Coupled-cluster method in Fock space. II. Brueckner-Hartree-Fock method

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The generalized coupled-cluster (CC) method of the preceding paper is cast into the form of the Brueckner-Hartree-Fock (BHF) method. In this approach the model vacuum Φ is optimized to become the maximum-overlap configuration for the reference eigenfunction Ψ. One of the approximation schemes of the preceding paper is applied to derive explicit algebraic equations which can be used for practical calculations of (approximate) energies of several states of a many-fermion system. These include the N-particle ground-state energy, energies of some $(N-1)$- and $(N+1)$-particle states, as well as energies of certain N-particle excited states. It is indicated that the numerical effort required in the present approach is comparable to that of the coupled-cluster singles and doubles (CCSD) method of Purvis and Bartlett [J. Chem. Phys. **76**, 1910 (1982)].

I. CHOICE OF MODEL VACUUM

In the preceding paper,[1] hereafter referred to as paper I, a generalization of the coupled-cluster (CC) method has been proposed. Although being essentially a single-reference approach, this generalized CC method may provide an access to an (in principle) arbitrary portion of the spectrum of the Fock-space Hamiltonian $\hat{H}$. When deriving the generalized CC equations (see Sec. VI of paper I) we found it convenient to assume that the reference configuration Φ (model vacuum) is the maximum-overlap configuration for some reference eigenfunction Ψ of $\hat{H}$. In the present paper we would like to reformulate the theory of paper I such that optimization of Φ towards the maximum-overlap configuration is taken into account. Another purpose of this paper is to apply one of the approximation schemes described in Sec. VII of paper I, and obtain a set of generalized CC equations suitable for practical computations. Solutions of these equations (CC amplitudes) may be used for calculating (approximate) values of the N-particle ground-state energy E and energies of some $(N-1)$- and $(N+1)$-particle states, as well as energies of certain excited N-particle states of a many-fermion system.

In Ref. 2 we showed how the usual single-reference CC method can be modified to allow for the above-mentioned optimization of Φ. We shall refer to this modified version of the CC method as the Brueckner-Hartree-Fock (BHF) method. A fairly extensive bibliography of the BHF method and related subjects can be found in Ref. 2. Below we shall combine results of Ref. 2 and paper I to formulate the BHF method in Fock space. The notation of paper I will be employed. When referring to a formula of paper I, we shall hereafter simply quote its number preceding it by the Roman numeral I.

It is instructive to consider first the usual Hartree-Fock (HF) method. Since the algebraic approximation is employed, one should speak rather of the Hartree-Fock-Roothaan[3] (HFR) method. Here, as in the case of the BHF method discussed further, the one-particle space $\mathcal{H}$ remains fixed, and only partition (I.24) is to be found. The HF condition reads [see Eq. (I.33)].

$$\langle \Phi | \hat{H} | \Phi \rangle \equiv \eta = \text{ minimum} . \tag{1}$$

The necessary condition for (1), η stationary, is equivalent to the requirement [see Eqs. (I.32b) and (I.32d)]

$$f_r^{\rho} \equiv \eta_{\rho r} = 0 , \tag{2}$$

Additional conditions may be imposed [see Eqs. (I.32c)]:

$$f_{\rho}^{\sigma} \equiv -\eta_{\sigma}^{\rho} = e_{\rho} \delta_{\rho}^{\sigma} , \tag{3a}$$

$$f_r^s \equiv \eta_r^s = e_r \delta_r^s . \tag{3b}$$

According to Koopmans's theorem,[4] $(-e_{\rho})$ approximates an energy of detachment of a particle from the N-particle system, and e_r approximates an energy of attachment of a particle to this system. Conditions (2) and (3) correspond to diagonalization of operator $\hat{f}$ of Eq. (I.34) within the space $\mathfrak{M}_1 = \mathcal{H}$ [see Eq. (I.11)]. Since $\hat{f}$ depends on its eigenfunctions, an iterative procedure known as the self-consistent-field (SCF) method is necessary in this case. The self-consistent eigenfunctions of $\hat{f}$ are known as the canonical HF spinorbitals.

