (38)] symmetry is taken into account, one can find that also all states $\Psi^{\rho\sigma\cdots}$ ("hole" indices only), and $\Psi^{rs\cdots}$ ("particle" indices only) correspond to

$$A_X{}^Y=0 , \quad x<y . \tag{87}$$

In this case Eq. (86c) reads

$$D_X{}^Y=-\sum_{\substack{V\\(v<x)}}C_X{}^V D_V{}^Y , \quad x<y . \tag{88}$$

It is seen that the rhs of the above equation contains parameters $D_V{}^Y$ with $v<x$. Hence, for $x=0,1,2,\ldots$,

$$D_X{}^Y=0 , \tag{89}$$

and, by a simple inductive argument, the above equality extends over all $x<y$. We see that Eqs. (87) and (89) are equivalent.

Returning to Eqs. (86), we know that Eq. (89) holds for $y=0$, and $y=1$, and we have the following:

(1) For Ψ $(y=0)$,

$$A\tilde{B}=1 \quad (x=y=0) , \tag{90a}$$

$$A_X\tilde{B}=C_X \quad (x>y=0) ; \tag{90b}$$

(2) for Ψ^j $(y=1)$,

$$A_i{}^k\tilde{B}_k{}^j=\delta_i{}^j \quad (x=y=1) , \tag{91a}$$

$$A_X{}^k\tilde{B}_k{}^j=C_X{}^j \quad (x>y=1) . \tag{91b}$$

These are simple linear equations which can be solved, provided that $A\neq 0$ [see Eq. (74)], and the following condition holds:

(iv) The submatrix of $\mathbf{A}$,

$$\mathbf{A}_1=\{A_i{}^j\} , \tag{92}$$

is nonsingular.

It can be observed in Eqs. (86), for $y\geq 2$, that nonlinear terms of the type

$$\sum_{\substack{V \\ (v<y)}} C_X{}^V D_V{}^Y \tag{93}$$

contain parameters $C_X{}^V$ only with $v<y$. Hence, when these equations are solved for $y \leq y_0$, equations for $y=y_0+1$ become linear in the unknown parameters. Because equations for $y=0$ [Eqs. (90)] and $y=1$ [Eqs. (91)] can be solved, a conclusion can be reached by induction that solving Eqs. (86) [and, hence, Eqs. (85)] can be traced down to solving a set of linear equations. Previously we learned that if there is a solution to Eqs. (85), it must be a unique one. Still, there is no definitive answer to the question whether such a solution exists. It is tempting, however, to make a conjecture that for any Hamiltonian $\hat{H}$ one can find such a form of $\hat{A}$ that representation (75) holds. In Sec. VII we show that this assumption is not crucial when an approximate treatment is introduced.

V. EFFECTIVE HAMILTONIAN

We assume here that the unitary operator $\hat{A}$ of Eq. (73) can be expressed in the form (75). Operator $\hat{A}^{-1}\hat{H}\hat{A}$ is a diagonal energy operator in basis (43)

$$\hat{A}^{-1}\hat{H}\hat{A}\Phi^X = E^X\Phi^X . \tag{94}$$

E^X is here the eigenvalue corresponding to eigenfunction Ψ^X of Hamiltonian $\hat{H}$. The effective Hamiltonian defined in Eq. (1) can now be written as

$$\hat{G}=\hat{B}(\hat{A}^{-1}\hat{H}\hat{A})\hat{B}^{-1} , \tag{95}$$

where the rhs of Eq. (95) obviously belongs to $\mathscr{F}^0$. Hence, $\hat{G}$ fulfills condition (41). We can express $\hat{G}$ as follows:

$$\hat{G}=\sum_X \sum_{\substack{Y \\ (y=x)}} g_X{}^Y \hat{X}^\dagger \hat{Y} , \tag{96}$$

and the meaning of parameters $g_X{}^Y$ can be understood better when matrix elements

$$G_X{}^Y = \langle \Phi^X | \hat{G} | \Phi^Y \rangle \tag{97}$$

are considered. One can write

$$\mathbf{G}=\bigoplus_{n=0}^{M} \mathbf{G}_n , \tag{98}$$

where

$$\mathbf{G}_n = \{ G_X{}^Y : \ x=y=n \} , \tag{99}$$

and diagonalization of these matrices yields eigenvalues of $\hat{H}$ [see Eqs. (94) and (95)]:

$$E^X\delta_X{}^Y = \sum_{\substack{V \\ (v=x)}} \sum_{\substack{W \\ (w=x)}} \tilde{B}_X{}^V G_V{}^W B_W{}^Y . \tag{100}$$

Let us consider explicitly a few special cases.

(i) For $x=y=0$,

$$G=g=E , \tag{101}$$

where E is the eigenvalue of $\hat{H}$, corresponding to the wave function Ψ;

(ii) for $x=y=1$,

$$G_1=\mathbf{G}_\mathrm{h}\oplus\mathbf{G}_\mathrm{p} , \tag{102}$$

where [see Eq. (B30) of Appendix B]

$$\mathbf{G}_\mathrm{h}=\{G_\rho{}^\sigma = E\delta_\rho{}^\sigma + g_\rho{}^\sigma\} , \tag{103a}$$

and

$$\mathbf{G}_\mathrm{p}=\{G_r{}^s = E\delta_r{}^s + g_r{}^s\} , \tag{103b}$$

and diagonalization of these matrices yields energies of $(N-1)$-particle states, E^ρ, and energies of $(N+1)$-particle states, E^r, respectively;

(iii) for $x=y=2$,

$$\mathbf{G}_2=\mathbf{G}_\mathrm{hh}\oplus\mathbf{G}_\mathrm{hp}\oplus\mathbf{G}_\mathrm{pp} , \tag{104}$$

where

$$\mathbf{G}_\mathrm{hh}=\{G_{\rho\sigma}{}^{\tau\upsilon},\ \rho<\sigma;\ \tau<\upsilon\} , \tag{105a}$$

$$\mathbf{G}_\mathrm{hp}=\{G_{\rho r}{}^{\sigma s}\} , \tag{105b}$$

$$\mathbf{G}_\mathrm{pp}=\{G_{rs}{}^{tu},\ r<s;\ t<u\} , \tag{105c}$$

and, in general [see Eq. (B30) of Appendix B],

$$G_{ij}{}^{kl} = E\delta_{ij}{}^{kl} + g_i{}^k\delta_j{}^l - g_i{}^l\delta_j{}^k + g_j{}^l\delta_i{}^k - g_j{}^k\delta_i{}^l + g_{ij}{}^{kl} , \tag{106}$$

and diagonalization of matrices (105) gives eigenvalues $E^{\rho\sigma}$, $E^{\rho r}$, and E^{rs}, corresponding to some $(N-2)$-, N-, and $(N+2)$-particle states, respectively.

One can see that once the effective Hamiltonian $\hat{G}$ is known, energies of states corresponding to a small number of quasiparticles (0, 1, and 2) can be calculated with ease. Moreover, the corresponding excitation energies can be determined directly, since the reference energy E may be subtracted from the diagonal of matrix $\mathbf{G}$ [see Eqs. (103) and (106)]. A minor complication is that matrices $\mathbf{G}_n$ are, in general, non-Hermitian for $n>0$. This is the price one has to pay when permitting a nonunitary operator $\hat{\Omega}$ in transformation (1).

Hamiltonian $\hat{H}$ of Eq. (16) and Hamiltonian $\hat{G}$ of Eq. (96) provide equivalent descriptions of the physical system under consideration. The picture associated with $\hat{G}$ is that of a system of interacting, stable quasiparticles. Here parameters $g_X{}^Y$ [for x $(=y)$ $=2,3,\ldots,M$] corresponds to x-quasiparticle interactions. In contrast, Hamiltonian $\hat{H}$ of the form of Eq. (31) describes our system in terms of quasiparticles which are unstable. Using the jargon of the quantum field theory we can say that the second picture involves "bare" quasiparticles, and the first one "dressed" quasiparticles. Accordingly, transformation (1) can be interpreted as a kind of renormalization procedure.

