Coupled-cluster method in Fock space. III. On similarity transformation of operators in Fock space

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A detailed and systematic presentation of algebraic and diagrammatic techniques introduced in paper I [L. Z. Stolarczyk and H. J. Monkhorst, Phys. Rev. A 32, 725 (1985)] is given. Performing a similarity transformation of an operator in Fock space, e.g., a Hamiltonian in the generalized coupled-cluster method (see paper I), leads to lengthy algebraic formulas for the linear parameters (amplitudes) of the transformed operator. These formulas can be expressed in a compact form by means of the so-called reduced diagrams. Precise rules are given for constructing such diagrams (related to the so-called directed graphs of the graph theory) and the algebraic expressions corresponding to them. In particular, rules for generating a connected-diagram expansion of the amplitudes of the transformed operator are formulated. Several examples illustrating the use of this diagrammatic-algebraic approach are considered.

I. INTRODUCTION

In the previous two papers (Refs. 1 and 2, hereafter referred to as papers I and II, respectively) we formulated a generalization of the coupled-cluster (CC) method[3-5] for a system of many fermions. This generalized CC method addresses the problem of calculating (a part of) the spectrum of the Fock-space Hamiltonian $\hat{H}$. The algebraic approach we proposed[1,2] involves expressing operator $\hat{H}$ through so-called quasiparticle fermion operators and performing a similarity transformation

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

yielding an effective Hamiltonian $\hat{G}$. The construction of the wave operator $\hat{\Omega}$ follows the characteristic prescription of the CC method:[3-5] $\hat{\Omega}$ is expressed through operator $\exp(\hat{\Theta})$, where the CC operator $\hat{\Theta}$ belongs to a certain nilpotent operator algebra. In the generalized CC method,[1] operator $\hat{\Theta}$ is determined from the condition that the effective Hamiltonian $\hat{G}$ conserves the number of quasiparticles in the system. Eigenvalues of $\hat{G}$ corresponding to states with a few quasiparticles can then be easily calculated. The well-known property of transformation (1) is that

$$\mathrm{Spec}(\hat{H}) = \mathrm{Spec}(\hat{G}) , \tag{2}$$

and, hence, a part of the spectrum of $\hat{H}$ is found that way. In other words, the generalized CC method effectively converts the many-particle problem associated with Hamiltonian $\hat{H}$ into a few-quasiparticle problem of Hamiltonian $\hat{G}$. The present paper is devoted to a study of a variant of transformation (1), namely,

$$\hat{H} \rightarrow \hat{\Gamma} = \exp(-\hat{\Theta}) \hat{H} \exp\hat{\Theta} , \tag{3}$$

where $\hat{H}$ and $\hat{\Theta}$ are some arbitrary operators acting in a finite-dimensional Fock space. The purpose of our analysis is to find a method for deriving algebraic formulas expressing the dependence of the linear parameters (amplitudes) of operator $\hat{\Gamma}$ on the amplitudes of operators $\hat{H}$ and $\hat{\Theta}$. A diagrammatic approach is devised to handle lengthy algebraic formulas, and precise rules are given for converting algebraic expressions into diagrams, and vice versa. The present study extends a preliminary one given in paper I, and will certainly be helpful in the better understanding of some details in the derivation of the generalized CC equations in that paper. We wish also to use results of the present paper to generate algebraic formulas for calculating expectation values and transition moments within the framework of the generalized CC method (see the following paper,[6] hereafter referred to as paper IV).

The content of the present paper is as follows. In Sec. II the algebraic structure of the Fock space and the corresponding Fermi-Dirac algebra are reviewed, along with the notation introduced in paper I. In Secs. III and IV algebraic expressions and the corresponding diagrams are derived for operator products and powers, respectively. Section V contains a discussion of algebraic and diagrammatic expressions for the amplitudes of the transformed operator defined in (3). Using the theory of Sec. V, we explain in Sec. VI how the generalized CC equations [the Brueckner-Hartree-Fock (BHF) equations] of paper II were derived. In Sec. VI we derive also additional generalized CC equations which are necessary in an extended version of the generalized CC method considered in paper IV. The results of the present paper are summarized in Sec. VII. Appendixes A–D contain supplementary derivations and discussions. Throughout the paper we shall refer to formulas of papers I, II, and IV by quoting an equation number preceded by the appropriate Roman numeral I, II, or IV.

II. FOCK SPACE AND FERMI-DIRAC ALGEBRA: NOTATION

The full Fock space for our fermion particles is a Cartesian product of Hilbert spaces spanned by n-particle

($n=0,1,\ldots,\infty$) wave functions, antisymmetric (for $n\geq 2$) with respect to permutations of particles. The Hilbert space corresponding to $n=0$ is spanned by a single-wave function Φ_0 called the physical vacuum. In the algebraic approximation[1] one chooses some M-element basis set of linearly independent spin orbitals, which spans an M-dimensional subspace $\aleph=\aleph(M)$ in the Hilbert space of the one-particle wave functions. Let

$$\{\phi_i\}_{i=1}^{i=M} \tag{4}$$

be an orthonormal basis in $\aleph$.

The annihilation operator $\hat{a}_i$ associated with spin orbital ϕ_i is a linear operator defined in the full Fock space; its action on an n-particle antisymmetric wave function Ψ gives an $(n-1)$-particle wave function $\hat{a}_i\Psi$:

$$\hat{a}_i\Psi(1,\ldots,n-1)=n^{1/2}\int d\tau_n\,\phi_i^*(n)\Psi(1,\ldots,n)\ , \tag{5}$$

where $\int d\tau_n$ denotes the integration over spatial and spin coordinates of the nth particle. It is also required that

$$\hat{a}_i\Phi_0=0\ , \tag{6}$$

for $i=1,\ldots,M$. The choice of the phase factor in Eq. (5) (as used in paper I) is the same as in Ref. 7, but a different choice is also frequently encountered, see, e.g., Ref. 8. For each annihilation operator $\hat{a}_i$ one defines the creation operator $\hat{a}^{\,i}$ as the Hermitian conjugate

$$\hat{a}^{\,i}\equiv(\hat{a}_i)^\dagger\ . \tag{7}$$

The annihilation and creation operators for fermion particles (the fermion operators, in brief) fulfill the following anticommutation relations:

$$[\hat{a}_i,\hat{a}_j]_+=[\hat{a}^{\,i},\hat{a}^{\,j}]_+=0\ , \tag{8a}$$

$$[\hat{a}_i,\hat{a}^{\,j}]_+=\delta_i^{\,j}\ . \tag{8b}$$

The set

$$\{\hat{a}_i,\hat{a}^{\,i}\}_{i=1}^{i=M} \tag{9}$$

generates an algebra $\mathcal{F}=\mathcal{F}(M)$ which we call the Fermi-Dirac algebra. One may choose another set of generators,

$$\{\hat{b}_i,\hat{b}^{\,i}\}_{i=1}^{i=M}\ , \tag{10}$$

fulfilling relations (7) and (8) by applying a similarity transformation

$$\hat{b}_i=\hat{U}^{-1}\hat{a}_i\hat{U}\ , \tag{11}$$

with a unitary operator $\hat{U}\in\mathcal{F}$. An analog of Eq. (6) also holds, with the physical vacuum Φ_0 replaced by the so-called model vacuum

$$\Phi=\hat{U}^{-1}\Phi_0\ . \tag{12}$$

One usually attempts to find operator $\hat{U}$ such that Φ is, in some sense, optimal, e.g., as an approximation to the ground state of a considered many-particle system (see paper II). In practice, the choice of $\hat{U}$ is most often limited to operators generating linear transformations of set (9) (see also the generalizations discussed in Ref. 9),

$$\hat{b}_i=\hat{a}_k K_i^k+\hat{a}^{\,k}L_{ki}\ , \tag{13}$$

where we use Einstein's summation convention. Transformation (13) is the Bogoliubov-Valatin transformation;[10] a special case of it is the particle-hole transformation [see Eqs. (I.27)]. Fermion operators of set (10) will be hereafter referred to as the quasiparticle fermion operators.

It follows from Wick's theorem[11] that any element of algebra $\mathcal{F}$ can be expressed as a linear combination of the so-called normal products, $\hat{X}^\dagger\hat{Y}$, of fermion operators. Here $\hat{X}$ and $\hat{Y}$ are products of annihilation operators of set (10); for example,

$$\hat{X}=\hat{b}_i\hat{b}_j\hat{b}_k\cdots\ . \tag{14}$$

According to the notation introduced in paper I, the string of indices corresponding to operator $\hat{X}$ of Eq. (14) will be denoted by

$$X=ijk\cdots\ , \tag{15}$$

and the number of annihilation operators in $\hat{X}$ by x. We also assume that for $x=0$ the corresponding index string X is empty and

$$\hat{X}=1\ . \tag{16}$$

Due to the anticommutation relation (8a), if index strings X and Y are of the same length ($x=y$) and differ only by a permutation of indices, then

$$\hat{X}=(-1)^p\hat{Y}\ , \tag{17}$$

where p is the parity (even or odd) of the permutation. Such strings will be called the equivalent index strings; this equivalency relation will be denoted by $X\sim Y$. It follows from Eq. (17) that $\hat{X}=0$ if there is a repetition of any index in string X, such a string will be called the degenerate index string. A nondegenerate string (15) corresponding to ordered indices $i<j<k<\cdots$ will be denoted by $\bar{X}$ and called the ordered index string. Obviously, $X\sim\bar{X}$, and the parity of the permutation which transforms X into $\bar{X}$ will be called the parity of X and denoted by $p(X)$. Now parameter p of Eq. (17) may be expressed as

$$p=p(X)+p(Y)\ . \tag{18}$$

Let us define also a very useful quantity we call the generalized Kronecker delta [see Eq. (I.47)]:

$$\delta_X^{\ Y}=\begin{cases}(-1)^{p(X)+p(Y)} & \text{for } X\sim Y \text{ and } X \text{ nondegenerate}\\ 0 & \text{otherwise}\ .\end{cases} \tag{19}$$

Using the above notation we define a finite-dimensional Fock space $\mathfrak{M}=\mathfrak{M}(M)$ (a subspace of the full fermion Fock space) spanned by an orthonormal basis set

$$\{\Phi^X=\hat{X}^\dagger\Phi:\ X=\bar{X}\}_{x=0}^{x=M}\ , \tag{20}$$

where Φ is the model vacuum of Eq. (12). The wave functions Φ^X are called (generalized) configurations; in the case when fermion quasiparticle operators of set (10) are obtained by using a particle-hole transformation, Φ^X are simply Slater's determinantal functions. The Fock space $\mathfrak{M}$ is a Hilbert space of dimension 2^M.

The Fermi-Dirac algebra $\mathcal{F}$ turns out to be the algebra of all linear operators acting in $\mathfrak{M}$. As a vector space, $\mathcal{F}$ is spanned by set

$$\{\hat{X}^{\dagger}\hat{Y}:\ X=\bar{X},\ Y=\bar{Y}\}_{x,y=0}^{x,y=M}\ , \tag{21}$$

and the dimension of the vector space $\mathcal{F}$ is equal to 2^{2M}. Any linear operator $\hat{H}\in\mathcal{F}$ can be expressed as a linear combination of operators of set (21),

$$\hat{H}=\eta+\eta^i\hat{b}_i+\eta_i\hat{b}^{\,i}+\eta_i{}^j\hat{b}^{\,i}\hat{b}_j+\tfrac{1}{2}\eta^{ij}\hat{b}_i\hat{b}_j + \tfrac{1}{2}\eta_{ij}\hat{b}^{\,j}\hat{b}^{\,i}+\cdots\ . \tag{22a}$$

As in papers I and II, we assume here that the linear coefficients in Eq. (22a) (η amplitudes), of a general form $\eta_X{}^Y$, are antisymmetric with respect to (separate) permutations of indices within strings X and Y. Thus, when the unrestricted (Einstein's convention) summation over x interchangeable indices is performed, one has to apply a "normalization" factor of $(x!)^{-1}$. Equation (22a) may be rewritten in a more compact form

$$\hat{H}=(x!y!)^{-1}\eta_X{}^Y\hat{X}^{\dagger}\hat{Y}\ , \tag{22b}$$

where the unrestricted summation over repeating indices is implicit. In some cases it is convenient to write a formula employing a restricted summation over repeating indices. Let us, for example, rewrite Eqs. (22a) and (22b) once more,

$$\hat{H}=\sum_X\sum_Y\eta_X{}^Y\hat{X}^{\dagger}\hat{Y}\ . \tag{22c}$$

The restricted summation used in Eq. (22c) has the following meaning: The first summation sign denotes a summation over all nondegenerate strings X, from $x=0$ to $x=M$, such that if a term corresponding to string X is taken into account in the summation, all the terms corresponding to strings which are equivalent to X are excluded from the summation. In other words, the restricted summation runs over the entire set (if no conditions are indicated) of nondegenerate, nonequivalent index strings. One of the possible variants of the restricted summation is to perform a summation over ordered strings $\bar{X}$.