In the case of the BHF method[2] the basic requirement is

$$\langle \Phi | \Psi \rangle = \text{ maximum} , \tag{4}$$

for Φ and Ψ both normalized to unity. The necessary condition for (4) means that the overlap integral is stationary. It can be shown[2] that in this case for the generalized CC operator $\hat{\Theta}$ of Eq. (I.116) one has

$$\theta_{ij} = \theta_{\rho r} = 0 , \tag{5}$$

for $\rho = 1,2,\ldots,N$, and $r = N+1, N+2, \ldots, M$. In Ref. 2 we showed that to impose the necessary condition for (4) one can assume that (5) holds and the Brueckner spin orbitals (corresponding to the maximum-overlap configuration Φ) can be determined from equations [see Eq. (I.113a), and Fig. 4(a) of paper I]:

$$\gamma_{ij} = \gamma_{\rho r} = 0 \tag{6}$$

for $\rho=1,2,\ldots,N$, and $r=N+1,N+2,\ldots,M$. Below we modify slightly the formulation of the BHF method given in Ref. 2. It will be useful to introduce the BHF operator $\hat{b}$ of the form

$$\hat{b}=b_i{}^j\hat{a}^i\hat{a}_j\ , \tag{7}$$

where we define [see Eq. (I.113b), and Fig. 6(b) of paper I] [operator $\hat{b}$ should not be confused with one of the fermion operators of Eqs. (I.27)]

$$b_r{}^\rho=(b_\rho{}^r)^*=\gamma_\rho{}^r\ , \tag{8a}$$

$$b_\rho{}^\sigma=(b_\sigma{}^\rho)^*=-\tfrac{1}{2}(\gamma_\rho{}^\sigma+\gamma_\sigma{}^\rho)\ , \tag{8b}$$

$$b_r{}^s=(b_s{}^r)^*=\tfrac{1}{2}(\gamma_r{}^s+\gamma_s{}^r)\ , \tag{8c}$$

and it is assumed that the generalized CC operator $\hat{\Theta}$ fulfills condition (5). By definition (8), operator $\hat{b}$ is Hermitian. Now, when $\hat{b}$ is made diagonal, condition (6) is automatically met. It should be stressed that also in this case a SCF procedure is needed. Since $\hat{b}$ depends not only on spin orbitals, but also on (generalized) CC amplitudes, the problem of so-called double self-consistency emerges in this case. One can notice that because of definition (8b) [(8c)] the Hermitian part of matrix $\mathbf{G}_{\rm h}$ ($\mathbf{G}_{\rm p}$) becomes diagonal when operator $\hat{b}$ is diagonalized [see Eqs. (I.113b), and Eqs. (I.102) and (I.103)]. This means that for this choice of (self-consistent) Brueckner spin orbitals (we shall call them canonical) one has

$$g_\rho{}^\sigma=-g_\sigma{}^\rho \tag{9a}$$

for $\rho\neq\sigma$, and

$$g_r{}^s=-g_s{}^r \tag{9b}$$

for $r\neq s$. It is seen that when anti-Hermitian contributions (9) are small, the set $\{-\epsilon_\rho\}$ of eigenvalues of $\hat{b}$ approaches exact particle-detachment energies of the N-particle system, whereas the set $\{\epsilon_r\}$ of eigenvalues of $\hat{b}$ approximates particle-attachment energies. When the above assumption is not justified, diagonalization of non-Hermitian matrices (I.103a) and (I.103b) should be performed.

In Sec. II explicit BHF equations will be derived using approximations introduced in Sec. VII of paper I.

II. APPROXIMATE VARIANTS OF BHF METHOD

Approximations described in Sec. VII of paper I can be applied equally well to the BHF method of Sec. I. In any approximation scheme, some model vacuum Φ (e.g., the HFR determinantal wave function) is assumed as a starting point. A truncated (generalized) CC operator $\hat{\Theta}$ (primes used in Sec. VII of paper I will be suppressed hereafter) is constructed assuming condition (5). The BHF operator (7) is then built according to definitions (8), and the eigenvalue problem for this operator is solved self-consistently [this includes solving a proper set of generalized CC equations (I.140)]. Finally, an effective Hamiltonian (I.141) is built following prescription (I.142), and its eigenvalues are calculated to approximate eigenvalues of Hamiltonian $\hat{H}$. Below two examples of approximate variants of the BHF method are considered.