The effective Hamiltonian $\hat{G}$ is dependent on the choice of the model vacuum Φ. In Appendix C we have proved that for Φ invariant with respect to the symmetry group $\mathscr{G}$ of Hamiltonian $\hat{H}$ one has also

$$[\hat{G},\hat{V}]_-=0 \tag{107}$$

for all $\hat{V}\in\mathscr{G}$. Findings of Appendix C may be employed in formulation of a spin-adapted version of the proposed method.

Now we wish to look more closely at the similarity transformation (1), with $\hat{\Omega}$ defined in Eq. (76). One can write

$$\hat{G}=(1+\hat{D}')(1+\hat{C}')\hat{H}(1+\hat{C})(1+\hat{D}) , \tag{108}$$

where [see Eqs. (71) and (72)]

$$1+\hat{C}'=(1+\hat{C})^{-1} , \tag{109a}$$

and

$$1+\hat{D}'=(1+\hat{D})^{-1} . \tag{109b}$$

We introduce an auxiliary effective Hamiltonian

$$\hat{\Gamma}=(1+\hat{C}')\hat{H}(1+\hat{C})=(1+\hat{D})\hat{G}(1+\hat{D}') , \tag{110}$$

and observe that the difference

$$\hat{\Gamma}-\hat{G}=\hat{D}\hat{G}+\hat{G}\hat{D}'+\hat{D}\hat{G}\hat{D}' \tag{111}$$

belongs to subalgebra $\mathscr{F}^{\downarrow}$(even). Thus, by expressing operator $\hat{\Gamma}$ in the form

$$\hat{\Gamma}=\sum_X \sum_Y \gamma_X{}^Y \hat{X}^\dagger \hat{Y} , \tag{112}$$

one finds immediately that

$$\gamma_X{}^Y=0 \tag{113a}$$

for $x>y$; and that

$$\gamma_X{}^Y=g_X{}^Y \tag{113b}$$

for $x=y$. The last equation indicates that the effective Hamiltonian $\hat{G}$ of the form (96) can be quite easily "extracted" from the auxiliary effective Hamiltonian $\hat{\Gamma}$. We write $\hat{\Gamma}$ as

$$\hat{\Gamma}=\hat{\Omega}_{\rm ex}^{-1}\hat{H}\hat{\Omega}_{\rm ex} , \tag{114}$$

where the excitation part of the universal wave operator $\hat{\Omega}$, $\hat{\Omega}_{\rm ex}=1+\hat{C}$, can be expressed using the exponential ansatz [see Eq. (69)]:

$$\hat{\Omega}_{\rm ex}=\exp(\hat{\Theta}) . \tag{115}$$

The generalized CC operator $\hat{\Theta}$ belongs to the excitation algebra $\mathscr{F}^{\uparrow}$(even):

$$\hat{\Theta}=\sum_X \sum_{\substack{Y \\ (y<x)}} \theta_X{}^Y \hat{X}^\dagger \hat{Y} . \tag{116}$$

The generalized CC amplitudes $\theta_X{}^Y$ $(x>y)$ are determined by conditions (113a); it is to be noticed that the number of these conditions is equal to the number of amplitudes $\theta_X{}^Y$. Parameters $\gamma_X{}^Y$ of the operator $\hat{\Gamma}$ can be expressed in terms of parameters $\eta_V{}^W$ of Hamiltonian $\hat{H}$ [see Eqs. (31) and (32)] and amplitudes $\theta_V{}^W$. In order to find explicit expressions the commutator expansion

$$\exp(-\hat{\Theta})\hat{H}\exp(\hat{\Theta}) = \hat{H}+[\hat{H},\hat{\Theta}]_-+(2!)^{-1}[[\hat{H},\hat{\Theta}]_-,\hat{\Theta}]_-+\cdots=\hat{\Gamma} \tag{117}$$

can be employed. The commutator series (117) can have only a finite number of nonzero terms; this is because expansion (69) is finite. The representation of $\hat{\Gamma}$ given in Eq. (117) indicates that each parameter $\gamma_X{}^Y$ can be expressed as a sum containing a finite number of linked products of parameters $\eta_V{}^W$ and $\theta_V{}^W$ [see Appendix B, Eq. (B21)]. This is also true if an approximate, truncated form of operator $\hat{\Theta}$ is used (as in Sec. VII). Therefore, unlinked terms do not appear in this approach.

A direct application of expansion (117) is not easy for a general CC operator of Eq. (116), and below a modified treatment is proposed. From Eq. (110) the following form of $\hat{\Gamma}$ can be obtained,

$$\hat{\Gamma}=\hat{H}+\hat{C}'\hat{H}+\hat{H}\hat{C}+\hat{C}'\hat{H}\hat{C} , \tag{118}$$

and parameters $\gamma_X{}^Y$ can be easily expressed through parameters $c_V{}^W$ [see Eq. (61)] and parameters $c'_V{}^W$ corresponding to operator $\hat{C}'$ [see Eq. (109a)]. Parameters $c_V{}^W$ and $c'_V{}^W$ can be, in turn, expressed via parameters $\theta_X{}^Y$ [see Eqs. (69) and (71)]. The pertinent expressions contain both linked and unlinked terms, and it is useful to introduce new parameters

$$\tau_X{}^Y=(c_X{}^Y)_{\rm linked} , \tag{119a}$$

$$\tau'_X{}^Y=(c'_X{}^Y)_{\rm linked} . \tag{119b}$$

It can be shown that parameters $c_X{}^Y$ $(c'_X{}^Y)$ can be expressed as polynomials in $\tau_V{}^W$ $(\tau'_V{}^W)$, with linear coefficients equal to 1:

$$c_X{}^Y=\tau_X{}^Y+\sum_{V_1}\sum_{V_2}\sum_{W_1}\sum_{W_2}\delta_X{}^{V_1V_2}\tau_{V_1}{}^{W_1}\tau_{V_2}{}^{W_2}\delta_{W_1W_2}{}^Y+\cdots , \tag{120}$$

etc. Obviously, the rhs of Eq. (120) contains, besides $\tau_X{}^Y$, only unlinked terms. Now we can express the rhs of Eq. (118) using parameters $\tau_V{}^W$ and $\tau'_V{}^W$. Each parameter $\gamma_X{}^Y$ can now be expressed as a polynomial in $\tau_V{}^W$ and $\tau_V{}^W$, with linear coefficients defined in Eqs. (32). Because of expansion (117), only linked contributions will survive. In Sec. VI we employ a diagrammatic approach to find linked expressions for parameters $\tau_V{}^W$ and $\tau'_V{}^W$, in terms of parameters $\theta_X{}^Y$, and for parameters $\gamma_X{}^Y$, in terms of parameters $\tau_V{}^W$ and $\tau'_V{}^W$. As indicated previously, the CC amplitudes $\theta_V{}^W$ can be calculated by solving (generalized) CC equations which follow from conditions (113a):

$$\gamma_X{}^Y(\{\theta_V{}^W\})=0 , \tag{121}$$

for $x>y$. Parameters $g_X{}^Y$ of the effective Hamiltonian $\hat{G}$ are then calculated according to Eq. (113b).