In paper I we showed that the vector space $\mathcal{F}$ can be expressed as a direct sum of vector spaces,

$$\mathcal{F}=\mathcal{F}^{\uparrow}\oplus\mathcal{F}^{0}\oplus\mathcal{F}^{\downarrow}\ , \tag{23}$$

where subspaces $\mathcal{F}^{\uparrow}$, $\mathcal{F}^{0}$, and $\mathcal{F}^{\downarrow}$ are spanned by the subsets of (21) subject to conditions $x>y$, $x=y$, and $x<y$, respectively [see Eqs. (I.54)]. $\mathcal{F}^{\uparrow}$, $\mathcal{F}^{0}$, and $\mathcal{F}^{\downarrow}$ are also subalgebras of algebra $\mathcal{F}$. Algebras $\mathcal{F}^{\uparrow}$ and $\mathcal{F}^{\downarrow}$, called the excitation and deexcitation algebra, respectively, are nilpotent algebras. It is to be noted that the decomposition (23) depends, in general, on the choice of the set of generators (10). Another decomposition of the vector space $\mathcal{F}$ will also be considered,

$$\mathcal{F}=\mathcal{F}(\text{even})\oplus\mathcal{F}(\text{odd})\ , \tag{24}$$

where subspaces $\mathcal{F}$(even) and $\mathcal{F}$(odd) are spanned by the subsets of (21) subject to conditions $x+y=\text{even}$ and $x+y=\text{odd}$, respectively. $\mathcal{F}$(even) appears also to be a subalgebra of algebra $\mathcal{F}$. As a vector space, $\mathcal{F}$(even) can be expressed in the form

$$\mathcal{F}(\text{even})=\mathcal{F}^{\uparrow}(\text{even})\oplus\mathcal{F}^{0}\oplus\mathcal{F}^{\downarrow}(\text{even})\ , \tag{25}$$

where $\mathcal{F}^{\uparrow}$(even) and $\mathcal{F}^{\downarrow}$(even) are subspaces (and subalgebras) of $\mathcal{F}^{\uparrow}$ and $\mathcal{F}^{\downarrow}$, respectively. The structure of the Fermi-Dirac algebra, given in Eqs. (23)–(25), is important for formulating the generalized CC method.[1]

III. OPERATOR PRODUCTS AND CORRESPONDING DIAGRAMS

In this section we shall consider operator products

$$\hat{\Lambda}=\hat{\Theta}_n\hat{\Theta}_{n-1}\cdots\hat{\Theta}_1\ , \tag{26}$$

where

$$\hat{\Lambda}=\sum_X\sum_Y\lambda_X{}^Y\hat{X}^{\dagger}\hat{Y}\ , \tag{27}$$

$$\hat{\Theta}_k=\sum_X\sum_Y[{}_X{}^Y]_k\hat{X}^{\dagger}\hat{Y}\ , \tag{28}$$

and it will be assumed that $\hat{\Theta}_k\in\mathcal{F}$(even), $k=1,\ldots,n$. Hence, in Eqs. (27) and (28), strings X and Y are subject to condition $x+y=\text{even}$. In this section we shall use the restricted-summation convention [see Eq. (22c) and the following discussion]. Below, formulas expressing the λ amplitudes of operator $\hat{\Lambda}$ through the $[\ ]_k$ amplitudes of operators $\hat{\Theta}_k$, for various n, are discussed. For $n=2$ and $n=3$, the pertinent formulas were given in Eqs. (I.B18) and (II.A9), respectively. We rewrite these formulas using the notation of Eqs. (26)–(28): (i) $n=2$,

$$\lambda_X{}^Y=\sum_{X_2}\sum_{X_1}\sum_{Y_2}\sum_{Y_1}\sum_{Z_{21}}\delta_X{}^{X_2X_1}[{}_{X_2}{}^{Y_2Z_{21}}]_2[{}_{Z_{21}X_1}{}^{Y_1}]_1\delta_{Y_2Y_1}{}^Y\ ; \tag{29}$$

(ii) $n=3$,

$$\lambda_X{}^Y=\sum_{X_3}\sum_{X_2}\sum_{X_1}\sum_{Y_3}\sum_{Y_2}\sum_{Y_1}\sum_{Z_{31}}\sum_{Z_{21}}(-1)^{x_2z_{31}}\delta_X{}^{X_3X_2X_1}[{}_{X_3}{}^{Y_3Z_{32}Z_{31}}]_3[{}_{Z_{32}X_2}{}^{Y_2Z_{21}}]_2[{}_{Z_{21}Z_{31}X_1}{}^{Y_1}]_1\delta_{Y_3Y_2Y_1}{}^Y\ . \tag{30}$$

Equation (29) is the basic formula in our algebraic technique since the formulas for $n>2$ can be derived from it by recursion. This procedure turns out to be quite cumbersome, however, which makes generation of the explicit formulas for $n>2$ worthwhile. In addition, we have found an error in the derivation of Eq. (A9) in paper II, though the final formula is correct. Therefore, in Appendix A we give a detailed derivation of Eq. (30), together with arguments which lead to the formula for general n.

A very convenient, compact representation of formulas (29), (30), and those for $n \geq 4$ may be given in the form of diagrams. Such a representation was introduced in paper I; now we are going to put it on a more formal basis. A simple diagram corresponding to a $[\ ]_k$ amplitude of operator $\hat{\Theta}_k$ is depicted in Fig. 1.

We write [see Eqs. (29) and (30)] the following: (i) $n=2$,

$$\lambda_X{}^Y = \sum_{a_2}\sum_{a_1}\sum_{b_2}\sum_{b_1}\sum_{c_{21}} J_X{}^Y(2;a_2,a_1;b_2,b_1;c_{21}) \; ; \tag{31}$$

(ii) $n=3$,

$$\lambda_X{}^Y = \sum_{a_3}\sum_{a_2}\sum_{a_1}\sum_{b_3}\sum_{b_2}\sum_{b_1}\sum_{c_{32}}\sum_{c_{31}}\sum_{c_{21}} J_X{}^Y(3;a_3,a_2,a_1;b_3,b_2,b_1;c_{32},c_{31},c_{21}) \; ; \tag{32}$$

where quantities (hereafter called simply diagrams)

$$J_X{}^Y(2;a_2,a_1;b_2,b_1;c_{21}) = \sum_{\substack{X_2\\(x_2=a_2)}} \sum_{\substack{X_1\\(x_1=a_1)}} \sum_{\substack{Y_2\\(y_2=b_2)}} \sum_{\substack{Y_1\\(y_1=b_1)}} \sum_{\substack{Z_{21}\\(z_{21}=c_{21})}} \delta_X{}^{X_2X_1}[{}_{X_2}{}^{Y_2Z_{21}}]_2[{}_{Z_{21}X_1}{}^{Y_1}]_1\delta_{Y_2Y_1}{}^Y \tag{33}$$

and

$$J_X{}^Y(3;a_3,a_2,a_1;b_3,b_2,b_1;c_{32},c_{31},c_{21}) = (-1)^{a_2c_{31}} \sum_{\substack{X_3\\(x_3=a_3)}} \sum_{\substack{X_2\\(x_2=a_2)}} \sum_{\substack{X_1\\(x_1=a_1)}} \sum_{\substack{Y_3\\(y_3=b_3)}} \sum_{\substack{Y_2\\(y_2=b_2)}} \sum_{\substack{Y_1\\(y_1=b_1)}} \sum_{\substack{Z_{32}\\(z_{32}=c_{32})}} \sum_{\substack{Z_{31}\\(z_{31}=c_{31})}}$$

$$\times \sum_{\substack{Z_{21}\\(z_{21}=c_{21})}} \delta_X{}^{X_3X_2X_1}[{}_{X_3}{}^{Y_3Z_{32}Z_{31}}]_3[{}_{Z_{32}X_2}{}^{Y_2Z_{21}}]_2[{}_{Z_{21}Z_{31}X_1}{}^{Y_1}]_1\delta_{Y_3Y_2Y_1}{}^Y \tag{34}$$

are given the diagrammatic representation in Fig. 2. In this representation the vertical ordering of terms, from the bottom to the top (traditionally referred to as the time ordering), corresponds to the horizontal ordering, from the right to the left, of the $[\ ]_k$ amplitudes in Eqs. (33) and (34). Symbols $a_1, a_2, \ldots$ indicate the numbers of outgoing lines, $b_1, b_2, \ldots$ stand for the numbers of ingoing lines, and $c_{21}, c_{31}, \ldots$ stand for the numbers of internal lines in a diagram. In the case of the formula corresponding to general n, one may write

$$\lambda_X{}^Y = \sum_{\text{out}}\sum_{\text{in}}\sum_{\text{intra}} J_X{}^Y(n;\text{out};\text{in};\text{intra}) \; , \tag{35}$$

where

$$\text{out} = a_n, \ldots, a_1 \; , \tag{36a}$$

$$\text{in} = b_n, \ldots, b_1 \; , \tag{36b}$$

$$\text{intra} = c_{n,n-1}, \ldots, c_{n,1}, c_{n-1,n-2}, \ldots, c_{n-1,1}, \ldots, c_{21} \; . \tag{36c}$$

The general algebraic form of a diagram reads [compare Eqs. (33) and (34), see also Appendix A]

$$J_X{}^Y(n;\text{out};\text{in};\text{intra}) = (-1)^P \sum_{\substack{X_n\\(x_n=a_n)}} \cdots \sum_{\substack{X_1\\(x_1=a_1)}} \sum_{\substack{Y_n\\(y_n=b_n)}} \cdots \sum_{\substack{Y_1\\(y_1=b_1)}} \sum_{\substack{Z_{n,n-1}\\(z_{n,n-1}=c_{n,n-1})}} \sum_{\substack{Z_{n1}\\(z_{n1}=c_{n1})}}$$

$$\times \sum_{\substack{Z_{n-1,n-2}\\(z_{n-1,n-2}=c_{n-1,n-2})}} \cdots \sum_{\substack{Z_{n-1,1}\\(z_{n-1,1}=c_{n-1,1})}} \cdots \sum_{\substack{Z_{21}\\(z_{21}=c_{21})}} \delta_X{}^{X_n\cdots X_1}[{}_{X_n}{}^{Y_nZ_{n,n-1}\cdots Z_{n1}}]_n$$

$$\times [{}_{Z_{n,n-1}X_{n-1}}{}^{Y_{n-1}Z_{n-1,n-2}\cdots Z_{n-1,1}}]_{n-1} \cdots [{}_{Z_{21}\cdots Z_{n1}X_1}{}^{Y_1}]_1 \delta_{Y_n\cdots Y_1}{}^Y \; , \tag{37}$$

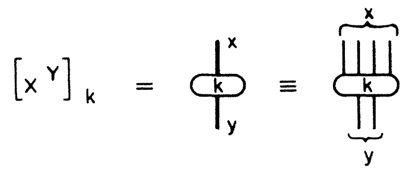

FIG. 1. Diagrammatic representation of a $[\ ]_k$ amplitude of operator $\hat{\Theta}_k$. Bold lines are used for multiple lines.

where what we call the parity of a diagram, P, is calculated as

$$P \equiv P(\text{out;intra}) = \sum_{1 \le i < j < k \le n} a_j c_{ki} + \sum_{1 \le i < j < k < l \le n} c_{lj} c_{ki} \ . \tag{38}$$

The above formula for P corresponds to the particular ordering of index strings (hereafter referred to as the standard ordering) we adopted on the right-hand side (rhs) of Eq. (37). The reader is asked to note a characteristic pattern of "interlocking" indices in both terms on the rhs of Eq. (38). Sets (36) are subject to conditions

$$\sum_{i=1}^{n} a_i = x \ , \tag{39a}$$

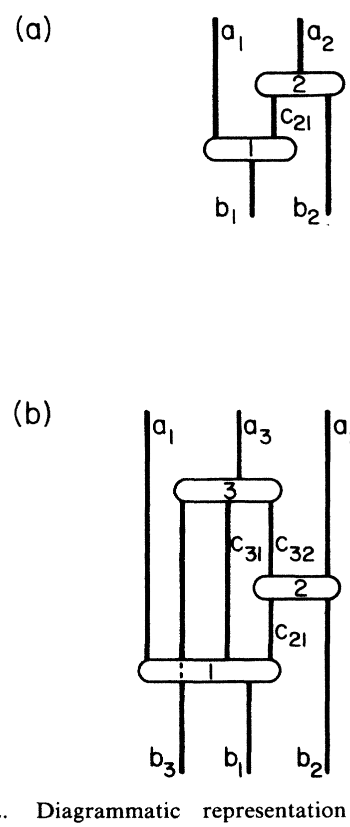

FIG. 2. Diagrammatic representation of (a) quantity $J_X{}^Y(2;a_2,a_1;b_2,b_1;c_{21})$ of Eq. (33); (b) quantity $J_X{}^Y(3;a_3,a_2,a_1;b_3,b_2,b_1;c_{32},c_{31},c_{21})$ of Eq. (34). Bold lines are used for multiple lines (see Fig. 1).

$$\sum_{i=1}^{n} b_i = y \ , \tag{39b}$$

and

$$a_j + b_j + \sum_{\substack{i=1 \\ (i<j)}}^{n} c_{ji} + \sum_{\substack{k=1 \\ (k>j)}}^{n} c_{kj} = \text{even} \ , \tag{39c}$$

for $1 < j < n$. Equation (39c) is a consequence of the requirement that each $\hat{\Theta}_j \in \mathcal{F}(\text{even})$. In general, if operators $\hat{\Theta}_2$ and $\hat{\Theta}_1$ are not confined to $\mathcal{F}(\text{even})$, formulas (29) and (33) need be modified by inserting an additional phase factor on their rhs's [see the derivation for formula (I.B18), in this case the phase factor is given in Eq. (I.B8)]. The corresponding phase factors for formulas (30), (34), and (37) can also be derived quite easily.