(i) The variant corresponding to $L=0$ and $K_0=4$. This is exactly the BHF(2) method described in Ref. 2. Here [see Eq. (I.139)]

$$\hat{\Theta}=\hat{\Theta}_{40}\ , \tag{10}$$

and the corresponding CC equations read [see Fig. 4(b) of paper I]

$$\gamma_{ijkl}=\gamma_{\rho\sigma rs}=0 \tag{11}$$

for $\rho<\sigma$ and $r<s$. Equations (6) are taken into account when the eigenproblem for the BHF operator (7) is considered.[2] In this approach only the ground-state energy E is determined.

(ii) The variant with $L=1$, $K_0=4$, and $K_1=3$. This is one step beyond the previous approximation scheme. We are going to discuss this variant in detail. For the CC operator one has formally

$$\hat{\Theta}=\hat{\Theta}_{40}+\hat{\Theta}_{31} \tag{12}$$

and, besides Eqs. (6) and (11), the following CC equations are to be solved [see Fig. 5(a) of paper I]:

$$\gamma_{ijk}{}^l=\begin{cases}\gamma_{\rho\sigma r}{}^\zeta=0 & \text{for } \rho<\sigma\\ \gamma_{\rho rs}{}^z=0 & \text{for } r<s\ .\end{cases} \tag{13}$$

One can notice that now Eqs. (6) and (11) contain more terms than in the case of variant (i). This is because in variant (i) all the CC amplitudes, except amplitudes $\theta_{\rho\sigma rs}$, are set equal to zero. In variant (ii) higher amplitudes τ_X for $x\geq 6$ [see Figs. 1(a) and 1(b)] can be approximated by linked terms built of amplitudes $\theta_{\rho\sigma r}{}^\zeta$ and $\theta_{\rho rs}{}^z$. The same applies to amplitudes $\tau_X{}^i$ for $x\geq 5$ [see Figs. 1(c) and 1(d)] which appear in Eqs. (13).

Variant (ii) seems to be the most general BHF method involving unknowns (CC amplitudes) which are at most four-indexed. It can be shown[5] that in this case construction of the left-hand sides (lhs's) of Eqs. (6), (11), and (13) can be reduced to procedures for which computation times scale approximately like M^6, where M is the dimension of the spin-orbital space $\mathcal{H}$. Hence, the numerical ef-

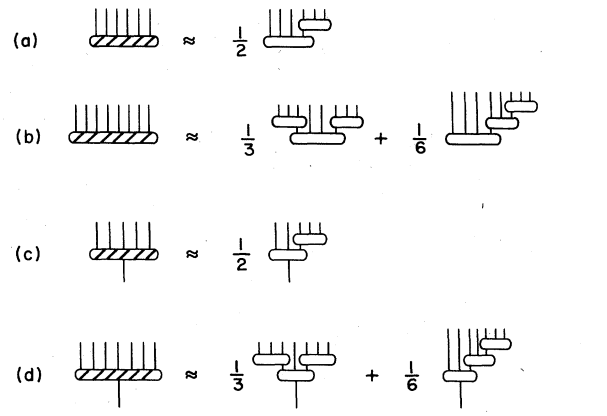

FIG. 1. Approximate diagrammatic expressions for parameters $\tau_X{}^Y$: (a) τ_{ijklmn}, (b) $\tau_{ijklmnpq}$, (c) $\tau_{ijklm}{}^n$, (d) $\tau_{ijklmnp}{}^q$. See also Figs. 1–3 of paper I.

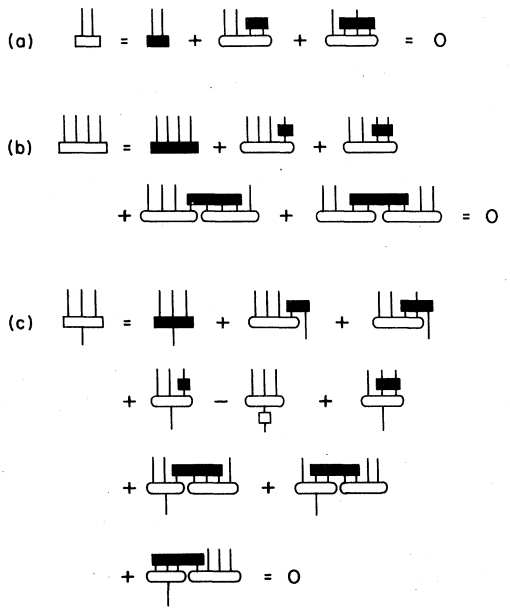

FIG. 2. Approximate BHF equations in the diagrammatic form: (a) $\gamma_{ij}=0$, (b) $\gamma_{ijkl}=0$, (c) $\gamma_{ijk}{}^{l}=0$. Compare with Figs. 4 and 5 of paper I.

