Coupled-cluster method in Fock space. IV. Calculation of expectation values and transition moments

Leszek Z. Stolarczyk* and Hendrik J. Monkhorst
Quantum Theory Project, Department of Physics, University of Florida, Gainesville, Florida 32611
(Received 9 March 1987; revised manuscript received 13 October 1987)

A method of calculating expectation values and transition moments within the framework of the generalized coupled-cluster (CC) method is described. This approach allows for a direct calculation of first- and second-order static properties, as well as response functions for a many-fermion system. Diagrammatic and algebraic techniques of the preceding paper are used to obtain explicit algebraic formulas for what is called one-particle CC density and transition matrices. From these quantities the ground-state expectation value and transition moments for an arbitrary one-particle operator can be easily computed.

I. INTRODUCTION

In this fourth paper of the series (Refs. 1–3, referred to as papers I, II, and III) we show that the generalized coupled-cluster (CC) method introduced in paper I can be extended to calculations of static and dynamic properties of a many-fermion system subject to an external perturbation. In a standard perturbation theory, basic ingredients needed for computing these properties are the spectrum of the unperturbed Hamiltonian $\hat{H}$, and expectation values and transition moments for the perturbation operator $\hat{V}$. The spectrum of $\hat{H}$ (in practice a part of it) is provided by the generalized CC method.[1,2] In the present paper a method for calculating the expectation values and transition moments will be described.

The standard CC method,[4–6] being neither variational nor perturbational, does not provide a simple prescription for calculating a system's properties. A systematic treatment of static and dynamic properties in a framework of the CC method was proposed by one of us.[7] In this approach,[7,8] suitable for calculating static first- and second-order properties, as well as dynamic response functions, an explicit dependence of the CC operator on the perturbation parameter (and time—when dynamic properties are considered) is assumed. Similar formalisms were also studied in Refs. 9–12. Arponen[13] initiated a different CC approach to static first-order properties by employing a variational principle; this approach has been further studied by Pal.[14] It is also worthwhile to mention a solution of the problem of analytical energy gradients in the CC method.[15] Last but not least, successful CC calculations of static properties of atomic and molecular systems has been performed by using a finite-field perturbation approach.[16]

A characteristic feature of the method we propose in the present paper is that it directly determines reduced density and transition matrices[17] (or, rather, certain equivalents called the CC density and transition matrices) for the unperturbed system. An obvious advantage of such an approach is that once the n-particle density and transition matrices are found, the expectation values and transition moments can easily be generated for an arbitrary n-particle operator $\hat{V}$. Here, explicit algebraic formulas are derived for the case $n=1$. Throughout the paper the formalism and notation of papers I, II, and III will be used. As before, we shall refer to equations contained in these papers by preceding a pertinent formula number with a proper Roman numeral (I, II, or III).

In Sec. II a brief summary of the generalized CC method[1] is presented. Section III contains basic formulas for expectation values and transition moments, and a system's properties expressible in terms of these quantities. The derivation of the CC formulas for expectation values and transition moments is given in Sec. IV. In Sec. V we employ diagrammatic and algebraic techniques from papers I and III to find explicit algebraic formulas for some one-particle CC density and transition matrices. An overview of the generalized CC method as a complete algebraic approach to the many-fermion problem is given in Sec. VI.

II. GENERALIZED CC METHOD—A SUMMARY

Throughout the paper we use the notation introduced in paper I and summarized in Sec. II of paper III. In the generalized CC method the Hamiltonian $\hat{H}$ for the system, given in Eq. (I.16), is first expressed in terms of the quasiparticle fermion operators [see Eqs. (I.26) and (I.27) and also Eqs. (III.10)–(III.13)] assuming the form given in Eq. (I.31). In this form $\hat{H}$ is manifestly a quasiparticle-number-nonconserving operator [see Eqs. (I.39) and (I.40)]. Then a similarity transformation (III.1) is performed, yielding the effective Hamiltonian $\hat{G}$ subject to the condition of being quasiparticle-number conserving [see Eq. (I.41)]. In other words, it is required that

$$\hat{G}\in\mathcal{F}^0 , \tag{1}$$

where $\mathcal{F}^0$ is a subalgebra of the Fermi-Dirac algebra [see Eq. (III.23)]. The wave operator $\hat{\Omega}$ appearing in Eq. (III.1) (called a universal wave operator, since it is—in

principle—defined for all the eigenstates of $\hat{H}$) is chosen in the following form:

$$\hat{\Omega}=\hat{\Omega}_{\rm ex}\hat{\Omega}_{\rm dx} , \tag{2}$$

where the excitation wave operator $\hat{\Omega}_{\rm ex}$ and the deexcitation wave operator $\hat{\Omega}_{\rm dx}$ are expressed in an exponential form,

$$\hat{\Omega}_{\rm ex}=\exp\hat{\Theta} , \tag{3a}$$

$$\hat{\Omega}_{\rm dx}=\exp\hat{\Xi} . \tag{3b}$$

Operators $\hat{\Theta}\in\mathcal{F}^{\uparrow}$ (even) and $\hat{\Xi}\in\mathcal{F}^{\downarrow}$ (even) [see Eqs. (III.23)–(III.25)] will be called the CC-excitation and CC-deexcitation operator, respectively, and may be expressed as

$$\hat{\Theta}=\sum_{\substack{X\\(x>y)}}\sum_{Y}\theta_X{}^Y\hat{X}^{\dagger}\hat{Y} , \tag{4a}$$

$$\hat{\Xi}=\sum_{\substack{X\\(x<y)}}\sum_{Y}\xi_X{}^Y\hat{X}^{\dagger}\hat{Y} \tag{4b}$$