In practical applications of formula (35), one first generates all possible diagrams for a given $\lambda_X{}^Y$ and then calculates their values using Eq. (37). We found it convenient[1] to rewrite formula (37) for each particular diagram as follows: (i) the generalized Kronecker deltas

$$\delta_X{}^{X_n \cdots X_1}, \quad \delta_{Y_n \cdots Y_1}{}^{Y}$$

are removed from the algebraic expression, (ii) the summations over strings $X_n, \ldots, X_1$ and $Y_n, \ldots, Y_1$ are replaced by the antisymmetrization of the resulting algebraic expression separately in lower and upper fixed indices (corresponding to strings X and Y, respectively), (iii) Einstein's convention of the unrestricted summation over repeating lower and upper indices (corresponding to strings Z_{kl}) is applied; every unrestricted summation over z_{kl} equivalent indices introduces a factor $(z_{kl}!)^{-1}$, see Eq. (22b). Several examples of such a treatment of formula (37) will be given in Sec. IV.

IV. OPERATOR POWERS AND CORRESPONDING DIAGRAMS

Results of Sec. III will now be applied to a special case of Eq. (26) with

$$\hat{\Theta}_n = \hat{\Theta}_{n-1} = \cdots = \hat{\Theta}_1 = \hat{\Theta} \ , \tag{40}$$

where we assume that $\hat{\Theta} \in \mathcal{F}(\text{even})$,

$$\hat{\Theta} = \sum_{\substack{X \\ (x+y=\text{even})}} \sum_{Y} \theta_X{}^Y \hat{X}^\dagger \hat{Y} \ . \tag{41}$$

The diagrammatic representation of the θ amplitudes of operators $\hat{\Theta}$ will be that given in Fig. 1, with letter k omitted. A new feature of the present case is that now diagrams with different structures may correspond to algebraic expressions that are closely related. Examples of such diagrams, differing only in the time ordering of their components, are given in Figs. 3 and 4. The algebraic expressions for the diagrams depicted in Fig. 3 read (see the remarks in the last paragraph of Sec. III) as follows: diagram (a1)

$$J_{ijk}{}^l(2;1,2;1,0;0) = \theta_i{}^l \theta_{jk} - \theta_j{}^l \theta_{ik} - \theta_k{}^l \theta_{ji} \ ; \tag{42a}$$

diagram (a2),

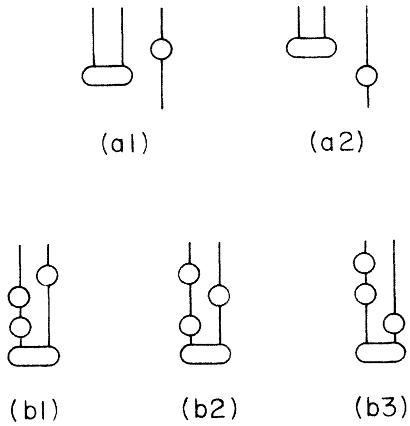

FIG. 3. Examples of diagrams differing in the time ordering of their components: (a1) and (a2) see Eqs. (42); (b1)–(b3) see Eqs. (43).

$$J_{ijk}{}^{l}(2;2,1;0,1;0)=\theta_{ij}\theta_k{}^l-\theta_{ik}\theta_j{}^l-\theta_{kj}\theta_i{}^l\ ; \qquad (42b)$$

diagram (b1),

$$J_{ij}(4;1,1,0,0;0,0,0,0;0,0,1,1,0,1)$$
$$=(-1)^1(\theta_i{}^k\theta_j{}^l\theta_l{}^m\theta_{mk}-\theta_j{}^k\theta_i{}^l\theta_l{}^m\theta_{mk})\ ; \qquad (43a)$$

diagram (b2),

$$J_{ij}(4;1,1,0,0;0,0,0,0;0,1,0,0,1,1)$$
$$=(-1)^2(\theta_i{}^k\theta_j{}^l\theta_k{}^m\theta_{ml}-\theta_j{}^k\theta_i{}^l\theta_k{}^m\theta_{ml})\ ; \qquad (43b)$$

diagram (b3),

$$J_{ij}(4;1,0,1,0;0,0,0,0;1,0,0,0,1,1)$$
$$=(-1)^1(\theta_i{}^k\theta_k{}^l\theta_j{}^m\theta_{ml}-\theta_j{}^k\theta_k{}^l\theta_i{}^m\theta_{ml})\ . \qquad (43c)$$

It is seen that the rhs's of Eqs. (42a) and (42b) are equal.

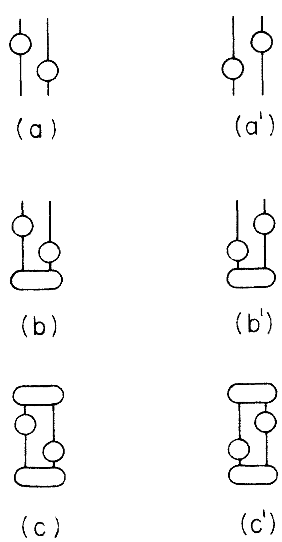

FIG. 4. Examples of symmetry-related diagrams: (a) and (a′) see Eq. (45); (b) and (b′) see Eq. (46); (c) and (c′) see Eq. (47).

A similar conclusion can also be reached in the case of Eqs. (43a)–(43c); here exchanging of some of the summation indices is necessary. In general, the following lemma can be proven (see Appendix B).

Lemma 1. Diagrams differing only in the time ordering of their components give identical contributions to sum (35).

The above lemma suggests that in the case of calculating operator powers, Eq. (35) may be modified such that only the contributions from nonequivalent (with respect to the time ordering) diagrams are taken into account, each contribution multiplied by an appropriate weight factor (called the time-ordering factor),

$$T\equiv T(\text{out};\text{in};\text{intra})\ , \qquad (44)$$

equal to the number of possible time orderings of the corresponding diagram. Things are a bit more subtle, however. Consider the algebraic expressions corresponding to the diagrams depicted in Fig. 4 (see the remarks in the last paragraph of Sec. III): diagrams (a) and (a′),

$$J_{ij}{}^{kl}(2;1,1;1,1;0)=\theta_i{}^k\theta_j{}^l-\theta_i{}^l\theta_j{}^k-\theta_j{}^k\theta_i{}^l+\theta_j{}^l\theta_i{}^k$$
$$=2(\theta_i{}^k\theta_j{}^l-\theta_j{}^k\theta_i{}^l)\ ; \qquad (45)$$

diagrams (b) and (b′),

$$J_{ij}(3;1,1,0;0,0,0;0,1,1)$$
$$=(-1)^1(\theta_i{}^k\theta_j{}^l\theta_{lk}-\theta_j{}^k\theta_i{}^l\theta_{lk})\ ; \qquad (46)$$

diagrams (c) and (c′),

$$J(4;0,0,0,0;0,0,0,0;1,1,0,0,1,1)$$
$$=(-1)^1\theta^{ij}\theta_i{}^k\theta_j{}^l\theta_{lk}\ . \qquad (47)$$

Clearly, due to a kind of symmetry (to be discussed later on in this section), in each case two apparently different diagrams correspond to a single algebraic expression [and a single term in sum (35)]. In general, if there are S such symmetry-related diagrams, the time-ordering factor (44) should be multiplied by the symmetry quotient

$$S^{-1}\equiv S^{-1}(\text{out};\text{in};\text{intra})\ . \qquad (48)$$

We propose, therefore, in the case of operator powers, the following modification of Eq. (35):

$$\lambda_X{}^Y(n)=\sum_{\text{out},\text{in},\text{intra}}{}' T(\text{out};\text{in};\text{intra})j_X{}^Y(n;\text{out};\text{in};\text{intra})\ , \qquad (49)$$

where the primed sum indicates that only one representative from each set of time-ordering-equivalent diagrams is to be taken into account. Quantity

$$j_X{}^Y(n;\text{out};\text{in};\text{intra})=S^{-1}(\text{out};\text{in};\text{intra})$$
$$\times J_X{}^Y(n;\text{out};\text{in};\text{intra}) \qquad (50)$$

will be called the reduced diagram. Its graphical representation will be the same as that for a usual diagram (see Figs. 2–4) except that now some amplitudes may be placed at the same level (see Fig. 5 of this paper and the figures in papers I and II). However, it is to be stressed that when a reduced diagram is to be written in the algebraic form given by formula (37), one has to choose one of possible time orderings of θ amplitudes and calculate parity (38) of the diagram accordingly.

We would like to discuss some topological properties of (reduced) diagrams. According to one important classification a diagram may be either connected or disconnected, and these two classes have obvious characteristics. A deeper insight into the structure of reduced diagrams can be obtained by using graph theory.[12] Consider the following transformation of a reduced diagram (see Fig. 5): (i) two auxiliary amplitudes, a "bottom" (b) and a "top" (t) are added to "absorb" the external lines, (ii) a common direction "up," indicated by arrows, is assinged to all the lines, and (iii) the graphical symbols of θ amplitudes are shrunk to points. It is to be stressed that arrows in (ii) have nothing to do with the usual symbols for particles and holes. What is obtained in steps (i)–(iii) is called the directed graph (digraph) (see Ref. 12, Chap. 7). A directed graph consists of a finite set of vertices (represented by points) and a finite family of ordered pairs of vertices called arcs (each represented by a line with an arrow). In general, reduced diagrams are equivalent to a certain class of digraphs.

It is seen that a connected diagram corresponds to a connected digraph; the reverse is not true, however. In accord with a popular terminology we shall call the diagrams which correspond to connected digraphs the linked diagrams, and those corresponding to disconnected digraphs, the unlinked diagrams. As seen in Fig. 5(c), some linked diagrams are disconnected (diagrams). In paper I we improperly used the term "linked" ("unlinked") in contexts where "connected" ("disconnected") would be appropriate.

Let us define the automorphism of a digraph[12] as a one-to-one mapping of the set of vertices into itself such that the corresponding mapping of the family of arcs is also a one-to-one mapping into itself. The automorphisms of a digraph form a group called the automorphism group of the digraph. It turns out that one can define parameter S of the symmetry quotient (48) as the order of the automorphism group of the digraph corresponding to a given reduced diagram. Examples of reduced diagrams, their characteristics, and the corresponding digraphs are shown in Fig. 5. It is seen that one has always $T \geq S$, where T is the time-ordering factor (44).

In the graphical representation a reduced diagram may be divided into connected parts. Below we shall find how

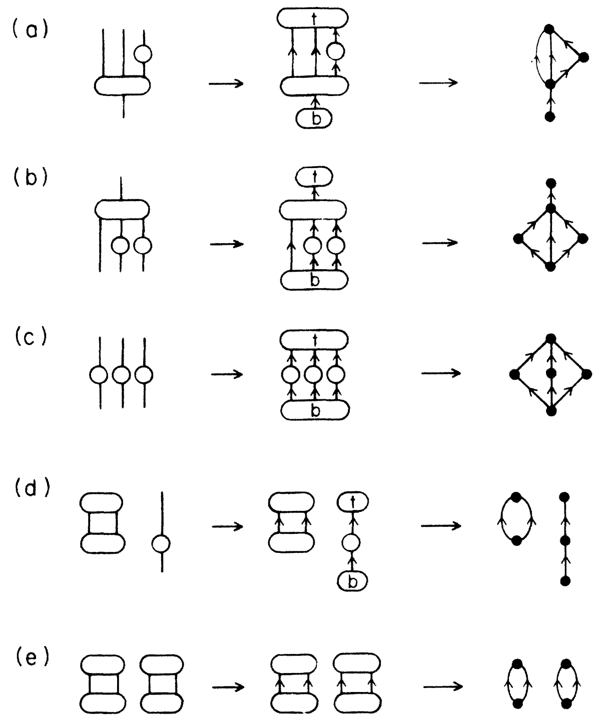

FIG. 5. Reduced diagrams and their transformation into digraphs (see text). The characteristics of the reduced diagrams: (a) connected, linked, $T=1$, $S=1$; (b) connected, linked, $T=2$, $S=2$; (c) disconnected, linked, $T=6$, $S=6$; (d) disconnected, unlinked, $T=3$, $S=1$; (e) disconnected, unlinked, $T=6$, $S=2$.

this obvious property can be translated into an algebraic language. We shall denote connected reduced diagrams by

$$\bar{j}_X{}^Y(n;\text{out};\text{in};\text{intra}) . \tag{51}$$

Now we assume that a reduced diagram of Eq. (50) can be divided into m connected parts ($m \geq 1$) and

$$n = n_m + \cdots + n_1 , \tag{52a}$$

$$\text{out} = \text{out}_m, \ldots, \text{out}_1 , \tag{52b}$$

$$\text{in} = \text{in}_m, \ldots, \text{in}_1 , \tag{52c}$$

$$\text{intra} = \text{intra}_m, \ldots, \text{intra}_1 , \tag{52d}$$

where symbols on the rhs of Eqs. (52) correspond to the connected parts of the diagram. In Appendix C we prove that the following formula applies:

$$j_X{}^Y(n;\text{out};\text{in};\text{intra}) = \tilde{S}^{-1} \sum_{V_m} \cdots \sum_{V_1} \sum_{W_m} \cdots \sum_{W_1} \delta_X{}^{V_m \cdots V_1} \bar{j}_{V_m}{}^{W_m}(n_m;\text{out}_m;\text{in}_m;\text{intra}_m) \cdots \times \bar{j}_{V_1}{}^{W_1}(n_1;\text{out}_1;\text{in}_1;\text{intra}_1) \delta_{W_m \cdots W_1}{}^Y . \tag{53}$$

In the above expression, $\tilde{S}$ is the number of symmetry operations which permute symmetry-related connected parts of the diagram in question. Again, in applications of formula (53) one may follow the suggestions given in the last paragraph of Sec. III.