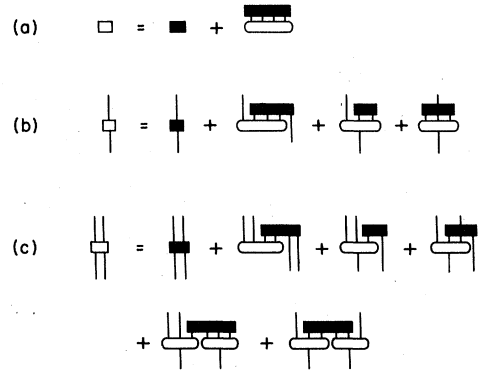

FIG. 3. Approximate BHF equations in the diagrammatic form: (a) $\gamma=g=E$, (b) $\gamma_{i}{}^{j}=g_{i}{}^{j}$, (c) $\gamma_{ij}{}^{kl}=g_{ij}{}^{kl}$. Compare with Fig. 6 of paper I.

fort required for solving the generalized CC equations in variant (ii) should be comparable to that in the coupled-cluster singles and doubles (CCSD) model.[5] Let us also notice that Eqs. (6), (11), and (13) of variant (ii) correspond exactly to those terms in Hamiltonian $\hat{H}$ of Eq. (I.31) which are responsible for $\hat{H}$ not being a quasiparticle-number–conserving operator.

It is difficult to assess now whether inclusion of terms depicted in Fig. 1 will improve the results (the energy spectrum) calculated in variant (ii). Hereafter we shall consider a simplified variant (ii) in which the amplitudes $\tau_{X}{}^{Y}$ shown in Fig. 1 are set equal to zero. The resulting diagrammatic CC equations are shown in Fig. 2. Parameters of the effective Hamiltonian [see Eqs. (I.141) and (I.142) are depicted in Fig. 3. We neglect here three- and higher-quasiparticle interactions. In Sec. III an algebraic form of the diagrammatic equations of Fig. 2 and 3 will be given. We shall refer to these equations as approximate BHF equations.

III. BHF EQUATIONS

The BHF equations depicted in Fig. 2 and 3 can be translated into an algebraic form with the help of formula (I.B18) and its analog derived in the appendix of the present paper [see Eq. (A9)]. An example of the application of Eq. (I.B18) is given in Fig. 2 of paper I. It should be pointed out that the generalized Kronecker deltas in Eqs. (I.B18) and (A9) are used simply to antisymmetrize the resulting algebraic expressions. Below the BHF equations of Figs. 2 and 3 are expressed in the algebraic form. Einstein's summation convention is employed; each unrestricted summation over n equivalent indices gives rise to the factor $(n!)^{-1}$. The equations of Fig. 2 read

$$\gamma_{ij}=\eta_{ij}+\tfrac{1}{2}\eta^{kl}\theta_{klij}+\tfrac{1}{6}(\eta_{i}{}^{klm}\theta_{klmj}-\eta_{j}{}^{klm}\theta_{klmi})=0\ , \tag{14a}$$

$$\begin{aligned}\gamma_{ijkl}=&\eta_{ijkl}+\eta_{i}{}^{m}\theta_{mjkl}-\eta_{j}{}^{m}\theta_{mikl}+\eta_{k}{}^{m}\theta_{mijl}\\&-\eta_{l}{}^{m}\theta_{mijk}+\tfrac{1}{2}(\eta_{ij}{}^{mn}\theta_{mnkl}+\eta_{jk}{}^{mn}\theta_{mnil}-\eta_{jl}{}^{mn}\theta_{mnik}-\eta_{ik}{}^{mn}\theta_{mnjl}+\eta_{il}{}^{mn}\theta_{mnjk}+\eta_{kl}{}^{mn}\theta_{mnij})\\&+(-1)^{9}\tfrac{1}{6}\eta^{mnpq}(\theta_{mijk}\theta_{npql}-\theta_{mjkl}\theta_{npqi}+\theta_{mikl}\theta_{npqj}-\theta_{mijl}\theta_{npqk})\\&+(-1)^{4}\tfrac{1}{4}\eta^{mnpq}(\theta_{mnij}\theta_{pqkl}+\theta_{mnjk}\theta_{pqil}-\theta_{mnik}\theta_{pqjl})=0\ ,\end{aligned} \tag{14b}$$