[see the comments to Eq. (III.22c)]. Due to form (2) assumed for the wave operator $\hat{\Omega}$ it is convenient to split transformation (III.1) into two steps. In the first one the auxiliary effective Hamiltonian $\hat{\Gamma}$ is found,

$$\hat{\Gamma}=\hat{\Omega}_{\rm ex}^{-1}\hat{H}\hat{\Omega}_{\rm ex} , \tag{5}$$

$$\hat{\Gamma}=\sum_{X}\sum_{Y}\gamma_X{}^Y\hat{X}^{\dagger}\hat{Y} , \tag{6}$$

and in the second step the proper effective Hamiltonian $\hat{G}$ is calculated,

$$\hat{G}=\hat{\Omega}_{\rm dx}^{-1}\hat{\Gamma}\hat{\Omega}_{\rm dx} , \tag{7}$$

$$\hat{G}=\sum_{X}\sum_{Y}g_X{}^Y\hat{X}^{\dagger}\hat{Y} . \tag{8}$$

Requirement (1) puts a constraint $x=y$ on the summation in Eq. (8); this turns out to be equivalent to conditions

$$\gamma_X{}^Y=0 \quad \text{for } x>y , \tag{9a}$$

$$g_X{}^Y=0 \quad \text{for } x<y . \tag{9b}$$

Conditions (9a) and (9b) compose two sets of equations from which θ and ξ amplitudes [see Eqs. (4)] can be determined, respectively. These generalized CC equations are nonlinear coupled algebraic equations (for details, see papers I, II, and III); it is to be noted that in each case the number of unknowns (the θ or ξ amplitudes) is equal to the number of equations. In paper I we show that when conditions (9a) are met one has also

$$g_X{}^Y=0 \quad \text{for } x>y , \tag{10a}$$

and

$$g_X{}^Y=\gamma_X{}^Y \quad \text{for } x=y . \tag{10b}$$

Equation (10b) brings about an important simplification: g amplitudes of operator $\hat{G}$ of Eq. (8) can be found without actually solving Eq. (9b). In other words, as long as one is interested only in the spectrum of $\hat{H}$ there is no need for knowing the deexcitation CC operator $\hat{\Xi}$. However, this operator will prove its usefulness in determining expectation values and transition moments (see Secs. IV and V of this paper). An explicit algebraic form of the generalized CC equation (9b), from which the ξ amplitudes of operator $\hat{\Xi}$ can be determined, is studied in paper III [see Eqs. (III.79) and (III.80)].

For the effective Hamiltonian $\hat{G}$ fulfilling condition (1) there can be found an operator $\hat{B}\in\mathcal{F}^0$ such that operator $\hat{B}^{-1}\hat{G}\hat{B}$ becomes diagonal in the basis set (III.20),

$$\hat{B}^{-1}\hat{G}\hat{B}\Phi^X=E^X\Phi^X ; \tag{11}$$

here $\{E^X\}$ is the spectrum of Hamiltonian $\hat{H}$. The orthonormal set of eigenfunctions of $\hat{H}$ can now be expressed as

$$\{\Psi^X=\hat{A}\Phi^X\} , \tag{12}$$

where operator

$$\hat{A}=\hat{\Omega}\hat{B} \tag{13}$$

is assumed to be unitary,

$$\hat{A}^{\dagger}\hat{A}=\hat{B}^{\dagger}\hat{\Omega}^{\dagger}\hat{\Omega}\hat{B}=1 . \tag{14}$$

For convenience, we rewrite Eqs. (11) and (14) using a matrix notation,

$$\sum_{\substack{Z_1\\(z_1=z_2=x=y)}}\sum_{Z_2}\tilde{B}_X{}^{Z_1}G_{Z_1}{}^{Z_2}B_{Z_2}{}^Y=E^X\delta_X{}^Y , \tag{15}$$

$$\sum_{\substack{Z_1\\(z_1=z_2=x=y)}}\sum_{Z_2}(B_{Z_1}{}^X)^*\langle\Phi^{Z_1}\mid\hat{\Omega}^{\dagger}\hat{\Omega}\Phi^{Z_2}\rangle B_{Z_2}{}^Y=\delta_X{}^Y , \tag{16}$$

where

$$G_X{}^Y=\langle\Phi^X\mid\hat{G}\Phi^Y\rangle , \tag{17}$$

$$B_X{}^Y=\langle\Phi^X\mid\hat{B}\Phi^Y\rangle , \tag{18}$$

$$\tilde{B}_X{}^Y=\langle\Phi^X\mid\hat{B}^{-1}\Phi^Y\rangle , \tag{19}$$

and $\delta_X{}^Y$ is the generalized Kronecker delta defined in Eq. (III.19). It is to be noted that because $\hat{G},\hat{B}\in\mathcal{F}^0$, strings X, Y, Z_1 and Z_2 [see definition (III.15)] in Eqs. (15) and (16) are of the same length: $x=y=z_1=z_2$. Hence, operator $\hat{G}$ is already block diagonal in the basis set (III.20). In paper I, Eqs. (I.101)–(I.106), the structure of matrices $\{G_X{}^Y\}$ was given for cases $x=y=0$, 1, and 2 (these numbers correspond to the numbers of quasiparticles in the system in each case). For $x=y=0$ (X,Y are the empty strings) there is no quasiparticle in the system and the corresponding wave function from set (III.20) is Φ, the model vacuum [see Eq. (III.12)]. In this case Eq. (15) reduces to

$$G=E , \tag{20}$$

where E is the ground-state energy of the system (actually, we do not insist that E is the lowest energy level, it serves rather as a reference from which excitation energies are calculated). Equation (16) leads to

$$B^*B=\langle\Phi\mid\hat{\Omega}^\dagger\hat{\Omega}\Phi\rangle^{-1}\ , \tag{21}$$

and hence $\mid B\mid$ serves as a normalization constant for the ground-state eigenfunction of $\hat{H}$,

$$\Psi=\mid B\mid\hat{\Omega}\Phi\ . \tag{22}$$

It is easy to verify that because of the definition (4b) of the CC deexcitation operator, one has

$$\hat{\Omega}_{\rm dx}\Phi=\Phi\ , \tag{23}$$

and thus, when the intermediate normalization for Ψ is assumed (B set equal to 1),

$$\Psi=\exp(\hat{\Theta})\Phi\ , \tag{24}$$

which is a well-known formula of the standard CC method[4–6] [see also the discussion in paper I, starting with Eq. (I.122)].