Concluding this section we would like to discuss certain properties of operator $\hat{\Omega}_{\rm ex}$, which shed some light on how the present method is related to previous CC theories. Let us consider wave functions

$$\tilde{\Psi}^X=\hat{\Omega}_{\rm ex}\Phi^X . \tag{122}$$

These functions, are, in general, neither normalized nor orthogonal. They fulfill the intermediate normalization condition

$$\langle \Phi^X | \tilde{\Psi}^Y \rangle = \delta_X{}^Y . \tag{123}$$

We can write operator $\hat{C}$ of Eq. (61) in the form

$$\hat{C} = \sum_{n=0}^{M-1} \hat{C}_n , \tag{124}$$

where

$$\hat{C}_n = \sum_{\substack{Y \\ (y=n)}} \sum_{\substack{X \\ (x>y)}} c_X^Y \hat{X}^\dagger \hat{Y} . \tag{125}$$

By substituting $\hat{\Omega}_{ex} = 1 + \hat{C}$ we can write Eq. (122) in the form

$$\tilde{\Psi}^X = (1 + \hat{C}_0 + \cdots + \hat{C}_X)\Phi^X . \tag{126}$$

For $x=0$ one has $\tilde{\Psi} = \langle \Phi | \Psi \rangle^{-1} \Psi$, and

$$\tilde{\Psi} = (1 + \hat{C}_0)\Phi . \tag{127}$$

Here $\hat{C}_0$ is the CI operator appearing in the single-reference CC method (see, e.g., Ref. 14). In the present notation the wave operator of this method reads

$$1 + \hat{C}_0 = \exp(\hat{T}_0) , \tag{128}$$

where

$$\hat{T}_0 = \sum_{\substack{X \\ (x>0)}} t_X X^\dagger , \tag{129}$$

and operators $\hat{X}^\dagger$ (corresponding to x even and $x_h = x_p$ because of the pseudocharge symmetry, see Sec. III) are the so-called particle-hole operators. These operators form a commutative subalgebra of the excitation algebra $\mathcal{F}^\dagger$(even). It can be found that

$$t_X = \tau_X , \tag{130}$$

where [see Eq. (119a)]

$$\tau_X = (c_X)_{\text{linked}} . \tag{131}$$

We can speculate that our operator $\hat{\Omega}_{ex}$ of Eq. (115) can be written in the form

$$\hat{\Omega}_{ex} = \exp(\hat{T}_0)\exp(\hat{T}_1)\cdots\exp(\hat{T}_{M-2}) , \tag{132}$$

where

$$\hat{T}_n = \sum_{\substack{Y \\ (y=n)}} \sum_{\substack{X \\ (x>y)}} t_X{}^Y \hat{X}^\dagger \hat{Y} . \tag{133}$$

Contrary to Eq. (130), for $y>0$ we have in general

$$t_X{}^Y \neq \tau_X{}^Y . \tag{134}$$

One can notice (see Ref. 10) that $\hat{\Omega}_{ex}$ of Eq. (132) is a generalization of the wave operator proposed by Offerman *et al.*,[17] whereas $\hat{\Omega}_{ex}$ of Eq. (115) generalizes the wave operator of Mukherjee *et al.*[6]

VI. GENERALIZED COUPLED-CLUSTER EQUATIONS IN DIAGRAMMATIC FORM

The generalized CC equations (121), and equations for the parameters of the effective Hamiltonian [Eq. (113b)] contain large numbers of (linked) terms. These terms can be conveniently expressed in the form of diagrams; the ones used in the present paper resemble the Hugenholtz diagrams.[16] The diagrammatic representation of basic parameters in our CC method is shown in Fig. 1.

When drawing a diagram, e.g., for a parameter $\gamma_X{}^Y$, one should remember that the number of quasiparticle lines on the top of the diagram (equal to x) and the number of quasiparticle lines on the bottom (equal to y) must fulfill the condition

$$x + y = \text{even} . \tag{135}$$

In general we shall suppress the indices and arrows ($\downarrow$ for "holes" and $\uparrow$ for "particles"); each diagram can be easily completed with these symbols. It should be noticed that the pseudocharge symmetry [see Eqs. (38) and (46) and Appendix C] requires

$$x_p - x_h = y_p - y_h . \tag{136}$$

Linked terms in Eqs. (121) and (113b) are represented by linked diagrams such as that shown in Fig. 2.

Algebraic representation of more complex diagrams (with the number of components greater than 2) requires multiple applications of the formula (B18); such a treatment will be applied in paper II.[11] This is the advantage of diagrammatic techniques—that they help to generate all the terms appearing in a given equation without the need of considering explicit algebraic expressions. The di-

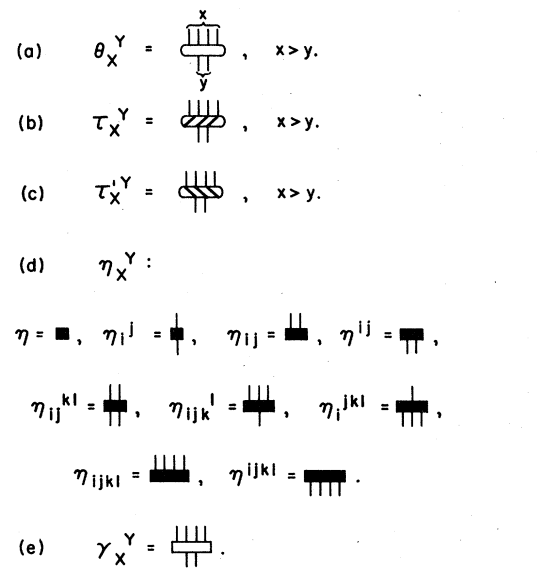

FIG. 1. The diagrammatic representations of (a) the CC amplitudes [see Eq. (116)], (b) and (c) parameters $\tau_X{}^Y$ and $\tau'_X{}^Y$ [see Eqs. (119)], (d) parameters of Hamiltonian $\hat{H}$ of Eq. (31), and (e) parameters of the auxiliary effective Hamiltonian $\hat{\Gamma}$ of Eq. (112).

FIG. 2. An example of a linked diagram and the corresponding algebraic expression. Here $\lambda_{ijk}{}^{l}$ is one of the contributions to the parameter $\gamma_{ijk}{}^{l}$ of the auxiliary Hamiltonian $\hat{\Gamma}$, originating from term $\hat{H}\hat{C}$ in Eq. (118) [see formula (B18) of Appendix B].

agrammatic expansion of a few parameters $\tau_X{}^Y$ is shown in Fig. 3.

In order to suppress the proliferation of terms in the diagrammatic expressions of Fig. 3 we assumed that our reference configuration Φ is the maximum-overlap configuration for the eigenfunction Ψ (see Refs. 11 and 14, and references therein), for in this case

$$c_{ij}=\tau_{ij}=\theta_{ij}=0\ , \tag{137}$$

for all $i<j$. Even so, the expression for $\tau_{ijklmnpq}$ [not shown in Fig. (3a)] contains already 54 terms. The numerical factors appearing in the diagrammatic expressions of Fig. 3 correspond to the factors $(n!)^{-1}$ in expansion (69). For higher values of n an additional factor, equal to the number of different "time orderings" of components of the diagram, may appear. Diagrammatic expressions for parameters $\tau'_X{}^Y$ are almost identical to those of Fig. 3, the only difference being due to the factor $(-1)^n$ originating from the expansion (69) applied to operator (71).

The generalized CC equations (121) are shown in a diagrammatic form in Figs. 4 and 5. Here parameters $\gamma_X{}^Y$ for $x>y$ are expressed in terms of parameters $\tau_V{}^W$ and $\tau'_V{}^W$.

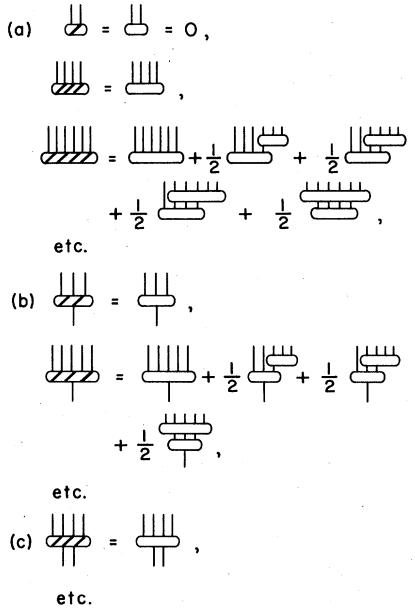

FIG. 3. Diagrammatic expansions for (a) τ_{ij}, τ_{ijkl}, and τ_{ijklmn}; (b) $\tau_{ijk}{}^{l}$ and $\tau_{ijklm}{}^{n}$; (c) $\tau_{ijkl}{}^{mn}$. See Eqs. (69), (119a), and (137).