It is also of interest to see how the time-ordering factor (44) corresponding to diagram (50) is related to time-ordering factors $T_m, \ldots, T_1$ corresponding to the connected diagrams appearing on the rhs of Eq. (53). In the case of $T_m = \cdots = T_1 = l$ one finds that T is equal to the number of permutations of all n θ amplitudes in diagram (50) subject to the condition that the ordering of amplitudes within each connected part remain unchanged. In the general case one finds that

$$T = \frac{n!}{n_m! \cdots n_1!} T_m \cdots T_1 \; . \tag{54}$$

Concluding this section we would like to note that connected (reduced) diagrams provide the basic building blocks for constructing algebraic formulas expressing λ amplitudes for operator powers.

V. SIMILARITY TRANSFORMATION: ALGEBRAIC AND DIAGRAMMATIC APPROACH

In this study of transformation (3) we restrict our considerations to the case when both operators $\hat{H}$ and $\hat{\Theta}$ [see Eqs. (22) and (41), respectively] belong to algebra $\mathcal{F}$(even). Obviously, in this case also operator

$$\hat{\Gamma} = \sum_X \sum_Y \gamma_X{}^Y \hat{X}^\dagger \hat{Y} \tag{55}$$

belongs to $\mathcal{F}$(even), and thus $\gamma_X{}^Y = 0$ for $x + y = \text{odd}$. Now we shall describe in greater detail the approach we proposed in paper I [see the discussion in Sec. V of that paper, Eqs. (I.117)–(I.120)]. Equation (I.117) gives the well-known commutator-series expansion of $\hat{\Gamma}$. Since in the present section we do not impose a condition that $\hat{\Theta}$ be nilpotent, this expansion may contain an infinite number of terms. An important conclusion which can be drawn from formula (I.117) is that any γ amplitude of operator $\hat{\Gamma}$ can be expressed as a sum of connected (in paper I we improperly used the term "linked," see comments in Sec. IV of the present paper) diagrams, linear in η amplitudes of operator $\hat{H}$ and, in general, nonlinear in θ amplitudes of operator $\hat{\Theta}$. Below we explain how this connected-diagram expansion can be generated.

The following representation will be useful in our considerations:

$$\exp\hat{\Theta} = 1 + \sum_{n=1}^{\infty} (n!)^{-1} \hat{\Theta}^n = 1 + \hat{C} \; , \tag{56a}$$

$$\exp(-\hat{\Theta}) = 1 + \sum_{n=1}^{\infty} (-1)^n (n!)^{-1} \hat{\Theta}^n = 1 + \hat{C}' \; . \tag{56b}$$

We write

$$\hat{C} = \sum_X \sum_Y c_X{}^Y \hat{X}^\dagger Y \; , \tag{57a}$$

$$\hat{C}' = \sum_X \sum_Y c'_X{}^Y \hat{X}^\dagger \hat{Y} \; , \tag{57b}$$

and the following formulas for the c and c' amplitudes:

$$c_X{}^Y = \sum_{n=1}^{\infty} (n!)^{-1} \lambda_X{}^Y(n) \; , \tag{58a}$$

$$c'_X{}^Y = \sum_{n=1}^{\infty} (-1)^n (n!)^{-1} \lambda_X{}^Y(n) \; , \tag{58b}$$

where parameters $\lambda_X{}^Y(n)$ are those defined in Eqs. (49) and (50). Now we choose Eq. (58a) to show how it can be transformed in order to express c amplitudes through connected diagrams built of θ amplitudes. We combine Eq. (58a) with Eqs. (49), (53), and (54) to obtain

$$c_X{}^Y = \sum_{n=1}^{\infty} \sum_{\text{out,in,intra}}' \tilde{S}^{-1} \frac{T_m \cdots T_1}{n_m! \cdots n_1!} \sum_{V_m} \cdots \sum_{V_1} \sum_{W_m} \cdots \sum_{W_1} \delta_X{}^{V_m \cdots V_1} \bar{j}_{V_m}{}^{W_m}(n_m;\text{out}_m;\text{in}_m;\text{intra}_m) \times \cdots$$
$$\times \bar{j}_{V_1}{}^{W_1}(n_1;\text{out}_1;\text{in}_1;\text{intra}_1) \delta_{W_m \cdots W_1}{}^Y \; . \tag{59}$$

The meaning of the primed summation in Eq. (59) is as follows: (i) For a given n one sums over all possible sets (36) subject to conditions (39) and the requirement that only diagrams nonequivalent with respect to time ordering are taken into account; (ii) each of the diagrams generated above is decomposed into $m\,(\geq 1)$ connected diagrams [see Eqs. (52)]. Now the summation over all nonequivalent diagrams, connected and disconnected, can be replaced by summations over nonequivalent connected diagrams,

$$\sum_{\text{out,in,intra}}' \tilde{S}^{-1} \rightarrow \sum_{m=1}^{n} (m!)^{-1} \sum_{\substack{n_m, \ldots, n_1 = 1 \\ (n_m + \cdots + n_1 = n)}} \sum_{\text{out}_m,\text{in}_m,\text{intra}_m}' \cdots \sum_{\text{out}_1,\text{in}_1,\text{intra}_1}' \; ; \tag{60}$$

here factor $(m!)^{-1}$ appears because now a diagram consisting of m disconnected parts is generated $(m!)\tilde{S}^{-1}$ times. We define also some useful parameters,

$$\tau_X{}^Y = \sum_{n=1}^{\infty} \sum_{\text{out,in,intra}}' \frac{T(\text{out;in;intra})}{n!} \bar{j}_X{}^Y(n;\text{out;in;intra}) \; , \tag{61a}$$

$$\tau'_X{}^Y = \sum_{n=1}^{\infty} \sum_{\text{out,in,intra}}' (-1)^n \frac{T(\text{out;in;intra})}{n!} \bar{j}_X{}^Y(n;\text{out;in;intra}) \; . \tag{61b}$$

It can be shown that, after substitution of (60) in Eq. (59), and appropriate grouping of terms, one arrives at the formula

$$c_X{}^Y=\tau_X{}^Y+(2!)^{-1}\sum_{V_2}\sum_{V_1}\sum_{W_2}\sum_{W_1}\delta_X{}^{V_2V_1}\tau_{V_2}{}^{W_2}\tau_{V_1}{}^{W_1}\delta_{W_2W_1}{}^Y+\cdots\ , \tag{62a}$$

where each term containing m τ parameters is preceded by factor $(m!)^{-1}$; by a mistake these factors are missing from formula (I.120), where this representation of the c amplitudes was first given. Quite similarly, for c' amplitudes the following formula is found:

$$c'_X{}^Y=\tau'_X{}^Y+(2!)^{-1}\sum_{V_2}\sum_{V_1}\sum_{W_2}\sum_{W_1}\delta_X{}^{V_2V_1}\tau'_{V_2}{}^{W_2}\tau'_{V_1}{}^{W_1}\delta_{W_2W_1}{}^Y+\cdots\ . \tag{62b}$$

Since parameters $\tau_X{}^Y$ and $\tau'_X{}^Y$ are expressed through connected diagrams [see Eqs. (61a) and (61b), respectively], it is evident from Eqs. (62) that they are the only connected contributions to $c_X{}^Y$ and $c'_X{}^Y$, respectively.

The relationships given in Eqs. (62) can be rewritten by employing the formalism described in Appendix D. Let us introduce operators

$$\hat{T}=\sum_X\sum_Y\tau_X{}^Y\hat{X}^\dagger\hat{Y} \tag{63a}$$

and

$$\hat{T}'=\sum_X\sum_Y\tau'_X{}^Y\hat{X}^\dagger\hat{Y}\ , \tag{63b}$$

where the τ and τ' amplitudes are defined in Eqs. (61a) and (61b), respectively. It can now be shown that the following representation applies:

$$1+\hat{C}=\exp*(\hat{T})\ , \tag{64a}$$

$$1+\hat{C}'=\exp*(\hat{T}')\ , \tag{64b}$$

where the "normal" exponential function of an operator is defined in Eq. (D14). One may check by using definition (D5) and (D6) that Eqs. (62) can be derived from Eqs. (64). The following formal relationships can also be derived from Eqs. (64):

$$\hat{T}=\ln*[\exp(\hat{\Theta})]\ , \tag{65a}$$

$$\hat{T}'=\ln*[\exp(-\hat{\Theta})]\ , \tag{65b}$$

where ln* of Eqs. (65) is the normal logarithm function, defined analogously to exp* of Eq. (D14). In principle, one can express operator $\hat{T}'$ through $\hat{T}$ [see Eqs. (65)], but it seems that, in general, τ' amplitudes of Eq. (61b) cannot be expressed through τ amplitudes of Eq. (61a) in a simple way. Therefore, in our approach, operators $\hat{T}$ and $\hat{T}'$ are only useful intermediates related to operator $\hat{\Theta}$ generating transformation (3).

After these preparations we write operator Γ' in the following form:

$$\hat{\Gamma}=\hat{H}+\hat{H}\hat{C}+\hat{C}'\hat{H}+\hat{C}'\hat{H}\hat{C}\ , \tag{66}$$

where

$$\hat{H}\hat{C}=\sum_{n=1}^{\infty}(n!)^{-1}\hat{H}(\hat{T}*)^n\ , \tag{67a}$$

$$\hat{C}'\hat{H}=\sum_{m=1}^{\infty}(m!)^{-1}(\hat{T}'*)^{m}\hat{H}\ , \tag{67b}$$

$$\hat{C}'\hat{H}\hat{C}=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(m!)^{-1}(n!)^{-1}(\hat{T}'*)^m\hat{H}(\hat{T}*)^n\ , \tag{67c}$$

invoking the normal product defined in Appendix D. The above formulas provide a starting point for deriving the connected-diagram expansion of γ amplitudes of operator $\hat{\Gamma}$. We shall use the diagrammatic approach described in Secs. III and IV. The following observations can be made.

(1) Each γ amplitude is a sum of connected diagrams built of η, τ, and τ' amplitudes. These diagrams are linear in η amplitudes, and, in general, nonlinear in τ and τ' amplitudes.

(2) There are no connections among τ amplitudes, and among τ' amplitudes in these diagrams. All other connections are permitted; in particular, $\tau(\tau')$ amplitudes may be connected solely to $\tau'(\tau)$ amplitudes.

(3) A diagram containing m τ' amplitudes and n τ amplitudes is multiplied by factor $(m!)^{-1}(n!)^{-1}$. However, the time-ordering factor (44) is in this case equal to $m!n!$ since there are exactly $m!$ and $n!$ possible time orderings of τ' and τ amplitudes, respectively. Hence, each reduced diagram appears with the unit weight in the connected-diagram expansion of a γ amplitude.

(4) If a diagram exhibits some symmetry with respect to permutations of τ and/or τ' amplitudes, the symmetry quotient (48) need be included in the definition of a reduced diagram [see formula (50)]. The problem of a diagram's symmetry is in this case a bit more complex than that discussed in Sec. IV, since a diagram is, in general, built of amplitudes of three different kinds. In Fig. 6 graphical symbols of η, γ, θ, τ, and τ' amplitudes are shown; we use here the same convention as introduced in paper I, Fig. 1. A typical reduced diagram appearing in the connected-diagram expansion of a γ amplitude is shown in Fig. 7. In order to write a reduced diagram in the algebraic form, one uses formula (37). As mentioned in Sec. IV, one has to choose one of the possible time orderings of τ and τ' amplitudes and calculate the parity

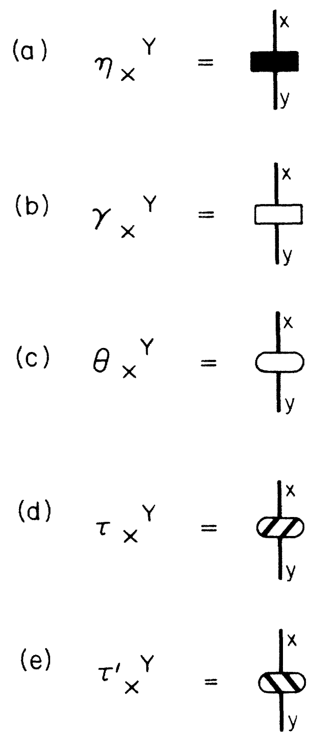

FIG. 6. Diagrammatic representation of η, γ, θ, τ, and τ' amplitudes. Bold lines are used for multiple lines (see Figs. 1 and 2).