It seems quite obvious that in the general case of $x=y=n$ one can solve Eq. (15) without imposing the normalization condition (16). However, we would like to make an observation which will prove helpful in our considerations in Sec. IV of this paper. Let us introduce matrices $\{C_X{}^Y, x=y\}$ such that

$$B_X{}^Y=\sum_{\substack{Z\\(z=x=y)}}C_X{}^Z\Lambda_Z{}^Y\ , \tag{25}$$

where

$$\Lambda_X{}^Y=\lambda_X\delta_X{}^Y \tag{26}$$

and λ_X are arbitrary nonzero parameters. After substituting Eq. (25) into Eq. (15), the following set of equations emerges:

$$\sum_{\substack{Z_1\,Z_2\\(z_1=z_2=x=y)}}\sum\tilde{C}_X{}^{Z_1}G_{Z_1}{}^{Z_2}C_{Z_2}{}^Y=E^X\delta_X{}^Y\ , \tag{27}$$

where matrix $\{\tilde{C}_X{}^Y\}$ is the inverse of matrix $\{C_X{}^Y\}$. Now matrix $\{C_X{}^Y\}$ represents a general solution to Eq. (15), not necessarily fulfilling Eq. (16). A simple identity following from Eqs. (25) and (26) will prove to be useful:

$$B_X{}^Z\tilde{B}_Z{}^Y=C_X{}^Z\tilde{C}_Z{}^Y \tag{28}$$

(note: there is no summation over strings Z in this equation).

Equation (27), for $x=y=n$ ($n=0,1,\ldots$ is the number of quasiparticles in the system), corresponds to the diagonalization of a non-Hermitian matrix $\{G_X{}^Y\}$ by means of a similarity transformation. The matrices involved are $\binom{M}{n}\times\binom{M}{n}$ matrices, where M is the dimension of the spin-orbital basis set (III.4). the dimension of the matrices can be reduced after symmetry properties of the Hamiltonian $\hat{H}$ are taken into account (see paper I). Obviously, in practice only a part of the spectrum $\{E^X\}$, corresponding to small n's, can be calculated this way.

III. EXPECTATION VALUES AND TRANSITION MOMENTS, AND SYSTEM'S PROPERTIES

Let us assume that operator $\hat{V}$ is a Hermitian operator representing a certain perturbation to our many-fermion system described by Hamiltonian $\hat{H}$. Quantity

$$V_X{}^Y=\langle\Psi^X\mid\hat{V}\Psi^Y\rangle \tag{29}$$

is for $X=Y$ called the expectation value of operator $\hat{V}$ in state Ψ^X, and for $X\neq Y$, called the transition moment of $\hat{V}$ for states Ψ^X and Ψ^Y; the states in question are orthonormal eigenstates of $\hat{H}$, taken from set (12). Below, a few examples of a system's properties which can be expressed in terms of integrals $V_X{}^Y$ are given.

Let us write the perturbed Hamiltonian for the system as

$$\hat{H}(\lambda)=\hat{H}+\lambda\hat{V}\ , \tag{30}$$

where λ is a perturbation parameter. The Rayleigh-Schrödinger perturbation theory applied to the ground state of $\hat{H}$ leads to the following expansion for an eigenvalue of $\hat{H}(\lambda)$:

$$E(\lambda)=E^{(0)}+\lambda E^{(1)}+\lambda^2E^{(2)}+\cdots\ , \tag{31}$$

where

$$E^{(0)}=E\ , \tag{32a}$$

$$E^{(1)}=V\ , \tag{32b}$$

$$E^{(2)}=-\sum_{\substack{X\\(x\neq0)}}\frac{\mid V^X\mid^2}{\Delta E^X}\ . \tag{32c}$$

In Eqs. (32) E is the ground-state energy of Eq. (20), V is the expectation value of $\hat{V}$ in the eigenstate Ψ [see Eq. (22)], V^X is the transition moment of $\hat{V}$ for states Ψ and Ψ^X, and ΔE^X is an excitation energy

$$\Delta E^X=E^X-E\ . \tag{33}$$

$E^{(1)}$ and $E^{(2)}$ correspond to first- and second-order static properties of the system.

In the case of a time- and frequency-dependent perturbation

$$\hat{V}(t,\omega)=\tfrac{1}{2}\hat{V}(e^{i\omega t}+e^{-i\omega t})e^{\alpha t}\ , \tag{34}$$

where $\alpha>0$, the dynamical behavior of the system may be described by the response function,[8]

$$\langle\langle V,V\rangle\rangle_\omega=\tfrac{1}{2}\sum_{\substack{X\\(x\neq0)}}\mid V^X\mid^2\left[\frac{1}{\omega-\Delta E^X}-\frac{1}{\omega+\Delta E^X}\right]\ . \tag{35}$$

It is seen that $\langle\langle V,V\rangle\rangle_\omega$ reduces to $E^{(2)}$ for $\omega\to0$.

The static and dynamic properties discussed here correspond to a perturbation-theory approach based on the full set of eigenstates of Hamiltonian $\hat{H}$, obtained in the algebraic approximation.[1] Due to computational limitations (see remarks at the end of Sec. II) one has to restrict the summations in Eqs. (32c) and (35). To assess the validity of such restrictions, the sum rule

$$\sum_X\mid V^X\mid^2=\langle\Psi\mid\hat{V}^2\Psi\rangle \tag{36}$$

might be used. It should be remembered, however, that the above sum rule is observed exactly only if set (12) is

complete, which is not the case in the algebraic approximation.

IV. CC FORMULAS FOR EXPECTATION VALUES AND TRANSITION MOMENTS

By employing representation (12) of the eigenstates of $\hat{H}$, one may write the general matrix element of Eq. (29) as

$$V_X{}^Y=\langle\Phi^X|\,\hat{A}^{\dagger}\hat{V}\hat{A}\Phi^Y\rangle=\langle\Phi^X|\,\hat{A}^{-1}\hat{V}\hat{A}\Phi^Y\rangle$$
$$=\langle(\hat{B}^{-1})^{\dagger}\Phi^X|\,\hat{\Omega}^{-1}\hat{V}\hat{\Omega}\hat{B}\Phi^Y\rangle\ . \tag{37}$$

One finds also that [see Eqs. (15) and (16), and definitions (18) and (19)]

$$\hat{B}\Phi^Y=\sum_{\substack{Z\\(z=y)}}\Phi^Z B_Z{}^Y\ , \tag{38a}$$

$$(\hat{B}^{-1})^{\dagger}\Phi^X=\sum_{\substack{Z\\(z=x)}}\Phi^Z(\tilde{B}_X{}^Z)^*\ . \tag{38b}$$