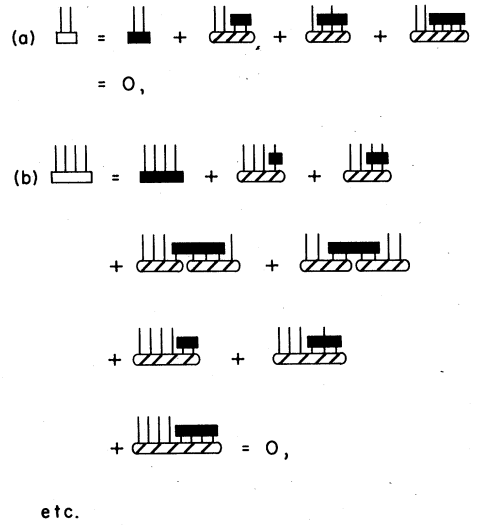

FIG. 4. The generalized CC equations in the diagrammatic form: (a) $\gamma_{ij}=0$, (b) $\gamma_{ijkl}=0$.

It is easy to find that the diagrammatic expressions in Fig. 4 are in fact identical with those appearing in the single-reference CC method based on the maximum-overlap configuration Φ. The graphical expression in Fig. 4(a) corresponds to the condition from which the so-called Brueckner spin-orbitals are determined (see Refs. 11 and 14, and references therein).

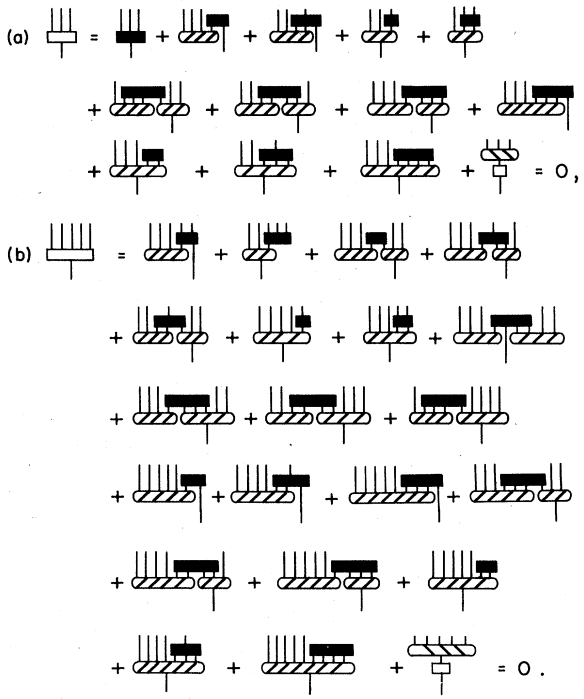

FIG. 5. The generalized CC equations in the diagrammatic form: (a) $\gamma_{ijk}{}^{l}=0$, (b) $\gamma_{ijklm}{}^{n}=0$. The last term in the diagrammatic expression for $\gamma_{ijk}{}^{l}$ ($\gamma_{ijklm}{}^{n}$) is $\tau'_{ijk}{}^{p}\gamma_p{}^{l}(\tau'_{ijklm}{}^{p}\gamma_p{}^{n})$, and parameters $\gamma_i{}^{j}$ are depicted in Fig. 6(b).

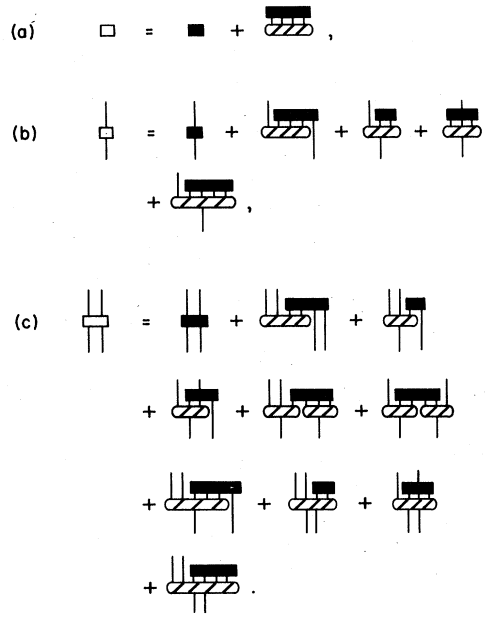

FIG. 6. The diagrammatic expressions for the parameters of the effective Hamiltonian $\hat{G}$ of Eq. (96): (a) $\gamma=g=E$, (b) ${\gamma_i}^j={g_i}^j$, (c) ${\gamma_{ij}}^{kl}={g_{ij}}^{kl}$.

Finally, in Fig. 6 we present diagrammatic equations determining the parameters of the effective Hamiltonian $\hat{G}$ [see Eq. (113b)].

Diagrammatic equations shown explicitly in Figs. 3–6 constitute only a very small fraction of the set of equations which can be, in principle, derived in our method. In paper II (Ref. 11) we shall formulate an approximate CC method using equations depicted in Figs. 3–6. Approximation schemes in the CC method are introduced in Sec. VII.

VII. APPROXIMATION SCHEMES

The generalized CC equations (121), a few of which were presented in the graphical form in Figs. 4 and 5, form a set of coupled nonlinear algebraic equations for the CC amplitudes ${\theta_X}^Y$. Their maximal rank can be found to be as high as N, the number of particles corresponding to the reference state Φ. Provided that Eqs. (85) have a solution, the generalized CC equations can have many solutions, corresponding to different choices of operator $\hat{A}$ of Eq. (73). Solving the full set of generalized CC equations seems to be an impossible task, even if N and M are not large. This would be also impractical, since, as already mentioned, only a small part of the spectrum of Hamiltonian $\hat{H}$ can be of interest. Below we discuss approximation schemes which may be employed in practical applications of the CC method described in preceding sections.

Consider a family of (truncated) CC operators

$$\hat{\Theta}'=\hat{\Theta}'(L;K_0,\ldots,K_L)=\sum_{l=0}^{L}\sum_{k\,(>l)}^{K_l}\hat{\Theta}'_{kl}\,, \tag{138}$$

where

$$\hat{\Theta}'_{kl}=\sum_{X\,(x=k)}\sum_{Y\,(y=l)}{\theta'_X}^Y\hat{X}^\dagger\hat{Y}\,, \tag{139}$$

and $L<M$, $l<K_l\leq M$. For each CC operator $\hat{\Theta}'$ of Eq. (138) we can construct the corresponding wave operator $\hat{\Omega}'_{\rm ex}$ and (auxiliary) effective Hamiltonian $\hat{\Gamma}'$ [see Eqs. (115) and (114), respectively]. Unknown CC amplitudes ${\theta'_X}^Y$ are now determined from a truncated set of generalized CC equations

$${\gamma'_X}^Y(\{{\theta'_V}^W\})=0\,, \tag{140}$$

for $0\leq y\leq L$, $y<x\leq K_y$. Again, the number of unknowns is equal to the number of equations. We can also construct an approximation to the effective Hamiltonian $\hat{G}$ of Eq. (96):

$$\hat{G}'=\sum_X\sum_Y{g'_X}^Y\hat{X}^\dagger\hat{Y}\,, \tag{141}$$

where [compare Eq. (113b)]

$${g'_X}^Y={\gamma'_X}^Y \tag{142}$$

for $x=y$. In the case of $L=M-1$, $K_0=K_1\cdots=K_{M-1}=M$ we have

$$\hat{\Theta}'=\hat{\Theta}\,, \tag{143}$$

and the full CC method is recovered. It is interesting to note that for approximate versions of this method corresponding to $L<M-1$, $K_0=K_1\cdots K_L=M$, one finds that

$${g'_X}^Y={g_X}^Y \tag{144}$$

for $x=y\leq L$. It means that in these cases exact values of eigenvalues E^X [see Eq. (94)] for $x\leq L$ can be obtained from $\hat{G}'$. In particular, for $L=0$ one has

$$g'=g=E \tag{145}$$

and

$$\hat{\Theta}=\hat{T}_0\,, \tag{146}$$

where $\hat{T}_0$, defined in Eq. (129), is the CC operator of the single-reference CC method.[3–5] It is seen that by taking $L=1,2,3\ldots$ we can gradually extend the single-reference CC method thus providing access to a certain portion of the spectrum of Hamiltonian $\hat{H}$. The corresponding eigenstates of $\hat{H}$ are in some sense "least excited" with respect to the reference eigenstate Ψ.