(38) of the diagram accordingly. Again the procedure described in the last paragraph of Sec. III is to be applied.

The connected-diagram expansions of τ and τ' amplitudes (in terms of θ amplitudes) are given in Eqs. (61a) and (61b), respectively. These expansions, when combined with the above-mentioned connected-diagram expansion for γ amplitudes, provide the final connected-diagram expansion of γ amplitudes in terms of η and θ amplitudes.

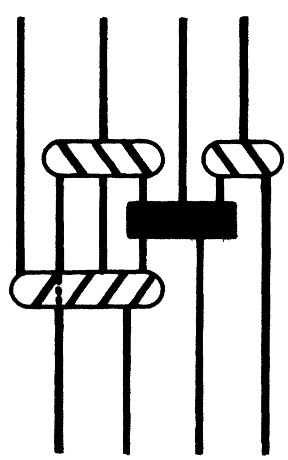

FIG. 7. Typical diagram appearing in the connected-diagram expansion of γ amplitudes in terms of η, τ, and τ' amplitudes. Single lines shown may represent multiple ones, as in Figs. 1 and 2.

VI. GENERALIZED CC METHOD: CALCULATION OF EFFECTIVE HAMILTONIAN

The generalized CC method was described in paper I; a variant of this approach called the Brueckner-Hartree-Fock method (an approximate version) was presented in paper II. A brief summary of the generalized CC method is given in Sec. II of paper IV. In order to avoid unnecessary repetitions, we shall refer to some formulas given in that paper (by preceding them with the Roman numeral IV).

Operators considered in the generalized CC method belong to algebra $\mathcal{F}$(even); no modification of the formalism discussed in the present paper is thus required. $\hat{H}$ is here the Hamiltonian for a many-fermion system [of the form given in Eq. (I.31)] and $\hat{G}$ is an effective Hamiltonian subject to condition (IV.1). Transformation (1) is performed in two steps [see Eqs. (IV.2)–(IV.8)]. In the first step an auxiliary effective Hamiltonian $\hat{\Gamma}$ is obtained via transformation (3). It is assumed that operator $\hat{\Theta}$ (the CC-excitation operator) belongs to the (nilpotent) excitation algebra $\mathcal{F}^{\dagger}$(even); hence, the θ amplitudes of operator $\hat{\Theta}$ are subject to the condition

$$\theta_X{}^Y=0 \quad \text{for } x \leq y \ . \tag{68}$$

These amplitudes can be determined by solving the generalized CC equations (IV.9a). In order to write down the connected-diagram expansions for the γ amplitudes of operator $\hat{\Gamma}$, it is convenient to rewrite Eq. (66) in the following form:

$$\hat{\Gamma}=\hat{H}(1+\hat{C})+\hat{C}\,'\hat{H}(1+\hat{C}) \ . \tag{69}$$

The connected-diagram expansions for some γ amplitudes corresponding to Eqs. (IV.9a) are shown in Figs. 4 and 5 of paper I. In Fig. 3 of that paper the connected-diagram expansions for some τ amplitudes are also given [see Eq. (61a)]. It is a characteristic feature of these expansions that they contain only a finite number of diagrams; this important simplification is a consequence of condition (68). In general, infinite connected-diagram expansions of γ, τ, and τ' amplitudes emerge unless operator $\hat{\Theta}$ is nilpotent.

A careful reader may notice that a few connected diagrams are missing from the diagrammatic equation (b) in Fig. 4 of paper I. We depicted these missing diagrams in Fig. 8 of the present paper; these terms vanish under the assumption that the diagrammatic equation (a) in Fig. 4 of paper I is fulfilled. Similar (vanishing) terms were also omitted in the diagrammatic equation (b) in Fig. 5 of paper I. It is seen that due to a special arrangement of terms in Eq. (69), an additional compactification of the diagrammatic expressions has been achieved.

In the BHF method,[2] the spin orbitals occupied in the model vacuum Φ are optimized in a self-consistent way until the following condition is fulfilled:

$$\theta_{ij}=0 \ , \tag{70}$$

for $i,j=1,\ldots,M$. In paper II we proposed an approximate variant of the BHF method; this variant can be generated by the diagrammatic equations depicted in Fig. 9

FIG. 8. Vanishing contribution to equation (b) in Fig. 4 of paper I (see text).

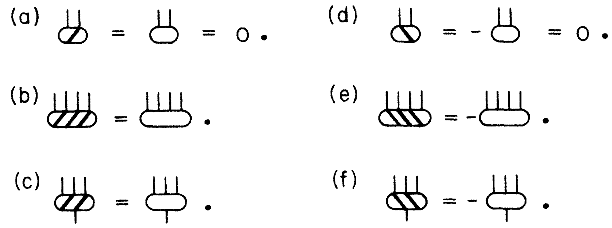

FIG. 9. Representation of τ and τ' amplitudes used to generate the approximate BHF equations shown in Figs. 2 and 3 of paper II. The approximation involved is that all the τ, τ', and θ amplitudes other than those shown in (a)–(f) above are set equal to zero (compare the diagrammatic equations in Fig. 3 of paper I).

of the present paper. It is seen that by substituting these equations for those in Figs. 4, 5, and 6 of paper I one obtains the approximate BHF equations written in the diagrammatic form in Figs. 2 and 3 of paper II. As an illustrative example of "translating" diagrams into algebraic formulas, let us consider two reduced diagrams appearing in equation (b) in Fig. 2 of paper II. These diagrams, for convenience drawn in Fig. 10 of the present paper, correspond to the quadratic terms in Čižek's CPMET equations (see Ref. 4). Both diagrams A and B correspond to the time-ordering factor $T=2$; however, as explained in Sec. V, each of these diagrams appears with the unit weight in the connected-diagram expansion of a γ amplitude [see Fig. 2(b) of paper II]. We use formula (34) [as a special case of the general formula (37)] and follow the routine discussed in the last paragraph of Sec. III. For each diagram the time ordering shown in Fig. 10 is assumed. For diagram A one finds the parity $P=3.3=9$; the symmetry quotient $S^{-1}=1$. For diagram B one finds the parity $P=2.2=4$; the symmetry quotient $S^{-1}=\frac{1}{2}$. Finally, one writes

$$
\begin{aligned}
A \equiv A_{ijkl} &= (-1)^9 (3!)^{-1} \eta^{mnpq} (\theta_{mijk}\theta_{npql} - \theta_{mljk}\theta_{npqi} - \theta_{milk}\theta_{npqj} - \theta_{mijl}\theta_{npqk}) \\
&= -\tfrac{1}{6}\eta^{mnpq}(\theta_{mijk}\theta_{npql} - \theta_{mjkl}\theta_{npqi} + \theta_{mikl}\theta_{npqj} - \theta_{mijl}\theta_{npqk}) ,
\end{aligned} \tag{71a}
$$

$$
\begin{aligned}
B \equiv B_{ijkl} &= \tfrac{1}{2}(-1)^4 (2!)^{-1}(2!)^{-1} \eta^{mnpq} (\theta_{mnij}\theta_{pqkl} - \theta_{mnkj}\theta_{pqil} - \theta_{mnlj}\theta_{pqki} - \theta_{mnik}\theta_{pqjl} - \theta_{mnil}\theta_{pqkj} + \theta_{mnkl}\theta_{pqij}) \\
&= \tfrac{1}{4}\eta^{mnpq}(\theta_{mnij}\theta_{pqkl} + \theta_{mnjk}\theta_{pqil} - \theta_{mnik}\theta_{pqjl}) .
\end{aligned} \tag{71b}
$$

In the case when the particle-hole transformation (I.27) is used to define the quasiparticle fermion operators (10), some amplitudes of operators $\hat{H}$, $\hat{\Gamma}$, $\hat{\Theta}$, etc. vanish identically because of the pseudocharge symmetry [see Eqs. (I.35)–(I.38)]. It can be shown that the nonzero amplitudes $\eta_X{}^Y$, $\gamma_X{}^Y$, $\theta_X{}^Y$, etc. are subject to condition (I.136),

$$
x_p - x_h = y_p - y_h , \tag{72}
$$

where $x_h(y_h)$ is the number of the "hole" indices (denoted by ρ, σ, etc.), and $x_p(y_p)$ is the number of the "particle" indices (denoted by r, s, etc.) in the index string $X(Y)$. Condition (72) can be imposed directly in algebraic expressions: For each term one generates simply all allowed combinations of "hole" and "particle" indices. For illustrative purposes we apply this procedure to quantities A and B of Eqs. (71):

$$
\begin{aligned}
A \equiv A_{\rho\sigma rs} &= -(\tfrac{1}{2}\eta^{t\tau v u}\theta_{t\rho\sigma r}\theta_{\tau v u s} - \tfrac{1}{2}\eta^{\tau v t u}\theta_{\tau\sigma rs}\theta_{vtu\rho} + \tfrac{1}{2}\eta^{\tau v t u}\theta_{\tau\rho rs}\theta_{vtu\sigma} - \tfrac{1}{2}\eta^{t\tau v u}\theta_{t\rho\sigma s}\theta_{\tau v u r}) \\
&= -\tfrac{1}{2}\eta^{\tau v t u}(-\theta_{\rho\sigma r t}\theta_{\tau v u s} + \theta_{\tau\rho r s}\theta_{\rho v t u} - \theta_{\tau\rho r s}\theta_{v\sigma t u} + \theta_{\rho\sigma s t}\theta_{\tau v u r}) ,
\end{aligned} \tag{73a}
$$

$$
\begin{aligned}
B \equiv B_{\rho\sigma rs} &= \tfrac{1}{4}\eta^{tu\tau v}\theta_{tu\rho\sigma}\theta_{\tau v rs} + \eta^{\tau u v t}\theta_{\tau u\sigma r}\theta_{vt\rho s} - \eta^{\tau t v u}\theta_{\tau t\rho r}\theta_{vu\sigma s} \\
&= \eta^{\tau v t u}(\tfrac{1}{4}\theta_{\rho\sigma t u}\theta_{\tau v r s} + \theta_{\sigma\tau u r}\theta_{\rho v t s} + \theta_{\rho\tau t r}\theta_{\sigma v u s}) .
\end{aligned} \tag{73b}
$$

The reader should note that the hole and particle indices are not equivalent, and therefore the numerical coefficients in Eqs. (73) are, in general, different from those in Eqs. (71). Equations (71) and (73) exemplify the way in which the BHF equations of paper II [see Eqs. (II.14)–(II.17)] were obtained. In Fig. 11 we show diagrammatic expressions for some γ amplitudes not considered in paper II (one will find an application for these amplitudes later on in this section). The γ amplitudes of Fig. 11 are, in general, nonzero since they are not subject

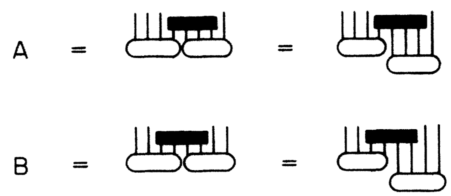

FIG. 10. Two diagrams contributing to equation (b) in Fig. 2 of paper II (see text).

to condition (IV.9a). In the algebraic form they read

$$\gamma^{ij}=\eta^{ij}+\tfrac{1}{6}(\eta^{iklm}\theta_{klm}{}^{j}-\eta^{jklm}\theta_{klm}{}^{i}) , \tag{74a}$$

$$\gamma^{ijkl}=\eta^{ijkl} , \tag{74b}$$

$$\gamma_i{}^{jkl}=\eta_i{}^{jkl}+\tfrac{1}{2}(\eta^{jkmn}\theta_{mni}{}^{l}+\eta^{klmn}\theta_{mni}{}^{j}-\eta^{jlmn}\theta_{mni}{}^{k}) . \tag{74c}$$

When the pseudocharge symmetry is taken into account [see condition (72)], Eqs. (74) may be rewritten as follows:

$$\gamma^{\rho r}=\eta^{\rho r}+\tfrac{1}{2}(\eta^{\rho\sigma st}\theta_{\sigma st}{}^{r}+\eta^{\sigma\tau sr}\theta_{\sigma\tau s}{}^{\rho}) , \tag{75a}$$

$$\gamma^{\rho\sigma rs}=\eta^{\rho\sigma rs} , \tag{75b}$$

$$\gamma_{\xi}{}^{\rho\sigma r}=\eta_{\xi}{}^{\rho\sigma r}+\tfrac{1}{2}\eta^{\rho\sigma tu}\theta_{\xi tu}{}^{r}+\eta^{\sigma\tau tr}\theta_{\xi\tau t}{}^{\rho}-\eta^{\rho\tau tr}\theta_{\xi\tau t}{}^{\sigma} , \tag{75c}$$

$$\gamma_z{}^{\rho rs}=\eta_z{}^{\rho rs}+\tfrac{1}{2}\eta^{\tau vrs}\theta_{\tau vz}{}^{\rho}+\eta^{\rho\tau tr}\theta_{\tau tz}{}^{s}-\eta^{\rho\tau ts}\theta_{\tau tz}{}^{r} . \tag{75d}$$