Note that in Eqs. (37) and (38) there is, in general, $x\neq y$, since $\hat{V}$ need not be a quasiparticle-number-conserving operator. By substituting Eqs. (38) into Eq. (37) one arrives at the formula

$$V_X{}^Y=\sum_{\substack{Z_1\\(z_1=x)}}\sum_{\substack{Z_2\\(z_2=y)}}\tilde{B}_X{}^{Z_1}W_{Z_1}{}^{Z_2}B_{Z_2}{}^Y\ , \tag{39}$$

where we denote

$$W_X{}^Y=\langle\Phi^X|\,\hat{\Omega}^{-1}\hat{V}\hat{\Omega}\Phi^Y\rangle\ . \tag{40}$$

There seems to be an apparent problem with formula (39) in that it requires the knowledge of matrices $\{B_X{}^Y\}$ subject to troublesome condition (16). This problem disappears in the case of calculating expectation values:

$$V_X{}^X=\sum_{\substack{Z_1\\(z_1=z_2=x)}}\sum_{Z_2}\tilde{B}_X{}^{Z_1}W_{Z_1}{}^{Z_2}B_{Z_2}{}^X$$
$$=\sum_{\substack{Z_1\\(z_1=z_2=x)}}\sum_{Z_2}\tilde{C}_X{}^{Z_1}W_{Z_1}{}^{Z_2}C_{Z_2}{}^X\ ; \tag{41}$$

the last equality follows from Eq. (28). In the case of a transition moment ($X\neq Y$), let us note that what is actually needed for calculating second-order properties [see, e.g., Eqs. (32c) and (35)] is the square of its absolute value,

$$|\,V_X{}^Y|^2=V_X{}^Y V_Y{}^X\ . \tag{42}$$

By substituting formula (39) into the above equation one finds that

$$V_X{}^Y V_Y{}^X=\sum_{\substack{Z_1\\(z_1=z_4=x)}}\sum_{Z_4}\sum_{\substack{Z_2\\(z_2=z_3=y)}}\sum_{Z_3}\tilde{B}_X{}^{Z_1}W_{Z_1}{}^{Z_2}B_{Z_2}{}^Y\tilde{B}_Y{}^{Z_3}W_{Z_3}{}^{Z_4}B_{Z_4}{}^X$$
$$=\sum_{\substack{Z_1\\(z_1=z_4=x)}}\sum_{Z_4}\sum_{\substack{Z_2\\(z_2=z_3=y)}}\sum_{Z_3}\tilde{C}_X{}^{Z_1}W_{Z_1}{}^{Z_2}C_{Z_2}{}^Y\tilde{C}_Y{}^{Z_3}W_{Z_3}{}^{Z_4}C_{Z_4}{}^X\ , \tag{43}$$

where, again, we have been able to use Eq. (28). It can be shown that matrices $\{B_X{}^Y\}$ can be eliminated in a similar way also from the formulas for higher-order properties.

Equations (41) and (43) are our basic CC formulas for expectation values and transition moments, respectively. For calculating matrix elements (40), one needs to know operator

$$\hat{W}=\hat{\Omega}^{-1}\hat{V}\hat{\Omega}\ , \tag{44}$$

$$\hat{W}=\sum_X\sum_Y w_X{}^Y\hat{X}^{\dagger}\hat{Y}\ . \tag{45}$$

Diagrammatic and algebraic expressions for some w amplitudes of operator $\hat{W}$ will be derived in Sec. V. Now we write a specific case of Eq. (41) corresponding to the first-order property (32b):

$$V=W=\langle\Phi|\,\hat{\Omega}^{-1}\hat{V}\hat{\Omega}\Phi\rangle\ . \tag{46}$$

By substituting Eqs. (2) and (3) into the above formula and taking into account property (23), one finds that

$$V=\langle\Phi|\,\exp(-\hat{\Xi})\exp(-\Theta)\hat{V}\exp(\hat{\Theta})|\,\Phi\rangle\ , \tag{47}$$

which is equivalent to the formula for expectation values derived by Arponen[13] (his "extended exp$S$" method). For the second-order properties (32c) and (35), Eq. (43) simplifies to

$$|\,V^X|^2=\sum_{\substack{Z_1\\(z_1=z_2=x)}}\sum_{Z_2}W^{Z_1}C_{Z_1}{}^X\tilde{C}_X{}^{Z_2}W_{Z_2}\ . \tag{48}$$

One also finds that the left-hand side (lhs) of Eq. (36) can be written as

$$\sum_X|\,V^X|^2=\sum_X W^X W_X\ . \tag{49}$$

Note that operator $\hat{W}$ of Eq. (44) is not Hermitian, and hence, in general, $W_X\neq(W^X)^*$. Parameters W, W^X, and W_X may be expressed in terms of w amplitudes of operator $\hat{W}$ [see Eq. (45)] by using formula (I.B30); in this case one gets, simply,

$$W=w\ , \tag{50a}$$

$$W^X=w^X\ , \tag{50b}$$

and

$$W_X=w_X\ . \tag{50c}$$

V. ONE-PARTICLE CC DENSITY AND TRANSITION MATRICES

In this section we assume that $\hat{V}$ is a one-particle operator in Fock space,

$$\hat{V}=u_i{}^j\hat{a}^i\hat{a}_j \ , \tag{51}$$

where $u_i{}^j=(u_j{}^i)^*$ are one-particle integrals, and the fermion operators are those of set (III.9) [see also Eqs. (I.16)–(I.19)]. When expressed through the quasiparticle fermion operators of set (III.10) corresponding to the particle-hole transformation (I.27), this operator reads

$$\hat{V}=v+v_i{}^j\hat{b}^i\hat{b}_j+\tfrac{1}{2}v^{ij}\hat{b}_i\hat{b}_j+\tfrac{1}{2}v_{ij}\hat{b}^j\hat{b}^i \ , \tag{52}$$

where the v amplitudes are given by [see Eqs. (I.31) and (I.32)]

$$v=u_\rho{}^\rho \ , \tag{53a}$$

$$v_i{}^j=\begin{cases} v_\rho{}^\sigma=-u_\sigma{}^\rho \\ v_r{}^s=u_r{}^s, \end{cases} \tag{53b}$$

$$v_{ij}=(v^{ij})^*=v_{\rho r}=-v_{r\rho}=u_r{}^\rho \ . \tag{53c}$$

In Eqs. (53) indices ρ and σ correspond to spin orbitals occupied in the wave function Φ (model vacuum), and indices r and s correspond to unoccupied spin orbitlas [see Eqs. (I.25)]. In Eqs. (51), (52), and (53a) Einstein's summation convention is used [see also Eqs. (III.22a) and (III.22b).