In practical applications of the proposed generalization of the CC method we must assume that parameters L and $K_0,K_1,\ldots,K_L$ are much smaller than their limiting values corresponding to Eq. (143). For the single-reference CC method ($L=0$) it was found[3–5] that in most cases the approximation with $K_0=4$ (this corresponds to the inclusion of double "particle"-"hole" excitations) is excellent. In paper II (Ref. 11) we shall describe a variant of the generalized CC method in which the approximation with $L=1$, $K_0=4$, and $K_1=3$ is employed. Our treatment will provide an extension of the

Brueckner-Hartree-Fock (BHF) version of the single-reference CC method.[14] It is to be pointed out that the problem of the existence of a solution of Eqs. (85) can be avoided when a variant with $L=1$ is considered. This is because in this case only Eqs. (90) and (91) need to be taken into account, and conditions (i)—(iv) [see Eqs. (74) and (92)] which are sufficient for the existence of their solutions can be met.

ACKNOWLEDGMENTS

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APPENDIX A: TRANSFORMATIONS OF FERMION OPERATORS, INDUCED BY TRANSFORMATIONS OF SPIN-ORBITAL BASIS

We consider a unitary transformation of basis (6):

$$\phi_j \rightarrow \phi'_j = \phi_i U^i{}_j \ , \tag{A1}$$

where the linear parameters define a unitary matrix $\mathbf{U}_1$ (the subscript 1 indicates a transformation of one-particle functions). As in Eq. (18a) there is a freedom in assigning covariant and contravariant positions to the indices in $U^i{}_j$. The inverse matrix $\mathbf{U}_1{}^{-1}=\mathbf{U}_1{}^{\dagger}$ will be denoted as $\tilde{\mathbf{U}}_1=\{\tilde{U}^i{}_j\}$, where

$$\tilde{U}^i{}_j=(U_j{}^i)^* \ . \tag{A2}$$

By substituting Eq. (A1) into definition (7), the following transformation of the annihilation operators can be deduced:

$$\hat{a}_j \rightarrow \hat{a}'_j = \hat{a}_i (U^i{}_j)^* = \tilde{U}_j{}^i \hat{a}_i \ . \tag{A3a}$$

The corresponding transformation of the creation operators [see Eq. (8)] reads

$$\hat{a}^j \rightarrow (\hat{a}^j)' = \hat{a}^i U_i{}^j \ . \tag{A3b}$$

Transformation (A1) induces also transformations of one- and two-particle integrals (17), but it can be shown that Hamiltonian $\hat{H}$ of Eq. (16) and operator $\hat{N}$ of Eq. (20) are invariant under transformation (A1).

In the quasiparticle representation determined by transformation (27) let us consider transformations (A1) for which

$$\mathbf{U}_1=\mathbf{U}_{\mathrm{h}}\oplus\mathbf{U}_{\mathrm{p}} \ , \tag{A4}$$

where $\mathbf{U}_{\mathrm{h}}=\{U^{\rho}{}_{\sigma}\}$ and $\mathbf{U}_{\mathrm{p}}=\{U^r{}_s\}$. The following transformations of quasiparticle annihilation operators emerge:

$$\hat{b}_{\sigma} \rightarrow \hat{b}'_{\sigma} = \hat{a}^{\rho} U_{\rho}{}^{\sigma} = \hat{b}_{\rho} U^{\rho}{}_{\sigma} \ , \tag{A5a}$$

$$\hat{b}_r \rightarrow \hat{b}'_r = \hat{a}_r (U^r{}_s)^* = \hat{b}_r (U^r{}_s)^* \ . \tag{A5b}$$

One can find that if $\mathbf{U}_1$ cannot be expressed in the form (A4), the resulting transformation of operators $\hat{b}_i$ is that of Bogoliubov-Valatin[15] (general type). Since we would like not to break the pseudocharge symmetry of quasiparticles [see the discussion after Eq. (38)], our further considerations will be restricted to transformations (A1) which fulfill condition (A4). It will be useful to introduce the matrix

$$\mathbf{V}_1=\mathbf{U}_{\mathrm{h}}{}^*\oplus\mathbf{U}_{\mathrm{p}} \ , \tag{A6}$$

and its inverse $\mathbf{V}_1{}^{-1}=\mathbf{V}_1{}^{\dagger}=\tilde{\mathbf{V}}_1$. Now the transformed annihilation operators of Eqs. (A5) can be written as

$$\hat{b}'_j = \hat{b}_i (V^i{}_j)^* = \tilde{V}_j{}^i \hat{b}_i \ , \tag{A7a}$$

and the corresponding transformed creation operators as

$$(\hat{b}^j)' = \hat{b}^i V_i{}^j \ . \tag{A7b}$$

It is seen that the form of the transformed fermion operators in Eqs. (A7) is the same as of those in Eqs. (A3).

The transformation of fermion operator strings from set (42) requires applying Eqs. (A7) to all the fermion operators in a given string:

$$\begin{aligned}\hat{X}^{\dagger}\hat{Y} \rightarrow (\hat{X}^{\dagger}\hat{Y})' &= \cdots (b^j)'(b^i)')b_k)'(b_l)'\cdots \\ &= \tilde{V}_k{}^p \tilde{V}_l{}^q \cdots [\cdots \hat{b}^n \hat{b}^m \hat{b}_p \hat{b}_q \cdots] V_m{}^i V_n{}^j \cdots \ .\end{aligned} \tag{A8}$$

In order to express the above transformation in a compact form we introduce matrix

$$\mathbf{V}=\bigoplus_{n=0}^{M}\mathbf{V}_n \ , \tag{A9}$$

where $\mathbf{V}_0=\{1\}$, $\mathbf{V}_1$ is defined in Eq. (A6), and, in general,

$$\mathbf{V}_n=\{V_X{}^Y:\ x=y=n\} \ , \tag{A10}$$

where

$$V_X{}^Y=(V_i{}^k V_j{}^l\cdots)_{\text{antisymmetrized}} \ , \tag{A11}$$

e.g.,

$$V_{ij}{}^{kl}=V_i{}^k V_j{}^l - V_j{}^k V_i{}^l \ . \tag{A12}$$

The same definition follows for matrix $\tilde{\mathbf{V}}=\mathbf{V}^{-1}=\mathbf{V}^{\dagger}$. Now we can write

$$(\hat{X}^{\dagger}\hat{Y})'=\sum_{\substack{W\\(w=x)}}\sum_{\substack{Z\\(z=y)}}\tilde{V}_Y{}^Z \hat{W}^{\dagger}\hat{Z} V_W{}^X \ . \tag{A13}$$

For a linear operator $\hat{\Lambda}$ of the form (50) transformation (A1) leads to a new representation

$$\hat{\Lambda}=(x!y!)^{-1}\lambda'_X{}^Y(\hat{X}^{\dagger}\hat{Y})' \ , \tag{A14}$$

where the transformed parameters $\lambda'_X{}^Y$ can be expressed as follows:

$$\lambda'_X{}^Y = \sum_{\substack{W \\ (w=x)}} \sum_{\substack{Z \\ (z=y)}} \tilde{V}_X{}^W \lambda_W{}^Z V_Z{}^Y . \tag{A15}$$

APPENDIX B: SOME USEFUL FORMULAS FOR OPERATORS BELONGING TO FD ALGEBRA

1. The contraction theorem (Ref. 17)

Consider two strings, $\hat{A}$ and $\hat{B}$, composed of fermion operators from set (26). The lengths of these strings are a and b, respectively. The contraction theorem involving these strings reads

$$\hat{B}\hat{A} = (-1)^{ab} \sum_{n=0}^{\min(a,b)} \underbrace{\hat{A}\hat{B}}_{(n)} , \tag{B1}$$

where

$$\underbrace{\hat{A}\hat{B}}_{(n)}$$

symbolizes a sum of all the possible contractions involving n-fermion operators from string $\hat{A}$, and the same number of fermion operators from string $\hat{B}$. Each of n-tuple contractions is a superposition of n single contractions. A single contraction within the string

$$\hat{A}\hat{B} = \hat{c}_1 \hat{c}_2 \cdots \hat{c}_{a+b} \tag{B2}$$

is defined as follows. If the contraction involves operators $\hat{c}_i$ and $\hat{c}_j$, they are removed from string (B2) and the resulting string of $(a+b-2)$-fermion operators is multiplied by a factor

$$(-1)^{i-j} [\hat{c}_i, \hat{c}_j]_+ . \tag{B3}$$

It is important that here an operator $\hat{c}_i$ is either an annihilation or creation operator from set (26), and index i is equal to the ordinal number of operator $\hat{c}_i$ in string (B2). In the case of multiple contractions ($n > 1$) the phase factor in (B3) is, for each successive single contraction, calculated according to the actual ordinal numbers of operators in the string. It can be shown that the definition of multiple contractions does not depend on the sequence in which the single contractions have been performed.