Concluding this section, we wish to derive a set of generalized CC equations from which ξ amplitudes of the CC-deexcitation operator $\hat{\Xi}$ [see Eq. (IV.4b)] can be calculated. These equations, corresponding to condition (IV.9b), have not been considered thus far since they are not indispensable in determining the effective Hamiltonian $\hat{G}$ [see the discussion below Eq. (IV.10b)]. However, the ξ amplitudes prove to be useful in calculating expectation values and transition moments (see paper IV). Operator $\hat{\Xi}$ belongs to algebra $\mathcal{F}^{\downarrow}(\text{even})$ and the ξ amplitudes are subject to condition

$$\xi_X{}^Y=0 \quad \text{for } x \geq y. \tag{76}$$

Equation (IV.7) may be rewritten as [compare Eq. (69)]

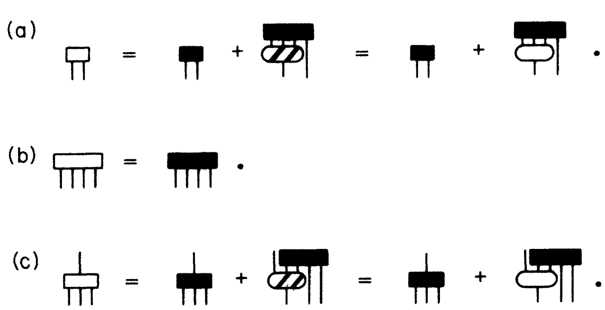

FIG. 11. Diagrammatic expressions for some γ amplitudes of operator $\hat{\Gamma}$ [see Eqs. (IV.5) and (IV.6): (a) γ^{ij}, (b) γ^{ijkl}, and (c) $\gamma_i{}^{jkl}$, obtained using the approximation set forth in Fig. 9.

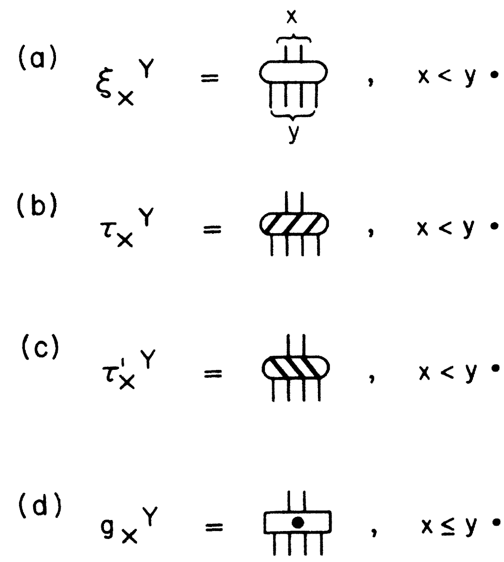

FIG. 12. Diagrammatic representations of (a) the ξ amplitudes of the CC-deexcitation operator $\hat{\Xi}$ [see Eq. (IV.4b)]; (b) and (c) τ and τ' amplitudes [see Eqs. (61)] related to ξ amplitudes; and (d) the g amplitudes of the effective Hamiltonian $\hat{G}$ [see Eqs. (IV.7) and (IV.8)].

$$\hat{G}=(1+\hat{D}\,')\hat{\Gamma}+(1+\hat{D}\,')\hat{\Gamma}\hat{D} , \tag{77}$$

where

$$1+\hat{D}=\exp(\hat{\Xi}) , \tag{78a}$$

$$1+\hat{D}\,'=\exp(-\hat{\Xi}) . \tag{78b}$$

Similarly, as in Eqs. (64), operators $\hat{D}$ and $\hat{D}\,'$ can be expressed through operators $\hat{T}$ and $\hat{T}\,'$, respectively (the τ and τ' amplitudes of these operators are now related to the ξ amplitudes of operator $\hat{\Xi}$). The graphical symbols of the ξ, τ, and τ' amplitudes, and the g amplitudes of operator $\hat{G}$ are shown in Fig. 12. We shall consider here an approximate operator $\hat{\Xi}$ in which only amplitudes of the forms ξ^{ij} and ξ^{ijkl} are different from zero; the corresponding τ and τ' amplitudes are depicted in Fig. 13. One can notice that there is no analog of condition (70) in the case of amplitudes ξ^{ij}. By employing the approximation set forth in Fig. 13, we derived the connected-diagram expansions of some g amplitudes (see Fig. 14). These are the CC equations for ξ amplitudes [see conditions (IV.9b)]. In the algebraic form, these equations read

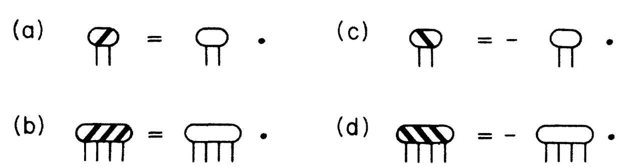

FIG. 13. Connected-diagram expansions (61) of some τ and τ' amplitudes in terms of ξ amplitudes (see Fig. 12). In further considerations we shall assume that the τ, τ', and ξ amplitudes other than those shown in (a)–(d) above are equal to zero.

$$g^{ij}=\gamma^{ij}-(\xi^{ik}\gamma_k{}^j-\xi^{jk}\gamma_k{}^i)-\tfrac{1}{2}\xi^{kl}\gamma_{kl}{}^{ij}=0\ , \tag{79a}$$

$$\begin{aligned} g^{ijkl}=\gamma^{ijkl}&-(\xi^{im}\gamma_m{}^{jkl}-\xi^{jm}\gamma_m{}^{ikl}+\xi^{km}\gamma_m{}^{ijl}-\xi^{lm}\gamma_m{}^{ijk})\\ &+(\xi^{im}\xi^{jn}\gamma_{nm}{}^{kl}-\xi^{km}\xi^{jn}\gamma_{nm}{}^{il}-\xi^{im}\xi^{kn}\gamma_{nm}{}^{jl}+\xi^{lm}\xi^{jn}\gamma_{nm}{}^{ik}+\xi^{im}\xi^{ln}\gamma_{nm}{}^{jk}+\xi^{km}\xi^{ln}\gamma_{nm}{}^{ij})\\ &-(\xi^{ijkm}\gamma_m{}^l-\xi^{jklm}\gamma_m{}^i+\xi^{iklm}\gamma_m{}^j-\xi^{ijlm}\gamma_m{}^k)\\ &-\tfrac{1}{2}(\xi^{ijmn}\gamma_{mn}{}^{kl}+\xi^{jkmn}\gamma_{mn}{}^{il}-\xi^{ikmn}\gamma_{mn}{}^{jl}+\xi^{ilmn}\gamma_{mn}{}^{jk}-\xi^{jlmn}\gamma_{mn}{}^{ik}+\xi^{klmn}\gamma_{mn}{}^{ij})=0\ . \end{aligned} \tag{79b}$$

By assuming the pseudocharge symmetry [see condition (72)], the following form of Eqs. (79) is obtained:

$$g^{\rho r}=\gamma^{\rho r}-(\xi^{\rho s}\gamma_s{}^r+\xi^{\sigma r}\gamma_\sigma{}^\rho)-\xi^{\sigma s}\gamma_{\sigma s}{}^{\rho r}=0\ , \tag{80a}$$

$$\begin{aligned} g^{\rho\sigma rs}=\gamma^{\rho\sigma rs}&-(\xi^{\rho t}\gamma_t{}^{\sigma rs}-\xi^{\sigma t}\gamma_t{}^{\rho rs}-\xi^{\tau r}\gamma_\tau{}^{\rho\sigma s}+\xi^{\tau s}\gamma_\tau{}^{\rho\sigma r})\\ &+(\xi^{\rho t}\xi^{\sigma u}\gamma_{ut}{}^{rs}-\xi^{\tau r}\xi^{\sigma t}\gamma_{\tau t}{}^{\sigma s}+\xi^{\rho t}\xi^{\tau r}\gamma_{\tau t}{}^{\sigma s}+\xi^{\tau s}\xi^{\sigma t}\gamma_{\tau t}{}^{\rho r}-\xi^{\rho t}\xi^{\tau s}\gamma_{\tau t}{}^{\sigma r}+\xi^{\tau r}\xi^{v s}\gamma_{v\tau}{}^{\rho\sigma})\\ &-(\xi^{\rho\sigma rt}\gamma_t{}^s+\xi^{\tau\sigma rs}\gamma_\tau{}^\rho-\xi^{\tau\rho rs}\gamma_\tau{}^\sigma-\xi^{\rho\sigma st}\gamma_t{}^r)\\ &-(\tfrac{1}{2}\xi^{\rho\sigma tu}\gamma_{tu}{}^{rs}+\xi^{\sigma\tau tr}\gamma_{\tau t}{}^{\rho s}-\xi^{\rho\tau tr}\gamma_{\tau t}{}^{\sigma s}+\xi^{\rho\tau ts}\gamma_{\tau t}{}^{\sigma r}-\xi^{\sigma\tau ts}\gamma_{\tau t}{}^{\rho r}+\tfrac{1}{2}\xi^{\tau v rs}\gamma_{\tau v}{}^{\rho\sigma})=0\ . \end{aligned} \tag{80b}$$

It is seen that Eqs. (80a) form a set of linear equations for amplitudes $\xi^{\rho r}$. After substituting the solutions of these equations into Eqs. (80b), a set of linear equations for amplitudes $\xi^{\rho\sigma rs}$ is obtained.

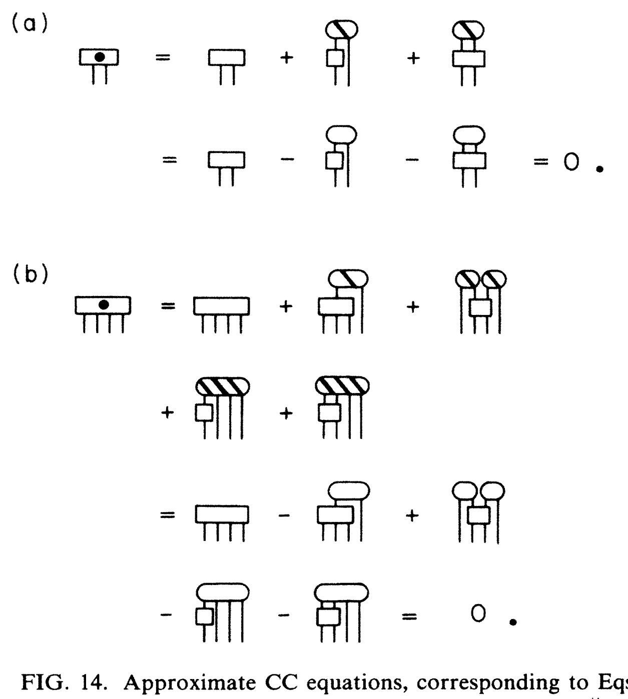

FIG. 14. Approximate CC equations, corresponding to Eqs. (IV.9b), from which ξ amplitudes can be calculated: (a) $g^{ij}=0$; (b) $g^{ijkl}=0$. Diagrammatic formulas for the γ amplitudes appearing in these equations can be found in Fig. 3 of paper II and in Fig. 11 of the present paper. It is also assumed that conditions (IV.9a) are fulfilled.

VII. SUMMARY

The present paper contains a complete presentation of the algebraic-diagrammatic formalism proposed, in a preliminary version, in paper I. This formalism is devised to facilitate calculations of products and powers of linear operators acting in a (finite-dimensional) Fock space for fermion particles. An important application of this formalism is in performing similarity transformations of operators in the Fock space.

Within this formalism one expresses all operators as linear combinations of normal products of fermion operators [in general, these are quasiparticle fermion operators, see Eqs. (11)–(13)]. For an operator, the linear coefficients in such an expansion are called amplitudes. The essence of the present formalism is to provide algebraic formulas expressing the amplitudes of an operator product *directly* in terms of the amplitudes of the operator factors. In this approach a certain algebra of amplitudes is defined; the basic equation of this algebra is Eq. (29) corresponding to a product of two operators. For convenience we have derived also explicit formulas corresponding to products of more than two operators; in these cases a diagrammatic representation of algebraic expressions turned out to be very useful. In the present paper both the algebraic expression and the corresponding graphical symbol are called simply a diagram. The diagram (its algebraic counterpart) corresponding to a product of n operators is given in Eq. (37).

In the case of operator powers, a new kind of diagram, called the reduced diagram, is introduced. We have shown in Sec. IV that reduced diagrams can be related to so-called directed graphs[12] (digraphs). This observation may be helpful in computer generation of reduced diagrams and determination of their time-ordering factors

(44) and symmetry quotients (48). Connected reduced diagrams provide the basis building blocks for constructing algebraic formulas for the amplitudes corresponding to an operator power.