$$\begin{aligned}\gamma_{ijk}{}^{l}=&\eta_{ijk}{}^{l}+\eta^{lm}\theta_{mijk}+\tfrac{1}{2}(\eta_{i}{}^{lmn}\theta_{mnjk}-\eta_{j}{}^{lmn}\theta_{mnik}+\eta_{k}{}^{lmn}\theta_{mnij})\\&+\eta_{i}{}^{m}\theta_{mjk}{}^{l}-\eta_{j}{}^{m}\theta_{mik}{}^{l}+\eta_{k}{}^{m}\theta_{mij}{}^{l}-\theta_{ijk}{}^{m}\gamma_{m}{}^{l}+\tfrac{1}{2}(\eta_{ij}{}^{mn}\theta_{mnk}{}^{l}+\eta_{jk}{}^{mn}\theta_{mni}{}^{l}-\eta_{ik}{}^{mn}\theta_{mnj}{}^{l})\\&+(-1)^{6}\tfrac{1}{6}\eta^{mnpq}(\theta_{mij}{}^{l}\theta_{npqk}+\theta_{mjk}{}^{l}\theta_{npqi}-\theta_{mik}{}^{l}\theta_{npqj})\\&+(-1)^{2}\tfrac{1}{4}\eta^{mnpq}(\theta_{mni}{}^{l}\theta_{pqjk}-\theta_{mnj}{}^{l}\theta_{pqik}+\theta_{mnk}{}^{l}\theta_{pqij})+(-1)^{0}\tfrac{1}{6}\eta^{mnpq}\theta_{mnp}{}^{l}\theta_{qijk}=0\ .\end{aligned} \tag{14c}$$

The BHF equations of Fig. 3 read

$$\gamma=\eta+\tfrac{1}{24}\eta^{ijkl}\theta_{ijkl}=g=E\ , \tag{15a}$$

$$\gamma_i{}^j=\eta_i{}^j+\tfrac{1}{6}\eta^{jklm}\theta_{klmi}+\tfrac{1}{2}\eta^{kl}\theta_{kli}{}^j+\tfrac{1}{6}\eta_i{}^{klm}\theta_{klm}{}^j=g_i{}^j\ , \tag{15b}$$

$$\begin{aligned}\gamma_{ij}{}^{kl}&=\eta_{ij}{}^{kl}+\tfrac{1}{2}\eta^{klmn}\theta_{mnij}+\eta^{km}\theta_{mij}{}^l-\eta^{lm}\theta_{mij}{}^k+\tfrac{1}{2}(\eta_i{}^{kmn}\theta_{mnj}{}^l-\eta_i{}^{lmn}\theta_{mnj}{}^k+\eta_j{}^{lmn}\theta_{mni}{}^k-\eta_j{}^{kmn}\theta_{mni}{}^l)\\&\quad+(-1)^6\tfrac{1}{6}\eta^{mnpq}(\theta_{mij}{}^k\theta_{npq}{}^l-\theta_{mij}{}^l\theta_{npq}{}^k)+(-1)^4\tfrac{1}{4}\eta^{mnpq}(\theta_{mni}{}^k\theta_{pqj}{}^l-\theta_{mni}{}^l\theta_{pqj}{}^k)\\&=g_{ij}{}^{kl}\ .\end{aligned} \tag{15c}$$