2. Multiplication of the normal products of fermion operators

The contraction theorem described in Sec. 1 of this appendix is applied here to calculation of the product

$$(\hat{X}_1^\dagger \hat{W}_1)(\hat{V}_2^\dagger \hat{Y}_2) = (-1)^{(x_1+w_1)v_2} \sum_{z=0}^{\min(v_2,w_1)} \underbrace{\hat{V}_2^\dagger \hat{X}_1^\dagger \hat{W}_1}_{(z)} \hat{Y}_2 , \tag{B4}$$

where $\hat{X}_1$, $\hat{W}_1$, $\hat{V}_2$, and $\hat{Y}_2$ are strings of annihilation operators $\{\hat{b}_i\}$. Here and below we make use of the notation introduced at the beginning of Sec. IV. For performing each z-tuple contraction in Eq. (B4), the following representation will be used:

$$\hat{W}_1 = \sum_{Y_1} \delta_{W_1}{}^{Y_1 Z} \hat{Y}_1 \hat{Z} , \tag{B5a}$$

$$\hat{V}_2 = \sum_{X_2} \delta_{V_2}{}^{Z X_2} \hat{Z} \hat{X}_2 , \tag{B5b}$$

where string $\hat{Z}$ contains those operators which will be contracted. In Eqs. (B5) the constrained summation over strings of indices is applied [see Eq. (49)], and therefore there is only a single term which survives in each Eq. (B5). Now we can write

$$(\hat{X}_1^\dagger \hat{W}_1)(\hat{V}_2^\dagger \hat{Y}_2) = (-1)^{(x_1+w_1)v_2} \times \sum_{X_2} \sum_{Y_1} \sum_{Z} \delta_{W_1}{}^{Y_1 Z} \delta_{Z X_2}{}^{V_2} \hat{X}_2^\dagger \underbrace{\hat{Z}^\dagger \hat{X}_1^\dagger \hat{Y}_1 \hat{Z}}_{(z)} \hat{Y}_2 , \tag{B6}$$

where the contraction theorem gives

$$\hat{X}_2^\dagger \underbrace{\hat{Z}^\dagger \hat{X}_1 \hat{Y}_1 \hat{Z}}_{(z)} \hat{Y}_2 = (-1)^{(x_1+y_1+1)z} X_2^\dagger X_1^\dagger \hat{Y}_1 \hat{Y}_2 . \tag{B7}$$

From Eqs. (B5) it follows that $w_1 = y_1 + z$, and $v_2 = x_2 + z$. The phase factors appearing in Eqs. (B6) and (B7) can be combined to give

$$(-1)^{(x_1+y_1+z)(x_2+z)} (-1)^{(x_1+y_1+1)z} = (-1)^{(x_1+y_1+z)x_2} = (-1)^{(x_1+w_1)x_2} , \tag{B8}$$

where we have used the fact that expression $2(x_1+y_1)z + z^2 + z$ is always even. Finally, we get

$$(\hat{X}_1^\dagger \hat{W}_1)(\hat{V}_2^\dagger Y_2) = \sum_{X_2} \sum_{Y_1} \sum_{Z} (-1)^{(x_1+w_1)x_2} \delta_{W_1}{}^{Y_1 Z} \delta_{Z X_2}{}^{V_2} \times (\hat{X}_1 \hat{X}_2)^\dagger \hat{Y}_1 \hat{Y}_2 . \tag{B9}$$

It is to be noted that if operator $\hat{X}_1^\dagger \hat{W}_1$ belongs to $\mathcal{F}$(even) [see set (59)], then $x_1 + w_1 =$ even, and

$$(-1)^{(x_1+w_1)x_2} = 1 . \tag{B10}$$

3. Calculation of products of linear operators in Fock space

From now on we restrict our attention only to operators belonging to subalgebra $\mathcal{F}$(even). Consider the product

$$\hat{C}\hat{D} = \hat{\Lambda} , \tag{B11}$$

where $\hat{\Lambda}$ is written in Eq. (49), and operators $\hat{C}$ and $\hat{D}$ are of the same form:

$$\hat{C} = \sum_{X_1} \sum_{W_1} c_{X_1}{}^{W_1} \hat{X}_1^\dagger \hat{W}_1 , \tag{B12a}$$

$$\hat{D} = \sum_{V_2} \sum_{Y_2} d_{V_2}{}^{Y_2} \hat{V}_2^\dagger \hat{Y}_2 . \tag{B12b}$$

After inserting Eqs. (B12) into Eq. (B11) we get

$$\hat{\Lambda} = \sum_{X_1} \sum_{W_1} \sum_{V_2} \sum_{Y_2} c_{X_1}{}^{W_1} d_{V_2}{}^{Y_2} (\hat{X}_1^\dagger \hat{W}_1)(\hat{V}_2^\dagger \hat{Y}_2) . \tag{B13}$$

Now we can use result (B9) with Eq. (B10). Since

$$\sum_{W_1} c_{X_1}{}^{W_1}\delta_{W_1}{}^{Y_1 Z}=c_{X_1}{}^{Y_1 Z}, \tag{B14}$$

and

$$\sum_{V_2} d_{V_2}{}^{Y_2}\delta_{ZX_2}{}^{V_2}=d_{ZX_2}{}^{Y_2}, \tag{B15}$$

we arrive at the formula

$$\hat{\Lambda}=\sum_{X_1}\sum_{X_2}\sum_{Y_1}\sum_{Y_2}\sum_{Z} c_{X_1}{}^{Y_1 Z} d_{ZX_2}{}^{Y_2}(\hat{X}_1\hat{X}_2)^{\dagger}\hat{Y}_1\hat{Y}_2 . \tag{B16}$$

Similarly, as in Eqs. (B5), we can write

$$\hat{X}_1\hat{X}_2=\sum_{X}\delta_{X_1X_2}{}^{X}\hat{X} , \tag{B17a}$$

$$\hat{Y}_1\hat{Y}_2=\sum_{Y}\delta_{Y_1Y_2}{}^{Y}\hat{Y} . \tag{B17b}$$

Finally, by comparing with Eq. (49), we find that

$$\lambda_X{}^{Y}=\sum_{X_1}\sum_{X_2}\sum_{Y_1}\sum_{Y_2}\sum_{Z}\delta_X{}^{X_1X_2}c_{X_1}{}^{Y_1Z}d_{ZX_2}{}^{Y_2}\delta_{Y_1Y_2}{}^{Y} . \tag{B18}$$

This is an important formula which can greatly simplify derivation of algebraic expressions appearing in many-fermion theories. Below, some applications of formula (B18) will be shown.