In Sec. V we have derived a connected-diagram expansion for the amplitudes of a similarity-transformed operator. Given in terms of reduced diagrams, such an expansion can be calculated for individual amplitudes of the transformed operator. The derivation of this connected-diagram expansion is greatly facilitated by introducing, after Jeziorski and Paldus,[13] a new kind of operator product in Fock space (see Appendix D).

The present algebraic-diagrammatic method of generating the connected-diagram expansion for a similarity-transformed operator was first employed in paper I where we derived a set of the generalized CC equations. In Sec. VI of the present paper we have discussed details of that derivation; by using the same technique we have also derived an additional set of CC equations corresponding to the deexcitation part of the wave operator (IV.2). We hope that these examples will prove helpful as a guide in using this new algebraic-diagrammatic approach.

We would like to conclude with a few remarks.

(i) The present formalism avoids explicit operations on fermion operators (involving the application of Wick's theorem[11] or the contraction theorem[14]). The use of the contraction theorem[14] is implicit here, see the derivation of Eq. (I.B18) [an equivalent of Eq. (29) of the present paper] in Appendix B of paper I.

(ii) The form of algebraic formulas derived in Secs. III–V is independent of the choice of the fermion operators (10). In particular, these formulas remain valid for fermion operators defined by means of a general Bogoliubov-Valatin transformation (13).

(iii) In the present approach the diagrams serve only as some helpful intermediates in generating explicit algebraic formulas.

ACKNOWLEDGMENTS

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APPENDIX A

In this appendix we would like to give a rigorous proof of formula (30). Arguments leading to the formula for general n [see Eqs. (35)–(39)] will also be presented.

For a product of $n=3$ operators one may write

$$\hat{\Lambda}=\hat{\Theta}_3\hat{K} , \tag{A1}$$

where

$$\hat{K}=\hat{\Theta}_2\hat{\Theta}_1 , \tag{A2a}$$

$$\hat{K}=\sum_{X}\sum_{Y}\kappa_X{}^Y\hat{X}^{\dagger}\hat{Y} . \tag{A2b}$$

By applying formula (29) to operators defined in Eqs. (A1) and (A2a) one finds λ and κ amplitudes,

$$\lambda_X{}^Y=\sum_{X_3}\sum_{V}\sum_{Y_3}\sum_{W}\sum_{Z}\delta_X{}^{X_3V}[{}_{X_3}{}^{Y_3Z}]_3\kappa_{ZV}{}^W\delta_{Y_3W}{}^Y , \tag{A3}$$

$$\kappa_{ZV}{}^W=\sum_{V_2}\sum_{V_1}\sum_{Y_2}\sum_{Y_1}\sum_{Z_{21}}\delta_{ZV}{}^{V_2V_1}[{}_{V_2}{}^{Y_2Z_{21}}]_2[{}_{Z_{21}V_1}{}^{Y_1}]_1 \times\delta_{Y_2Y_1}{}^W . \tag{A4}$$

We now follow the procedure introduced in the Appendix of paper II, allowing for a direct coupling of $[\ ]_3$ amplitudes in Eq. (A3) to $[\ ]_2$ and $[\ ]_1$ amplitudes in Eq. (A4). We use identity

$$\delta_{ZV}{}^{V_2V_1}=\sum_{X_2}\sum_{X_1}\sum_{Z_{32}}\sum_{Z_{31}}\delta_{Z_{32}Z_{31}X_2X_1}{}^{Z_{32}X_2Z_{31}X_1} \times\delta_Z{}^{Z_{32}Z_{31}}\delta_V{}^{X_2X_1}\delta_{Z_{32}X_2}{}^{V_2} \times\delta_{Z_{31}X_1}{}^{V_1} , \tag{A5}$$

which can be derived from an analog of Eq. (II.A4). However, the subsequent formula (II.A5) is correct only in cases when the index strings of the Kronecker δ are nondegenerate [compare definition (19)]. Therefore, formula (II.A6) appears to be incorrect. Instead, one may rewrite Eq. (A5) in the form

$$\delta_{ZV}{}^{V_2V_1}=\sum_{X_2}\sum_{X_1}\sum_{Z_{32}}\sum_{Z_{31}}(-1)^{x_2z_{31}} \times\delta_{Z_{32}X_1}{}^{Z_{32}X_1}\delta_{Z_{31}X_2}{}^{Z_{31}X_2} \times\delta_Z{}^{Z_{32}Z_{31}}\delta_V{}^{X_2X_1} \times\delta_{Z_{32}X_2}{}^{V_2}\delta_{Z_{31}X_1}{}^{V_1} , \tag{A6}$$

where, in comparison with the form of Eq. (II.A6), a new factor

$$\delta_{Z_{32}X_1}{}^{Z_{32}X_1}\delta_{Z_{31}X_2}{}^{Z_{31}X_2} \tag{A7}$$

appears. This factor is responsible for deleting from sum (A6) those terms which correspond to "overlapping" strings Z_{32} and X_1, and/or Z_{31} and X_2. By substituting Eqs. (A6) and (A4) into Eq. (A3), one arrives at the formula which resembles Eq. (30), except for factor (A7), which now enters the formula. Below we show that factor (A7) can be dropped from this formula and Eq. (30) is recovered. In order to prove this we shall take formula (30) as the starting point and show that the terms corresponding to overlapping strings Z_{32} and X_1 and/or Z_{31} and X_2 cancel mutually. Let us write

$$Z_{32}=C_{32}S_{21}\ , \tag{A8a}$$

$$X_1=S_{21}A_1\ , \tag{A8b}$$

$$Z_{31}=C_{31}S_{12}\ , \tag{A8c}$$

$$X_2=S_{12}A_2\ , \tag{A8d}$$

where the index string S_{21} (S_{12}) represents an overlap between strings Z_{32} and X_1 (Z_{31} and X_2). Now we substitute Eqs. (A8) into Eq. (30), making also substitution

$$\sum_{X_2}\sum_{X_1}\sum_{Z_{32}}\sum_{Z_{31}} \to \sum_{A_2}\sum_{A_1}\sum_{C_{32}}\sum_{C_{31}}\sum_{S_{21}}\sum_{S_{12}} \delta_{C_{32}A_1}{}^{C_{32}A_1}\delta_{C_{31}A_2}{}^{C_{31}A_2}\ , \tag{A9}$$

where the factor analogous to (A7) is introduced to assure that the common part of Z_{32} and X_1 is contained in S_{21}, and the common part of Z_{31} and X_2 is contained in S_{12}. We write

$$(-1)^{x_2z_{31}}=(-1)^{s_{12}^2+c_{31}s_{12}+s_{12}a_2+a_2c_{31}}\ , \tag{A10a}$$

$$\delta_X{}^{X_3X_2X_1}=\delta_X{}^{X_3A_2S_{12}S_{21}A_1}(-1)^{s_{12}a_2}\ , \tag{A10b}$$

$$[x_{X_3}{}^{Y_3Z_{32}Z_{31}}]_3=[x_{X_3}{}^{Y_3C_{32}C_{31}S_{12}S_{21}}]_3(-1)^{c_{31}s_{12}+s_{12}s_{21}}\ , \tag{A10c}$$

$$[z_{Z_{32}X_2}{}^{Y_2Z_{21}}]_2=[c_{C_{32}S_{12}S_{21}A_2}{}^{Y_2Z_{21}}]_2(-1)^{s_{12}s_{21}}\ , \tag{A10d}$$

$$[z_{Z_{21}Z_{31}X_1}{}^{Y_1}]_1=[z_{Z_{21}C_{31}S_{12}S_{21}A_1}{}^{Y_1}]_1\ . \tag{A10e}$$

The final phase factor emerging after multiplying the rhs's of Eqs. (A10) amounts to

$$(-1)^{s_{12}^2+a_2c_{31}}=(-1)^{s_{12}}(-1)^{a_2c_{31}}\ . \tag{A11}$$

Let us note that all the terms on the rhs's of Eqs. (A10b)–(A10e) contain string $S_{12}S_{21}$ and therefore one may assume that strings S_{12} and S_{21} have no common indices [otherwise the rhs of Eqs. (A10b)–(A10e) would vanish]. Thus, a nondegenerate string T_{12} can be found such that

$$T_{12}\sim S_{12}S_{21}\ . \tag{A12}$$

We now rewrite the quantities on the rhs's of Eqs. (A10b)–(A10e) in the form

$$\delta_X{}^{X_3A_2S_{12}S_{21}A_1}=\sum_{T_{12}}\delta_X{}^{X_3A_2T_{12}A_1}\delta_{T_{12}}{}^{S_{12}S_{21}}\ , \tag{A13}$$

etc. After all these preparations, Eq. (30) may be written as

$$\lambda_X{}^Y=\sum_{T_{12}}\left[\sum_{X_3}\sum_{A_2}\sum_{A_1}\sum_{Y_3}\sum_{Y_2}\sum_{Y_1}\sum_{C_{32}}\sum_{C_{31}}\sum_{Z_{21}}\delta_{C_{32}A_1}{}^{C_{32}A_1}\delta_{C_{31}A_2}{}^{C_{31}A_2}\Delta_X{}^Y(X_3,A_2,A_1;Y_3,Y_2,Y_1;C_{32},C_{31},Z_{21};T_{12})\right]\ , \tag{A14}$$

where

$$\Delta_X{}^Y(X_3,A_2,A_1;Y_3,Y_2,Y_1;C_{32},C_{31},Z_{21};T_{12})=(-1)^{a_2c_{31}}\delta_X{}^{X_3A_2T_{12}A_1}[x_{X_3}{}^{Y_3C_{32}C_{31}T_{12}}]_3$$
$$\times[c_{C_{32}T_{12}A_2}{}^{Y_2Z_{21}}]_2[z_{Z_{21}C_{31}T_{12}A_1}{}^{Y_1}]_1\delta_{Y_3Y_2Y_1}{}^Y\sum_{S_{12}}\sum_{S_{21}}(-1)^{s_{12}}(\delta_{T_{12}}{}^{S_{12}S_{21}})^4\ . \tag{A15}$$

We now show that the quantity defined in Eq. (A15) vanishes if string T_{12} is nonempty ($t_{12}\neq 0$). One may write

$$\sum_{S_{12}}\sum_{S_{21}}(-1)^{s_{12}}(\delta_{T_{12}}{}^{S_{12}S_{21}})^4=\sum_{\substack{S_{12}\ S_{21}\\ (S_{12}S_{21}\sim T_{12})}}(-1)^{s_{12}}\ , \tag{A16}$$

where on the rhs of this equation the summation runs over all substrings of T_{12}. There are exactly

$$\begin{vmatrix} t_{12} \\ s_{12} \end{vmatrix}=\frac{t_{12}!}{s_{12}!(t_{12}-s_{12})!} \tag{A17}$$

nonequivalent strings S_{12} of the length s_{12} which are substrings of T_{12}. But for $t_{12}>0$, the rhs of Eq. (A16) vanishes due to identity

$$\sum_{s_{12}=0}^{t_{12}}\begin{vmatrix} t_{12} \\ s_{12} \end{vmatrix}(-1)^{s_{12}}=0\ . \tag{A18}$$

We thus find that in Eq. (A14), the only surviving terms correspond to the empty string T_{12}. That leads to our final conclusion: In Eq. (30) all the terms in which strings Z_{32} and X_1, and/or Z_{31} and X_2, overlap cancel mutually. This makes the inclusion of factor (A7) in this formula unnecessary.

Using essentially the same technique as above, we have also found an analog of Eq. (30) for $n=4$. Derivations for $n=2$, 3, and 4 pave the road for the formula for a general n value. The pattern of index strings in Eq. (37) emerges as a natural generalization of those for the cases $n=2$, 3, and 4, and so does the formula (38) for the parity of a diagram; the validity of this formula can be proved by induction. As for the case of $n=3$, in the derivation of the formula (37) unwanted factors of the type

$$\delta_{Z_{np}X_q}{}^{Z_{np}X_q}\delta_{Z_{nq}X_p}{}^{Z_{nq}X_p}\ , \tag{A19}$$

analogous to factor (A7), emerge. Those factors appear for all the pairs $p\neq q$; $p,q<n$ and can be eliminated, one at a time, using the procedure we described in detail for factor (A7).