As the effective Hamiltonian $\hat{G}$ [see Eqs. (5) and (7)], the transformed operator $\hat{W}$ of Eqs. (44) and (45) is calculated in two steps. First, the auxiliary transformed operator $\hat{\Upsilon}$ is found:

$$\hat{\Upsilon}=\hat{\Omega}_{\rm ex}^{-1}\hat{V}\hat{\Omega}_{\rm ex} \ , \tag{54}$$

$$\hat{\Upsilon}=\sum_X\sum_Y v_X{}^Y\hat{X}^\dagger\hat{Y} \ , \tag{55}$$

and then operator $\hat{W}$ is determined as

$$\hat{W}=\hat{\Omega}_{\rm dx}^{-1}\hat{\Upsilon}\hat{\Omega}_{\rm dx} \ . \tag{56}$$

It is very advantageous that to calculate the system's properties described in Sec. III; one needs to know only a small subset of W amplitudes [see Eqs. (50)]. Below we shall find explicit algebraic formulas for the amplitudes w, w^{ij}, and w_{ij}.

We shall use diagrammatic and algebraic techniques described in paper III. A graphical representation of the v amplitudes of operator $\hat{V}$, the v amplitudes of operator Υ, and the w amplitudes of operator $\hat{W}$ is shown in Fig. 1. Diagrammatic expressions for some v amplitudes are given in Fig. 2 and those for w amplitudes in Fig. 3. The final diagrammatic formulas for the amplitudes w, w_{ij}, and w^{ij}, expressing them in terms of v, θ, and ξ amplitudes, are given in Fig. 4. The approximations used to obtain these formulas are those employed in papers II and III. Now we write down these formulas in the algebraic form according to the rules set forth in paper III:

$$w=v-\tfrac{1}{2}\xi^{ij}v_{ij}-\tfrac{1}{4}\xi^{ij}v^{kl}\theta_{klij}+\tfrac{1}{2}\xi^{ij}\xi^{kl}v_k{}^m\theta_{mlij}-\tfrac{1}{6}\xi^{ijkl}v_i{}^m\theta_{mjkl} \ , \tag{57a}$$

$$w_{ij}=v_{ij}+\tfrac{1}{2}v^{kl}\theta_{klij}-\tfrac{1}{2}(\xi^{kl}v_i{}^m\theta_{mklj}-\xi^{kl}v_j{}^m\theta_{mkli})-\xi^{kl}v_k{}^m\theta_{mlij} \ , \tag{57b}$$

$$\begin{aligned} w^{ij}=v^{ij}&-(\xi^{ik}v_k{}^j-\xi^{jk}v_k{}^i)-\tfrac{1}{2}(\xi^{ik}v^{lm}\theta_{lmk}{}^j-\xi^{jk}v^{lm}\theta_{lmk}{}^i)-\tfrac{1}{2}(\xi^{kl}v^{im}\theta_{mkl}{}^j-\xi^{kl}v^{jm}\theta_{mkl}{}^i) \\ &-\tfrac{1}{6}(\xi^{iklm}v^{jn}\theta_{nklm}-\xi^{jklm}v^{in}\theta_{nklm})-\tfrac{1}{2}(\xi^{iklm}v_k{}^n\theta_{nlm}{}^j-\xi^{jklm}v_k{}^n\theta_{nlm}{}^i)-\tfrac{1}{2}\xi^{ijkl}v_{kl}-\tfrac{1}{4}\xi^{ijkl}v^{mn}\theta_{nmkl} \ . \end{aligned} \tag{57c}$$

It is seen that the right-hand sides (rhs's) of the above equations are linear in v amplitudes, so these equations may be rewritten as follows:

$$w=v+v_i{}^jD_j{}^i(\ |\ )+\tfrac{1}{2}v^{ij}D_{ij}(\ |\ )+\tfrac{1}{2}v_{ij}D^{ij}(\ |\ ) \ , \tag{58a}$$

$$\begin{aligned} w_{ij}=v_{ij}&+\tfrac{1}{2}v^{kl}D_{klij}(ij\ |\ )+[v_i{}^kD_{kj}(ij\ |\ )-v_j{}^kD_{ki}(ij\ |\ )] \\ &+v_k{}^lD_{lij}{}^k(ij\ |\ ) \ , \end{aligned} \tag{58b}$$

$$\begin{aligned} w^{ij}=v^{ij}&+\tfrac{1}{2}v^{kl}D_{kl}{}^{ij}(\ |\ ij) \\ &+[v^{ik}D_k{}^j(\ |\ ij)-v^{jk}D_k{}^i(\ |\ ij)] \\ &+v_k{}^lD_l{}^{kij}(\ |\ ij)+[v_k{}^iD^{jk}(\ |\ ij)-v_k{}^jD^{ik}(\ |\ ij)] \\ &+\tfrac{1}{2}v_{kl}D^{kl}(\ |\ ij) \ . \end{aligned} \tag{58c}$$

Here we have introduced quantities $D_{Z_1}{}^{Z_2}(X\ |\ Y)$ which form what we call the one-particle CC density (for $X=Y$) and transition (for $X\neq Y$) matrices:

$$D_j{}^i(\ |\ )=\tfrac{1}{2}\xi^{lm}\xi^{ik}\theta_{jklm}-\tfrac{1}{6}\xi^{iklm}\theta_{jklm} \ , \tag{59a}$$

$$D_{ij}(\ |\ )=-\tfrac{1}{2}\xi^{kl}\theta_{klij} \ , \tag{59b}$$

$$D^{ij}(\ |\ )=-\xi^{ij} \ , \tag{59c}$$

$$D_{klij}(ij\ |\ )=\theta_{klij} \ , \tag{59d}$$

$$D_{kj}(ij\ |\ )=-\tfrac{1}{2}\xi^{lm}\theta_{lmkj} \ , \tag{59e}$$

$$D_{ki}(ij\ |\ )=-\tfrac{1}{2}\xi^{lm}\theta_{lmki} \ , \tag{59f}$$

$$D_{lij}{}^k(ij\ |\ )=\xi^{km}\theta_{mlij} \ , \tag{59g}$$

$$\begin{aligned} D_{kl}{}^{ij}(\ |\ ij)=&-(\xi^{im}\theta_{klm}{}^j-\xi^{jm}\theta_{klm}{}^i) \\ &-\tfrac{1}{2}\xi^{ijmn}\theta_{mnkl} \ , \end{aligned} \tag{59h}$$