4. Calculation of a commutator

In this section we calculate a commutator

$$[\hat{C},\hat{D}]_-=\hat{C}\hat{D}-\hat{D}\hat{C} . \tag{B19}$$

By denoting $\hat{\Lambda}'=\hat{D}\hat{C}$ we find from Eq. (B18) that

$$\lambda'_X{}^{Y}=\sum_{X_1}\sum_{X_2}\sum_{Y_1}\sum_{Y_2}\sum_{Z}\delta_X{}^{X_2X_1}d_{X_2}{}^{Y_2Z}c_{ZX_1}{}^{Y_1}\delta_{Y_2Y_1}{}^{Y} . \tag{B20}$$

For commutator (B19), we substitute $\hat{\Lambda}''=\hat{\Lambda}-\hat{\Lambda}'$ and obtain the formula

$$\lambda''_X{}^{Y}=\sum_{X_1}\sum_{X_2}\sum_{Y_1}\sum_{Y_2}\sum_{\substack{Z\\(z>0)}}(\delta_X{}^{X_1X_2}c_{X_1}{}^{Y_1Z}d_{ZX_2}{}^{Y_2}\delta_{Y_1Y_2}{}^{Y}-\delta_X{}^{X_2X_1}d_{X_2}{}^{Y_2Z}c_{ZX_1}{}^{Y_1}\delta_{Y_2Y_1}{}^{Y}) . \tag{B21}$$

It is to be noticed that terms corresponding to $z=0$ are missing from the rhs of Eq. (B21). This happens because (x_1+y_1) and (x_2+y_2) are even in that case, and this leads to

$$\delta_X{}^{X_1X_2}\delta_{Y_1Y_2}{}^{Y}=\delta_X{}^{X_2X_1}\delta_{Y_2Y_1}{}^{Y} . \tag{B22}$$

Thus, due to cancellation of terms with $z=0$, the rhs of Eq. (B21) contains only so-called linked terms.

5. Calculation of matrix elements

Here we show calculation of matrix elements

$$C_X{}^{Y}=\langle\Phi^X|\hat{C}\Phi^Y\rangle , \tag{B23}$$

where operator $\hat{C}$ is of the general form shown in Eq. (B12a). We can write [see Eq. (44)]

$$\hat{C}\Phi^Y=\hat{C}\hat{D}\Phi , \tag{B24}$$

where

$$\hat{D}=\hat{Y}^{\dagger} , \tag{B25}$$

and in Eq. (B12b) we must set

$$d_{V_2}{}^{Y_2}=0 \tag{B26}$$

for $y_2>0$, and

$$d_{V_2}=\delta_{V_2}{}^{Y} . \tag{B27}$$

We also take advantage of Eq. (B11) to write Eq. (B23) in the form

$$C_X{}^{Y}=\langle\Phi^X|\hat{\Lambda}\Phi\rangle=\lambda_X . \tag{B28}$$

Let us notice that operator $\hat{D}$ defined Eq. (B25) is not necessarily confined to $\mathscr{F}$(even). However, since we assume that operator $\hat{C}\in\mathscr{F}$(even), equality (B10) holds and we can use Eq. (B18) to obtain

$$\lambda_X=\sum_{X_1}\sum_{X_2}\sum_{Z}\delta_X{}^{X_1X_2}c_{X_1}{}^{Z}d_{ZX_2} . \tag{B29}$$

By combining Eqs. (B28), (B29), and (B27) we finally find

$$C_X{}^{Y}=\sum_{X_1}\sum_{X_2}\sum_{Z}\delta_X{}^{X_1Z}c_{X_1}{}^{X_2}\delta_{X_2Z}{}^{Y} , \tag{B30}$$

where symbols X_2 and Z have been exchanged in order to obtain a more symmetrical expression.

Equation (B30) determines a linear mapping $\{c_{X_1}{}^{X_2}\}\rightarrow\{C_X{}^{Y}\}$. It is easy to find that any parameter $c_{X_1}{}^{X_2}$ can contribute only to matrix elements $C_X{}^{Y}$ for which $x=x_1+z$ and y_1+z $(z\geq 0)$. This means that if, for example, operator $\hat{C}\in\mathscr{F}^{\dagger}$(even), all the matrix elements $C_X{}^{Y}$ corresponding to $x\leq y$ are identically zero.

APPENDIX C: SYMMETRY PROPERTIES OF THE UNIVERSAL WAVE OPERATOR

In the algebraic approximation space $\mathfrak{M}$ is usually chosen to be invariant with respect to the symmetry group of Hamiltonian $\hat{\mathscr{H}}$. In this case the symmetry group of the projected Hamiltonian $\hat{H}$ is the same as that of $\hat{\mathscr{H}}$. The symmetry of Hamiltonian (3) includes the permutational, particle-number, spin and spatial, as well as time-

reversal symmetry. In nucleonic systems the spin symmetry also occurs. For the system of fermions, the permutational symmetry is fully taken into account when $\mathfrak{M}$ is constructed as a Fock space (see Sec. II). Thus, this symmetry need not be discussed further. In the quasiparticle formalism (see Sec. III) the particle-number symmetry is replaced by the pseudocharge symmetry represented by operator $\hat{Q}$ of Eq. (36), and Hamiltonian $\hat{H}$ is found to commute with $\hat{Q}$ [see Eq. (38)]. The remaining symmetries of $\mathscr{H}$ can be analyzed at the level of one-particle wave functions; here the corresponding symmetry operations are represented by one-particle operators $\hat{U}_1$. We make the assumption (see Sec. III) that our one-particle space $\mathfrak{X}$ is invariant with respect to all the symmetry operators $\hat{U}_1$. With this assumption fulfilled, we may state that the Fock space $\mathfrak{M}$ and Hamiltonian $\hat{H}$ of Eq. (31) are invariant with respect to the symmetry group of Hamiltonian (3).

In Sec. III we have chosen a certain eigenfunction of $\hat{H}$ as a reference and assumed that Ψ belongs to the fully symmetric representation of the symmetry group of $\hat{H}$ (the permutational symmetry is not considered here). Now we assume that our model vacuum Φ possess the same property. This is by no means an obvious assumption, since a "broken-symmetry" determinantal wave function can provide a better approximation to Ψ in certain cases.[18] The symmetry breaking may not only pertain to the symmetries described by operators $\hat{\mathbf{U}}_1$, but also to the pseudocharge symmetry.[15]

In the case of a fully symmetrical Φ not only $\mathfrak{X}$, but also each of subspaces $\mathfrak{X}_h$ and $\mathfrak{X}_p$ [see Eq. (24)] is invariant with respect to all the operators $\hat{U}_1$. The corresponding transformations of basis (6) can now be described as in Appendix A, Eq. (A1), with condition (A4) fulfilled. [We exclude the time-reversal symmetry operator from our further considerations, since it corresponds to an antiunitary transformation of basis (6). The problem of the time-reversal symmetry in the single-reference CC method was analyzed in Ref. 14; an extension of this analysis to the generalized CC method is straightforward.] Using the results of Appendix A one can find that for each one-particle symmetry operator $\hat{U}_1$ its extension $\hat{V}$ onto the Fock space can be constructed:

$$\hat{V}\Phi^Y=(y!)^{-1}\Phi^X V_X{}^Y , \tag{C1}$$

where matrix elements $V_X{}^Y=\langle\Phi^X|\hat{V}|\Phi^Y\rangle$ can be constructed as in Eq. (A11). The symmetry operators $\hat{V}$ are unitary and fulfill the commutation relations

$$[\hat{H},\hat{V}]_-=0 , \tag{C2a}$$

$$[\hat{Q},\hat{V}]_-=0 . \tag{C2b}$$

We can include unitary operators $\exp(i\alpha\hat{A})$, $0\le\alpha\le 2\pi$, in the set

$$\mathscr{G}=\{\hat{V}\} \tag{C3}$$

containing the symmetry operators of Hamiltonian $\hat{H}$; we shall refer to $\mathscr{G}$ as to the symmetry group of $\hat{H}$.