The phase factors in Eqs. (14) and (15) stem from the use of formula (A9): in Eq. (14b) factor $(-1)^9$ corresponds to $z_{13}=3$ and $x_2=3$, etc. Equations (14) and (15) are written in a very general form which is good also when the general Bogoliubov-Valatin[6] transformation is used to define new fermion operators in Eq. (I.26); in this case only the definitions (I.32) should be generalized. When the usual particle-hole transformation (I.27) is employed, the pseudocharge symmetry [see Eq. (I.136)] can be used to simplify Eqs. (14) and (15). The resulting equations read

$$\gamma_{\rho r}=\eta_{\rho r}+\eta^{\sigma s}\theta_{\rho\sigma sr}+\tfrac{1}{2}(\eta_\rho{}^{\sigma\tau s}\theta_{\sigma\tau sr}+\eta_r{}^{\sigma st}\theta_{\rho\sigma st})=0\ , \tag{16a}$$

$$\begin{aligned}\gamma_{\rho\sigma rs}&=\eta_{\rho\sigma rs}+\eta_\rho{}^\tau\theta_{\tau\sigma rs}-\eta_\sigma{}^\tau\theta_{\tau\rho rs}-\eta_r{}^t\theta_{\rho\sigma st}+\eta_s{}^t\theta_{\rho\sigma rt}+\tfrac{1}{2}\eta_{\rho\sigma}{}^{\tau\upsilon}\theta_{\tau\upsilon rs}+\eta_{\sigma r}{}^{\tau t}\theta_{\rho\tau ts}-\eta_{\sigma s}{}^{\tau t}\theta_{\rho\tau tr}-\eta_{\rho r}{}^{\tau t}\theta_{\sigma\tau ts}+\eta_{\rho s}{}^{\tau t}\theta_{\sigma\tau tr}\\&\quad+\tfrac{1}{2}\eta_{rs}{}^{tu}\theta_{\rho\sigma tu}-\tfrac{1}{2}\eta^{\tau\upsilon tu}(\theta_{\rho\sigma ru}\theta_{\tau\upsilon ts}+\theta_{\tau\sigma rs}\theta_{\rho\upsilon tu}-\theta_{\tau\rho rs}\theta_{\sigma\upsilon tu}-\theta_{\rho\sigma su}\theta_{\tau\upsilon tr})\\&\quad+\tfrac{1}{4}\eta^{\tau\upsilon tu}\theta_{\rho\sigma tu}\theta_{\tau\upsilon rs}+\eta^{\tau\upsilon tu}\theta_{\sigma\tau ur}\theta_{\rho\upsilon ts}-\eta^{\tau\upsilon tu}\theta_{\rho\tau tr}\theta_{\sigma\upsilon us}=0\ .\end{aligned} \tag{16b}$$

Equation (14c) splits into two types of equations:

$$\begin{aligned}\gamma_{\rho\sigma r}{}^\zeta&=\eta_{\rho\sigma r}{}^\zeta-\eta^{\xi t}\theta_{\rho\sigma rt}+\eta_\rho{}^{\xi\tau t}\theta_{\sigma\tau tr}-\eta_\sigma{}^{\xi\tau t}\theta_{\rho\tau tr}+\tfrac{1}{2}\eta_r{}^{\xi tu}\theta_{\rho\sigma tu}+\eta_\rho{}^\tau\theta_{\tau\sigma r}{}^\zeta-\eta_\sigma{}^\tau\theta_{\tau\rho r}{}^\zeta+\eta_r{}^t\theta_{\rho\sigma t}{}^\zeta-\theta_{\rho\sigma r}{}^\tau\gamma_\tau{}^\zeta\\&\quad+\tfrac{1}{2}\eta_{\rho\sigma}{}^{\tau\upsilon}\theta_{\tau\upsilon r}{}^\zeta+\eta_{\sigma r}{}^{\tau t}\theta_{\rho\tau t}{}^\zeta-\eta_{\rho r}{}^{\tau t}\theta_{\sigma\tau t}{}^\zeta+\tfrac{1}{2}\eta^{\tau\upsilon tu}(\theta_{\rho\sigma t}{}^\zeta\theta_{\tau\upsilon ur}-\theta_{\tau\sigma r}{}^\zeta\theta_{\rho\upsilon tu}+\theta_{\tau\rho r}{}^\zeta\theta_{\sigma\upsilon tu})\\&\quad-\eta^{\tau\upsilon tu}(\theta_{\rho\tau t}{}^\zeta\theta_{\sigma\upsilon ur}-\theta_{\sigma\tau t}{}^\zeta\theta_{\rho\upsilon ur}-\tfrac{1}{4}\theta_{\tau\upsilon r}{}^\zeta\theta_{\rho\sigma tu})-\tfrac{1}{2}\eta^{\tau\upsilon tu}\theta_{\tau\upsilon t}{}^\zeta\theta_{\rho\sigma ru}=0\ ,\end{aligned} \tag{16c}$$