$$D_k{}^j(\ |\ ij)=-\tfrac{1}{2}\xi^{lm}\theta_{lmk}{}^j+\tfrac{1}{6}\xi^{jlmn}\theta_{klmn} \ , \tag{59i}$$

$$D_k{}^i(\ |\ ij)=-\tfrac{1}{2}\xi^{lm}\theta_{lmk}{}^i+\tfrac{1}{6}\xi^{ilmn}\theta_{klmn} \ , \tag{59j}$$

$$D_l{}^{kij}(\ |\ ij)=-\tfrac{1}{2}(\xi^{ikmn}\theta_{lmn}{}^j-\xi^{jkmn}\theta_{lmn}{}^i) \ , \tag{59k}$$

$$D^{jk}(\ |\ ij)=\xi^{jk} \ , \tag{59l}$$

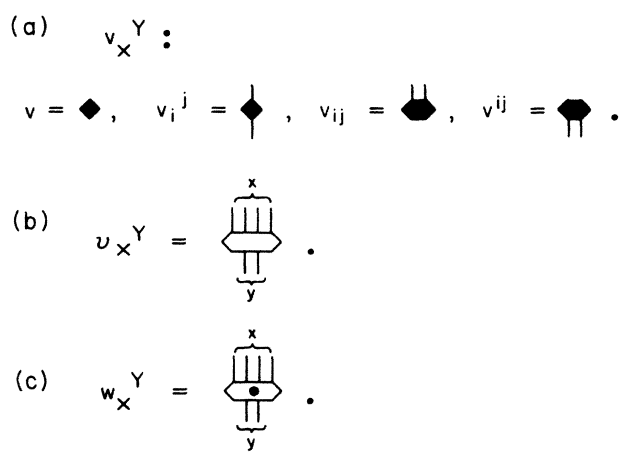

FIG. 1. Diagrammatic representation of (a) the v amplitudes of operator $\hat{V}$ [see Eqs. (52) and (53)], (b) the v amplitudes of operator $\hat{\Upsilon}$ [see Eqs. (54) and (55)], and (c) the w amplitudes of operator $\hat{W}$ [see Eqs. (44) and (45)].

$$D^{ik}(\,|\,ij)=\xi^{ik}\,, \tag{59m}$$

$$D^{kl}(\,|\,ij)=-\xi^{ijkl}\,. \tag{59n}$$

It is seen that quantities $D_{Z_1}{}^{Z_2}(X\,|\,Y)$ are antisymmetric with respect to permutations of indices within strings Z_1 and Z_2. In the case when the quasiparticle fermion

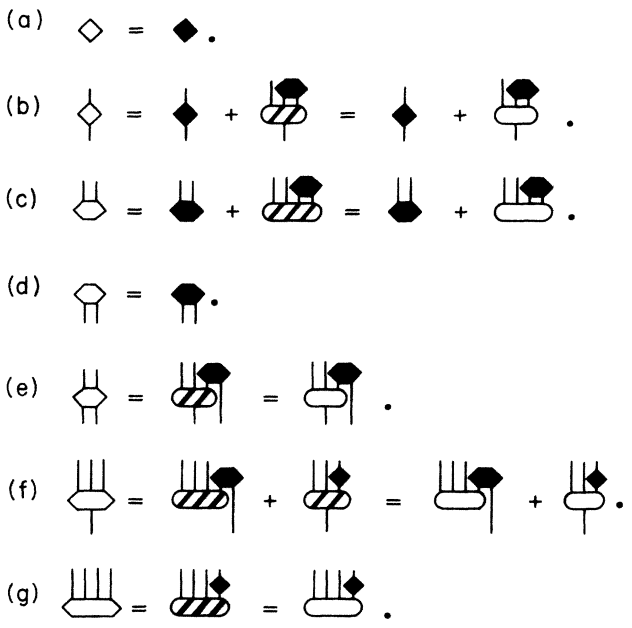

FIG. 2. Diagrammatic expressions for v amplitudes of operator $\hat{\Upsilon}$: (a) v, (b) $v_i{}^j$, (c) v_{ij}, (d) v^{ij}, (e) $v_{ij}{}^{kl}$, (f) $v_{ijk}{}^l$, and (g) v_{ijkl}. The graphical symbols for parameters $\tau_X{}^Y$, and the θ amplitudes of operator $\hat{\Theta}$ [see Eq. (4a)] appearing in these expressions are shown in Fig. 1 of paper I. In the derivation of (a)–(g) the approximation set forth in Fig. 9 of paper III is assumed; the v amplitudes other than (a)–(g) are assumed to be equal to zero.

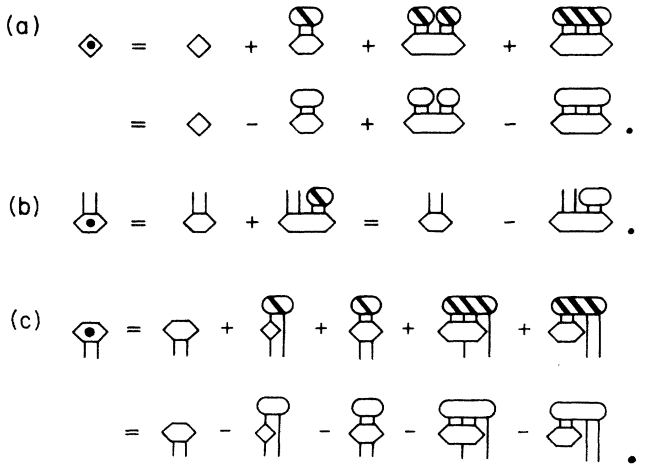

FIG. 3. Diagrammatic expressions for w amplitudes of operator $\hat{W}$: (a) w, (b) w_{ij}, and (c) w^{ij}. The graphical symbols for parameters $\tau'_X{}'^Y$ and ξ amplitudes of operator Ξ [see Eq. (4b)] appearing in these expressions are shown in Fig. 12 of paper III. Expressions (a)–(c) have been derived using the approximation set forth in Fig. 13 of paper III and Fig. 2 of the present paper.