Consider an operator $\hat{\Lambda}$, expressed as in Eq. (50), which commutes with some operator $\hat{V}\in\mathscr{G}$. In this case

$$\hat{V}\hat{\Lambda}\hat{V}^{-1}=\hat{\Lambda} , \tag{C4}$$

and $\hat{\Lambda}$ can be written as

$$\hat{\Lambda}=(x!y!)^{-1}\lambda_X{}^Y(\hat{X}^\dagger\hat{Y})' , \tag{C5}$$

where operators

$$(\hat{X}^\dagger\hat{Y})'=\hat{V}\hat{X}^\dagger\hat{Y}\hat{V}^{-1} \tag{C6}$$

can also be expressed as in Eq. (A13). By comparing Eqs. (50) and (C5), the following invariance can be proved [compare Eq. (A15)]:

$$\lambda_W{}^Z=(x!y!)^{-1}V_W{}^X\lambda_X{}^Y\tilde{V}_Y{}^Z . \tag{C7}$$

Similarly, for matrix elements (52) one finds

$$\Lambda_W{}^Z=(x!y!)^{-1}V_W{}^X\Lambda_X{}^Y\tilde{V}_Y{}^Z . \tag{C8}$$

After these preparations we can discuss symmetry properties of operators $\hat{A}$, $\hat{B}$, $\hat{C}$, and $\hat{D}$ introduced in Sec. IV. We know that, because of Eq. (C2a), eigenfunctions of $\hat{H}$ belong to irreducible representations of the symmetry group $\mathscr{G}$:

$$\hat{V}\Psi^Y=(x!)^{-1}\Psi^X K_X{}^Y , \tag{C9}$$

where matrices $\mathbf{K}$ [of the structure similar to matrices $\mathbf{V}$ of Eq. (A9)] are block-diagonal, each block being an irreducible matrix "image" of operator $\hat{V}$. Here it is assumed that condition (ii) for operator $\hat{A}$ (see Sec. IV) is fulfilled. From Eq. (81) one gets

$$\hat{V}\Psi^Y=(x!)^{-1}(\hat{V}\Phi^X)A_X{}^Y , \tag{C10}$$

and by comparing Eqs. (C9) and (C10) [see also Eq. (C1)] one finds

$$(x!)^{-1}\Psi^X K_X{}^Y=(x!z!)^{-1}\Phi^Z V_Z{}^X A_X{}^Y . \tag{C11}$$

Again, we compare the above equation with Eq. (81) and arrive at the following symmetry-invariance formula for the CI amplitudes:

$$A_Z{}^W=(x!z!)^{-1}V_Z{}^X A_X{}^Y\tilde{K}_Y{}^W , \tag{C12}$$

where $\tilde{\mathbf{K}}=\tilde{\mathbf{K}}^{-1}=\mathbf{K}^\dagger$. Now we can apply Eq. (C12) to transform both sides of Eqs. (85), the resulting equations are the following: For $x=y$,

$$A_X{}^Y=B'_X{}^Y+\sum_{\substack{W\\(w=y)}}\sum_{\substack{V\\(v<y)}}C'_X{}^V D'_V{}^W B'_W{}^Y ; \tag{C12'}$$

for $x>y$,

$$A_X{}^Y=\sum_{\substack{W\\(w=y)}}C'_X{}^W B'_W{}^Y+\sum_{\substack{W\\(w=y)}}\sum_{\substack{V\\(v<y)}}C'_X{}^V D'_V{}^W B'_W{}^Y ; \tag{C12''}$$

and for $x<y$,

$$A_X{}^Y=\sum_{\substack{W\\(w=y)}}D'_X{}^W B'_W{}^Y+\sum_{\substack{W\\(w=y)}}\sum_{\substack{V\\(v<x)}}C'_X{}^V D'_V{}^W B'_W{}^Y , \tag{C12'''}$$

where

$$B'_Z{}^W=(x!y!)^{-1}V_Z{}^X B_X{}^Y \tilde{K}_Y{}^W , \tag{C13a}$$

$$C'_Z{}^W=(x!y!)^{-1}V_Z{}^X C_X{}^Y \tilde{V}_Y{}^W , \tag{C13b}$$

$$D'_Z{}^W=(x!y!)^{-1}V_Z{}^X D_X{}^Y \tilde{V}_Y{}^W . \tag{C13c}$$

In Sec. IV [see Eqs. (75)—(80), and the discussion at the end of the section] we have shown that Eqs. (C12) can have only one solution (and we assume that it exists). Thus

$$B'_Z{}^W=B_Z{}^W , \tag{C14a}$$

$$C'_Z{}^W=C_Z{}^W , \tag{C14b}$$

$$D'_Z{}^W=D_Z{}^W . \tag{C14c}$$

The last two equalities, combined with Eqs. (C13b) and (C13c), respectively, prove [see Eq. (C8)] that

$$[\hat{C},\hat{V}]_-=0 , \tag{C15a}$$

$$[\hat{D},\hat{V}]_-=0 . \tag{C15b}$$

Hence, we have [see Eq. (76)]

$$[\hat{\Omega},\hat{V}]_-=0 , \tag{C16a}$$

and, therefore,

$$[\hat{G},\hat{V}]_-=0 . \tag{C16b}$$

From Eq. (C15a) it follows also that [see Eq. (67)]

$$[\hat{\Theta},\hat{V}]_-=0 , \tag{C17a}$$

and [see Eq. (114)]

$$[\hat{\Gamma},\hat{V}]_-=0 . \tag{C17b}$$

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[1]S. Wilson and D. M. Silver, Phys. Rev. A **14**, 1949 (1976).

[2]W. Kutzelnigg, Chem. Phys. Lett. **83**, 156 (1981); J. Chem. Phys. **77**, 3081 (1982); W. Kutzelnigg and S. Koch, *ibid.* **79**, 4315 (1983); W. Kutzelnigg, *ibid.* **80**, 822 (1984).

[3]F. Coester, Nucl. Phys. **7**, 421 (1958); H. Kümmel, K. H. Lührmann, and J. G. Zabolitzky, Phys. Rep. **36C**, 1 (1978), and references therein.

[4]J. Čížek, J. Chem. Phys. **45**, 4256 (1966); J. Paldus, in *New Horizons of Quantum Chemistry,* edited by P.-O. Löwdin and B. Pullman (Reidel, Dordrecht, 1983), pp. 31—60, and references therein.

[5]R. J. Bartlett, Annu. Rev. Phys. Chem. **32**, 359 (1981), and references therein.

[6]D. Mukherjee, R. K. Moitra, and A. Mukhopadhyay, Pramana **4**, 247 (1975); Mol. Phys. **30**, 1861 (1975); **33**, 955 (1977).

[7]R. Offermann, W. Ey, and H. Kümmel, Nucl. Phys. **A273**, 349 (1976); R. Offermann, *ibid.* **A273** 368 (1976); W. Ey, *ibid.* **A296**, 189 (1978).

[8]I. Lindgren, Int. J. Quantum Chem. **S12**, 33 (1978).

[9]K. Emrich, Nucl. Phys. **A351**, 379 (1981); **A351**, 397 (1981); K. Emrich and J. G. Zabolitzky, *ibid.* **51**, 439 (1981).

[10]B. Jeziorski and H. J. Monkhorst, Phys. Rev. A **24**, 1668 (1981), and references therein.

[11]L. Z. Stolarczyk and H. J. Monkhorst, following paper, Phys. Rev. A **32**, 743 (1985).

[12]L. Z. Stolarczyk and H. J. Monkhorst (unpublished).

[13]C. C. J. Roothaan, Rev. Mod. Phys. **23**, 69 (1951).

[14]L. Z. Stolarczyk and H. J. Monkhorst, Int. J. Quantum Chem. Symp. **18**, 267 (1984).

[15]N. N. Bogoliubov, Zh. Eksp. Teor. Fiz. **34**, 58 (1958) [Sov. Phys.—JETP **7**, 41 (1958)]; J. G. Valatin, Nuovo Cimento **7**, 843 (1958).

[16]J. Paldus and J. Čížek, Adv. Quantum Chem. **9**, 105 (1975).

[17]F. E. Harris, B. Jeziorski, and H. J. Monkhorst, Phys. Rev. A **23**, 1632 (1981).

[18]P.-O. Löwdin, Adv. Chem. Phys. **14**, 283 (1969); J. Paldus, J. Čížek, and B. A. Keating, Phys. Rev. A **8**, 640 (1973).