APPENDIX B

In our proof of lemma 1 of Sec. IV we shall use Eq. (37) with amplitudes $[{}_X{}^Y]_k$ replaced by $\theta_X{}^Y$. It is seen that changing the time ordering of θ amplitudes in a diagram can be performed stepwise, with two adjacent amplitudes exchanged at a time. Assume that diagram $J_X'{}^Y$ is obtained from diagram $J_X{}^Y$ by exchanging pth and $(p+1)$th amplitudes, followed by reordering of some index strings to recover the standard ordering given in formula (37). Such reordering is possible only if

$$c_{p+1,p}=0\ , \tag{B1}$$

i.e., there are no lines connecting the pth and $(p+1)$th amplitudes in the graphical representation of the diagram. It is evident that $J_X{}^Y$ and $J_X'{}^Y$ may only differ in sign. We thus write

$$J_X'{}^Y(n;\text{out}';\text{in}';\text{intra}')=(-1)^{\Delta}J_X{}^Y(n;\text{out};\text{in};\text{intra})\ , \tag{B2}$$

where the primed and unprimed symbols, of Eqs. (36) in general, correspond to different strings of numbers than the unprimed ones [see examples given in Eqs. (42) and (43)]. It will be useful to consider Δ as a sum of four terms

$$\Delta=\Delta_1+\Delta_2+\Delta_3+\Delta_4\ . \tag{B3}$$

Here Δ_1 corresponds to a difference of the parities of diagrams $J_X{}^Y$ and $J_X'{}^Y$:

$$\Delta_1=P-P'\ . \tag{B4}$$

By applying definition (38) with condition (B1) one finds that

$$\begin{aligned}\Delta_1=&\sum_{\substack{i=1\\(i<p)}}^{n}(a_pc_{p+1,i}-a_{p+1}c_{pi})+\sum_{\substack{k=1\\(k>p+1)}}^{n}(a_{p+1}c_{kp}-a_pc_{k,p+1})+\sum_{\substack{i=1\\(i<p)}}^{n}\sum_{\substack{l=1\\(l>p+1)}}^{n}(c_{lp}c_{p+1,i}-c_{l,p+1}c_{pi})\\&+\sum_{\substack{1\le i<j\le n\\(i,j<p)}}(c_{p+1,j}c_{pi}-c_{pj}c_{p+1,i})+\sum_{\substack{1\le k<l\le n\\(k,l>p+1)}}(c_{l,p+1}c_{kp}-c_{lp}c_{k,p+1})\ .\end{aligned} \tag{B5}$$

Quantity Δ_2 corresponds to the change in the ordering of index strings in the generalized Kronecker deltas in Eq. (37),

$$\delta_X{}^{X_n\cdots X_pX_{p+1}\cdots X_1}=(-1)^{x_px_{p+1}}\delta_X{}^{X_n\cdots X_{p+1}X_p\cdots X_1}\ , \tag{B6a}$$

$$\delta_{Y_n\cdots Y_pY_{p+1}\cdots Y_1}{}^Y=(-1)^{y_py_{p+1}}\delta_{Y_n\cdots Y_{p+1}Y_p\cdots Y_1}{}^Y\ , \tag{B6b}$$

where the quantities on the left-hand sides (lhs's) correspond to $J_X'{}^Y$. Because $x_p=a_p$, $x_{p+1}=a_{p+1}$, $y_p=b_p$, and $y_{p+1}=b_{p+1}$ [see Eq. (37)], one finds that

$$\Delta_2=a_pa_{p+1}+b_pb_{p+1}\ . \tag{B7}$$

A similar analysis performed for the θ amplitudes in Eq. (37), corresponding to the ordinal numbers smaller than p, gives contribution

$$\Delta_3=\sum_{\substack{i=1\\(i<p)}}^{n}c_{pi}c_{p+1,i}\ ; \tag{B8}$$

the contribution corresponding to the θ amplitudes with the ordinal numbers greater than $p+1$ reads

$$\Delta_4=\sum_{\substack{k=1\\(k>p+1)}}^{n}c_{kp}c_{k,p+1}\ . \tag{B9}$$

In order to simplify the expression for Δ obtained by substituting Eqs. (B5) and (B7)–(B9) into Eq. (B3), let us introduce quantities

$$A_p=\sum_{\substack{j=1\\(j>p+1)}}^{n}c_{jp}\ , \tag{B10a}$$

$$B_p=\sum_{\substack{i=1\\(i<p)}}^{n}c_{pi}\ , \tag{B10b}$$

$$A_{p+1}=\sum_{\substack{j=1\\(j>p+1)}}^{n}c_{j,p+1}\ , \tag{B10c}$$

$$B_{p+1}=\sum_{\substack{i=1\\(i<p)}}^{n} c_{p+1,i} \ . \tag{B10d}$$

We shall also modify the rhs of Eq. (B5) by changing all the minus signs into plus signs; obviously this operation does not change the parity of Δ_1. It can now be shown that the following expression is obtained:

$$\Delta=(a_p+A_p+B_p)(a_{p+1}+A_{p+1}+B_{p+1})+b_pb_{p+1} \ . \tag{B11}$$

Because of our assumption that $\hat{\Theta}\in\mathcal{F}(\text{even})$ [see Eq. (41)], conditions (39c) apply. Taking into account Eq. (B1), one may write

$$a_p+b_p+A_p+B_p=2q \ , \tag{B12a}$$

$$a_{p+1}+b_{p+1}+A_{p+1}+B_{p+1}=2q' \ , \tag{B12b}$$

where q and q' are some integer numbers. By combining Eq. (B11) with Eqs. (B12), one finds that

$$\Delta=(2q-b_p)(2q'-b_{p+1})+b_pb_{p+1} \ , \tag{B13}$$

and, hence, Δ turns out to be even. Finally, Eq. (B2) is shown to read

$$J_X'^{\,Y}=J_X^{\,Y} \ , \tag{B14}$$

which concludes the proof of lemma 1.

APPENDIX C

In this appendix, formula (53), expressing a reduced diagram in terms of connected reduced diagrams, is derived. An arbitrary reduced diagram (50) may be written as

$$j_X^{\,Y}(n\,;\text{out};\text{in};\text{intra}) =S^{-1}(-1)^P \sum_{\substack{X_n\\(x_n=a_n)}}\cdots\sum_{\substack{X_1\\(x_1=a_1)}}\sum_{\substack{Y_n\\(y_n=b_n)}}\cdots\sum_{\substack{Y_1\\(y_1=b_1)}} \delta_X^{\,X_n\cdots X_1}K_{X_n\cdots X_1}^{\,Y_n\cdots Y_1}(n\,;\text{out};\text{in};\text{intra})\delta_{Y_n\cdots Y_1}^{\,Y} \ , \tag{C1}$$

where the form of

$$K_{X_n\cdots X_1}^{\,Y_n\cdots Y_1}(n\,;\text{out};\text{in};\text{intra})$$

can easily be inferred from Eq. (37). We shall consider the case when diagram (C1) consists of two connected parts (subdiagrams); this corresponds to $m=2$ [see Eqs. (52)]. Now one may choose a particular time ordering of θ amplitudes in diagram (37) such that

$$\begin{aligned}K_{X_n\cdots X_1}^{\,Y_n\cdots Y_1}&(n\,;\text{out};\text{in};\text{intra})\\ &=\bar{K}_{X_n\cdots X_{k+1}}^{\,Y_n\cdots Y_{k+1}}(n_2;\text{out}_2;\text{in}_2;\text{intra}_2)\\ &\quad\times\bar{K}_{X_k\cdots X_1}^{\,Y_k\cdots Y_1}(n_1;\text{out}_1;\text{in}_1;\text{intra}_1) \ ,\end{aligned} \tag{C2}$$

where $k\equiv n_1$ and the symbols with bars on the rhs of Eq. (C2) correspond to the connected parts of the diagram. The following identities for the generalized Kronecker deltas will be useful:

$$\delta_X^{\,X_n\cdots X_1}=\sum_{V_2}\sum_{V_1}\delta_X^{\,V_2V_1}\delta_{V_2}^{\,X_n\cdots X_{k+1}}\delta_{V_1}^{\,X_k\cdots X_1} \ , \tag{C3a}$$

$$\delta_{Y_n\cdots Y_1}^{\,Y}=\sum_{W_2}\sum_{W_1}\delta_{W_2W_1}^{\,Y}\delta_{Y_n\cdots Y_{k+1}}^{\,W_2}\delta_{Y_k\cdots Y_1}^{\,W_1} \ . \tag{C3b}$$

Because of the assumed disconnected character of diagram (C1), one has

$$c_{ji}=0 \tag{C4}$$

for $j>n_1$ and $i\le n_1$. It can be checked that in this case [see formula (38)] the parity of diagram (C1) can be expressed as

$$P=P_2+P_1 \ , \tag{C5}$$

where P_2 and P_1 are the parities of the connected subdiagrams. For the symmetry quotient (48) one finds

$$S^{-1}=S_2^{-1}S_1^{-1}\tilde{S}^{-1} \ , \tag{C6}$$

where S_1^{-1} and S_2^{-1} are the symmetry quotients for the connected subdiagrams. Quantity $\tilde{S}$ is equal to 2 if the subdiagrams are related by symmetry, $\tilde{S}=1$ otherwise. In general, $\tilde{S}\le m!$, where m is the number of the connected subdiagrams of a diagram. It is to be noted that Eq. (C6), or its generalization for $m>2$, may not be applicable to the case when the constituting subdiagrams are chosen to be disconnected. This is because in such a case a part of a subdiagram may be symmetry related to another subdiagram or its part and this makes the interpretation of quantity $\tilde{S}$ dependent on the inner structure of the subdiagrams.

It is easy to check that by substituting Eqs. (C2), (C3), (C5), and (C6) into Eq. (C1), formula (53) for the case $m=2$ is obtained. A generalization of this derivation for $m>2$ is obvious.

APPENDIX D

A product of fermion operators, e.g., those of set (9), can be formally put into the form of the normal product $\hat{X}^{\dagger}\hat{Y}$ by suitably reordering fermion operators in the initial product under the assumption that the rhs of Eq. (8b) is equal to zero. This operation, often denoted by enclosing the operator product in a curly bracket, is sometimes used to define a "normal product" of two (or more) operators, e.g.,

$$\hat{\Lambda}=\{\hat{\Theta}_2\hat{\Theta}_1\} \ . \tag{D1}$$

The above definition is ambiguous, however. Consider two pairs of operators,

$$\hat{\Theta}_2=\hat{a}^{\,i}\hat{a}_i, \quad \hat{\Theta}_1=\hat{a}^{\,i}\hat{a}_j \tag{D2a}$$

and

$$\hat{\Theta}'_2=1, \quad \hat{\Theta}'_1=\hat{a}^{\,i}\hat{a}_j \ . \tag{D2b}$$

It is easy to check that

$$\hat{\Theta}_2\hat{\Theta}_1=\hat{\Theta}'_2\hat{\Theta}'_1 \tag{D3}$$

but

$$\{\hat{\Theta}_2\hat{\Theta}_1\}\neq\{\hat{\Theta}'_2\hat{\Theta}'_1\} \ . \tag{D4}$$

In general, expression (D1) is undefined unless the structure of the operator in the curly brackets is specified.

Aware of deficiencies of definition (D1), Jeziorski and Paldus[13] recently proposed a rigorous algebraic definition of the normal product. We rewrite their definition for operators from $\mathcal{F}$(even) using the notation of the present paper [see Eqs. (27) and (28)]:

$$\hat{\Lambda}=\hat{\Theta}_2 * \hat{\Theta}_1 \ , \tag{D5}$$

where

$$\lambda_X{}^Y=\sum_{X_2}\sum_{X_1}\sum_{Y_2}\sum_{Y_1}\delta_X{}^{X_2X_1}[{}_{X_2}{}^{Y_2}]_2[{}_{X_1}{}^{Y_1}]_1\delta_{Y_2Y_1}{}^{Y} \ . \tag{D6}$$

It is seen that formula (D6) can be obtained from Eq. (29) after suppressing on the rhs of that equation all the terms corresponding to nonempty strings Z_{21}. After applying the above definition to operators

$$\hat{\Theta}_2=\hat{X}_2^{\dagger}\hat{Y}_2 \tag{D7a}$$

and

$$\hat{\Theta}_1=\hat{X}_1^{\dagger}\hat{Y}_1 \ , \tag{D7b}$$

one finds that

$$(\hat{X}_2^{\dagger}\hat{Y}_2) * (\hat{X}_1^{\dagger}\hat{Y}_1)=(\hat{X}_2\hat{X}_1)^{\dagger}\hat{Y}_2\hat{Y}_1 \ , \tag{D8}$$

which justifies the name "normal product" for the operation (D6). It is easy to check that this operation is commutative:

$$\hat{\Theta}_2 * \hat{\Theta}_1=\hat{\Theta}_1 * \hat{\Theta}_2 \ . \tag{D9}$$

The normal product (D6) introduces a new algebraic structure in $\mathcal{F}$(even) corresponding to a commutative algebra we denote by $\mathcal{F}$(even$*$). Within this new algebra we define the normal power of an operator, for integer n:

$$(\hat{T} *)^n\equiv\hat{T} * (\hat{T} *)^{n-1} \ , \tag{D10}$$

with

$$(\hat{T} *)^0\equiv 1 \ . \tag{D11}$$

In the same vein

$$(\hat{T} *)^{-1} \ , \tag{D12}$$

if it exists, will be interpreted as the normal inverse of operator $\hat{T}$. It can be shown that algebra $\mathcal{F}$(even$*$) is a nilpotent algebra: For arbitrary $\hat{T}$ one finds that

$$(\hat{T} *)^n=0 \tag{D13}$$

for $n\geq M$. Hence, any series of normal powers contains a finite number of terms and thus converges. For any operator function, expressible through operator power series, one may define its normal counterpart, e.g.,

$$\exp * (\hat{T} *)\equiv\sum_{n=0}(n!)^{-1}(\hat{T} *)^n \ . \tag{D14}$$

Operator $\exp * (\hat{T})$ is related to Lindgren's[15] operator

$$\{\exp(\hat{T})\} \tag{D15}$$

in the same sense as definition (D5) is related to (D1).

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