operators of set (III.10) are obtained by using the particle-hole transformation [see Eq. (I.27)], the pseudocharge symmetry imposes restrictions (III.72), and in this case Eqs. (59) read [see also Eqs. (53)]

$$D_\sigma{}^\rho(\,|\,)=\xi^{\tau t}\xi^{\rho r}\theta_{\sigma\tau tr}-\tfrac{1}{2}\xi^{\rho\tau tu}\theta_{\sigma\tau tu}\,, \tag{60a}$$

$$D_s{}^r(\,|\,)=\xi^{\tau t}\xi^{\rho r}\theta_{\rho\tau ts}-\tfrac{1}{2}\xi^{\rho\sigma tr}\theta_{\rho\sigma ts}\,, \tag{60b}$$

$$D_{\rho r}(\,|\,)=-\xi^{\sigma s}\theta_{\rho\sigma sr}\,, \tag{60c}$$

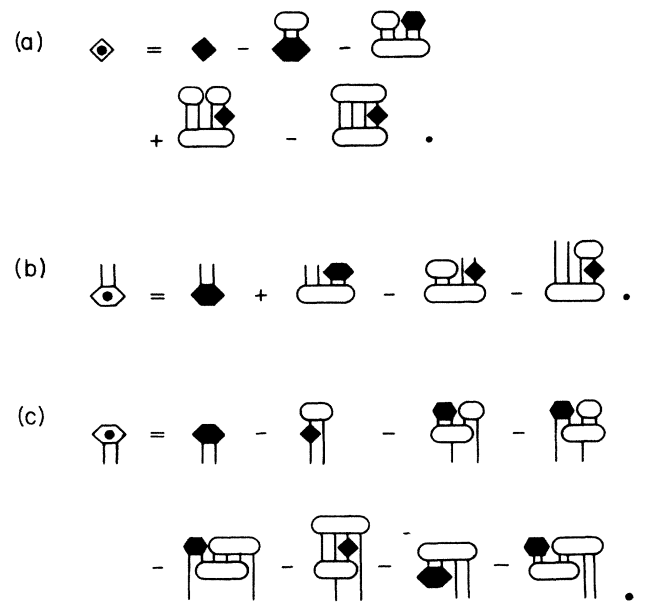

FIG. 4. Diagrammatic expressions for w amplitudes of operator $\hat{W}$, obtained by substituting the expressions given in Fig. 2 for those of Fig. 3.

$$D^{\rho r}(\,|\,) = -\xi^{\rho r}\ , \tag{60d}$$

$$D_{\rho\sigma rs}(\rho r\,|\,) = \theta_{\rho\sigma rs}\ , \tag{60e}$$

$$D_{\sigma r}(\rho r\,|\,) = -\xi^{\tau t}\theta_{\sigma\tau tr}\ , \tag{60f}$$

$$D_{\rho s}(\rho r\,|\,) = -\xi^{\tau t}\theta_{\rho\tau ts}\ , \tag{60g}$$

$$D_{\sigma\rho r}{}^{\tau}(\rho r\,|\,) = -\xi^{\tau t}\theta_{\sigma\rho rt}\ , \tag{60h}$$

$$D_{\rho rs}{}^{t}(\rho r\,|\,) = -\xi^{\tau t}\theta_{\tau\rho rs}\ , \tag{60i}$$

$$D_{\sigma s}{}^{\rho r}(\,|\,\rho r) = -(\xi^{\rho t}\theta_{\sigma st}{}^{r} + \xi^{\tau r}\theta_{\tau\sigma s}{}^{\rho}) - \xi^{\tau\rho rt}\theta_{\tau\sigma st}\ , \tag{60j}$$

$$D_{\sigma}{}^{\rho}(\,|\,\rho r) = -\xi^{\tau t}\theta_{\sigma\tau t}{}^{\rho} + \tfrac{1}{2}\xi^{\rho\tau rs}\theta_{\sigma\tau rs}\ , \tag{60k}$$

$$D_{s}{}^{r}(\,|\,\rho r) = -\xi^{\tau t}\theta_{\tau ts}{}^{r} + \tfrac{1}{2}\xi^{\rho\sigma tr}\theta_{\rho\sigma ts}\ , \tag{60l}$$

$$D_{\tau}{}^{\sigma\rho r}(\,|\,\rho r) = -\tfrac{1}{2}\xi^{\rho\sigma st}\theta_{\tau st}{}^{r} + \xi^{\sigma vur}\theta_{\tau vu}{}^{\rho}\ , \tag{60m}$$

$$D_{t}{}^{\rho rs}(\,|\,\rho r) = -\xi^{\rho vus}\theta_{vut}{}^{r} + \tfrac{1}{2}\xi^{\sigma\tau rs}\theta_{\sigma\tau t}{}^{\rho}\ , \tag{60n}$$

$$D^{\sigma r}(\,|\,\rho r) = \xi^{\sigma r}\ , \tag{60o}$$

$$D^{\rho s}(\,|\,\rho r) = \xi^{\rho s}\ , \tag{60p}$$

$$D^{\sigma s}(\,|\,\rho r) = \xi^{\rho\sigma rs}\ . \tag{60q}$$

There are our final formulas for the one-particle CC density and transition matrices. The derivation of the two-particle CC density and transition matrices can be performed similarly; such a derivation would produce approximately twice the number of terms in Eqs. (60).

Our one-particle CC density and transition matrices are defined merely as sets of linear coefficients (59) and (60) corresponding to formulas (58). In order to show how they are related to the usual density and transition matrices,[17] let us consider the case of the ordinary one-particle density matrix corresponding to our ground-state wave function Ψ [see Eqs. (22) and (24)]. The expectation value [compare Eq. (29)]

$$V = \langle\,\Psi\,|\,\hat{V}\Psi\,\rangle\langle\,\Psi\,|\,\Psi\,\rangle^{-1} \tag{61}$$

for the one-particle operator $\hat{V}$ of Eq. (51) can be written in the following form:

$$V = u_i{}^j\Delta_j{}^i\ , \tag{62}$$

where

$$\Delta_j{}^i = (\Delta_i{}^j)^*\ , \tag{63}$$

and matrix Δ represents the one-particle density matrix[17] for the wave function Ψ. In order to facilitate the comparison between the ordinary and the CC density matrix, we rewrite Eq. (62) by using different indices for occupied and unoccupied spin orbitals [compare Eqs. (53)]:

$$V = u_{\sigma}{}^{\rho}\Delta_{\rho}{}^{\sigma} + u_r{}^s\Delta_s{}^r + u_{\rho}{}^r\Delta_r{}^{\rho} + u_r{}^{\rho}\Delta_{\rho}{}^r\ . \tag{64}$$

With the same operation performed on Eq. (58a) and by taking into account relations (46) and (50a), one arrives at the formula

$$V = v + v_{\rho}{}^{\sigma}D_{\sigma}{}^{\rho}(\,|\,) + v_r{}^sD_s{}^r(\,|\,) + v^{\rho r}D_{\rho r}(\,|\,) + v_{\rho r}D^{\rho r}(\,|\,)\ , \tag{65}$$

where the quantities appearing on the rhs of this equation are defined in Eqs. (53) and (60a)–(60d). The comparison of formulas (64) and (65) reveals the following relations:

$$\Delta_{\rho}{}^{\sigma} = \delta_{\rho}{}^{\sigma} - D_{\sigma}{}^{\rho}(\,|\,)\ , \tag{66a}$$

$$\Delta_s{}^r = D_s{}^r(\,|\,)\ , \tag{66b}$$

$$\Delta_r{}^{\rho} = D_{\rho r}(\,|\,)\ , \tag{66c}$$

$$\Delta_{\rho}{}^r = D^{\rho r}(\,|\,)\ . \tag{66d}$$

Matrix Δ calculated by using Eqs. (66) is exactly Hermitian [see Eq. (63)] only in the case when the generalized CC equations (9) have been solved exactly. Because our Eqs. (60a)–(60d) correspond to an approximate solution of Eqs. (9), an average procedure yielding

$$\Delta_r{}^{\rho} = (\Delta_{\rho}{}^r)^* = \tfrac{1}{2}\{D_{\rho r}(\,|\,) + [D^{\rho r}(\,|\,)]^*\}\ , \tag{67}$$

etc., can be applied.

VI. GENERALIZED CC METHOD—AN OVERVIEW

In papers I, II, and III and this paper (paper IV), the formalism of the generalized CC method has been presented. This method provides a systematic treatment of the many-fermion problem studied in the algebraic approximation (i.e., with the Fock space generated by a chosen finite basis set of spin orbitals). A hierarchy of coupled nonlinear algebraic equations (the generalized CC equations) is obtained, with the amplitudes of the CC excitation and deexcitation operators as unknowns. By solving these equations the amplitudes of the effective Hamiltonian and the CC density and transition matrices can be determined. These quantities may then be used for calculating the energy spectrum and static and dynamic properties of a given many-fermion system. In papers I and III we developed special algebraic and diagrammatic techniques for deriving and handling of numerous algebraic formulas which appear in the generalized CC method. The approximation schemes described in paper I, employing truncated CC operators, effectively decouple certain subsets of the generalized CC equations; this makes the many-fermion problem in question computationally tractable. This hierarchy of approximations (closely related to that of the generalized CC equations) begins with the Hartree-Fock approximation and ends at the exact solution. It is fair to say that the approximations studied in paper I, and implemented in papers II, III, and IV, are suitable for many-fermion systems with soft-core interactions such as electronic systems. For systems with a hard-core interparticle potential, as considered in nuclear physics, other approximation schemes might be developed, see the article by Kümmel *et al.* in Ref. 4.

Apart from providing a well-defined hierarchy of approximations suitable for practical applications, the generalized CC method offers also a new insight into the quasiparticle model for a system of many fermions. This model emerges here not as a semiphenomenological approximation but rather as a rigorous scheme in which every eigenstate of the system's Hamiltonian $\hat{H}$ is assigned a new quantum number equal to the number of

quasiparticles. Such an assignment can be achieved by applying a mathematical procedure we describe in detail in paper I, Sec. III–V. In the case of a "normal" system, for which the Hartree-Fock (HF) approximation is qualitatively correct for a N-particle ground state, our quasiparticles (in this case "particles" and "holes") correspond to some $(N\pm1)$-particle states of the system. As eigenstates of $\hat{H}$, these states are stationary states of the system that lead to infinite lifetimes for the corresponding quasiparticles. At this point the reader may note a difference between the present quasiparticle model and that of the Green's function method,[18] where the lifetimes of quasiparticles are, in general, finite. In our model the description of a many-particle system, given in the terms of quasiparticles, parallels that given in the terms of particles, the Hamiltonian $\hat{H}$ for the particles corresponds to the Hamiltonian $\hat{G}$ for the quasiparticles, the physical vacuum Φ_0 (the vacuum for the particles) corresponds to the model vacuum Φ (the vacuum for the quasiparticles). By design [see Eqs. (III.1) and (III.2)], the spectra of $\hat{H}$ and $\hat{G}$ are identical, and in the present paper we have shown how the expectation values and transition moments corresponding to eigenstates of $\hat{H}$ can be calculated by employing some quantities associated with Hamiltonian $\hat{G}$. It is to be stressed that the choice of the model vacuum Φ is (to some extent) arbitrary from the mathematical point of view; it depends on the choice of the reference eigenstate Ψ [see Eqs. (22) and (24)]. Ψ is usually chosen to be the eigenstate of $\hat{H}$ corresponding to the ground state of the system. Such an assignment may depend, however, on the value of the chemical potential for the system. In our approach (see paper II), Φ is an approximation to the Brueckner (or maximum overlap) configuration corresponding to Ψ. It can be determined iteratively[2] starting, e.g., from the appropriate HF wave function.

We conclude that the generalized CC method offers a consistent and complete approach to the many-fermion problem in the algebraic approximation and may provide an alternative to the Green's function method[18] which still dominates in the field of the quantum many-body theory.

ACKNOWLEDGMENTS

This work was supported in part by the U.S. Office of Naval Research–Defense Advanced Research Projects Agency (ONR–DARPA) Grant No. 160658212, the U.S. National Science Foundation (NSF) Grant No. CHE-85-05733, and the Polish Academy of Sciences Grant No. CPBP-01-12.

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*Permanent address: Department of Chemistry, University of Warsaw, Pasteura 1, PL-02-093 Warsaw, Poland.

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