and

$$\begin{aligned}\gamma_{\rho rs}{}^z&=\eta_{\rho rs}{}^z-\eta^{\tau z}\theta_{\tau\rho rs}+\tfrac{1}{2}\eta_\rho{}^{\tau\upsilon z}\theta_{\tau\upsilon rs}-\eta_r{}^{\tau tz}\theta_{\rho\tau ts}+\eta_s{}^{\tau tz}\theta_{\rho\tau tr}+\eta_\rho{}^\tau\theta_{\tau rs}{}^z\\&\quad+\eta_r{}^t\theta_{\rho st}{}^z+\eta_s{}^t\theta_{\rho rt}{}^z-\theta_{\rho rs}{}^t\gamma_t{}^z+\eta_{\rho r}{}^{\tau t}\theta_{\tau ts}{}^z+\tfrac{1}{2}\eta_{rs}{}^{tu}\theta_{\rho tu}{}^z-\eta_{\rho s}{}^{\tau t}\theta_{\tau tr}{}^z\\&\quad+\tfrac{1}{2}\eta^{\tau\upsilon tu}(\theta_{\rho rt}{}^z\theta_{\tau\upsilon us}-\theta_{\tau rs}{}^z\theta_{\rho\upsilon tu}-\theta_{\rho st}{}^z\theta_{\tau\upsilon ur})+\eta^{\tau\upsilon tu}(\tfrac{1}{4}\theta_{\rho tu}{}^z\theta_{\tau\upsilon rs}+\theta_{\tau tr}{}^z\theta_{\rho\upsilon us}-\theta_{\tau ts}{}^z\theta_{\rho\upsilon ur})\\&\quad-\tfrac{1}{2}\eta^{\tau\upsilon tu}\theta_{\upsilon tu}{}^z\theta_{\tau\rho rs}=0\ .\end{aligned} \tag{16d}$$

Equation (15a) becomes

$$\gamma=\eta+\tfrac{1}{4}\eta^{\rho\sigma rs}\theta_{\rho\sigma rs}=g=E\ . \tag{17a}$$

Equation (15b) splits into

$$\gamma_\rho{}^\sigma=\eta_\rho{}^\sigma-\tfrac{1}{2}\eta^{\sigma\tau tu}\theta_{\rho\tau tu}+\eta^{\tau t}\theta_{\rho\tau t}{}^\sigma+\tfrac{1}{2}\eta_\rho{}^{\tau\upsilon t}\theta_{\tau\upsilon t}{}^\sigma=g_\rho{}^\sigma \tag{17b}$$

and

$$\gamma_r{}^s=\eta_r{}^s-\tfrac{1}{2}\eta^{\tau\upsilon ts}\theta_{\tau\upsilon tr}+\eta^{\tau t}\theta_{\tau tr}{}^s+\tfrac{1}{2}\eta_r{}^{\tau tu}\theta_{\tau tu}{}^s=g_r{}^s\ . \tag{17c}$$

There are three types of two-quasiparticle potentials [see Eqs. (I.104) and (I.105)], but we shall be interested only in the hole-particle one:

$$\begin{aligned}\gamma_{\rho r}{}^{\sigma s}&=\eta_{\rho r}{}^{\sigma s}+\eta^{\sigma\tau ts}\theta_{\rho\tau tr}+\eta^{\sigma t}\theta_{\rho rt}{}^s+\eta^{\tau s}\theta_{\tau\rho r}{}^\sigma+\eta_\rho{}^{\sigma\tau t}\theta_{\tau tr}{}^s-\tfrac{1}{2}\eta_\rho{}^{\tau\upsilon s}\theta_{\tau\upsilon r}{}^\sigma+\eta_r{}^{\tau ts}\theta_{\rho\tau t}{}^\sigma-\tfrac{1}{2}\eta_r{}^{\sigma tu}\theta_{\rho tu}{}^s\\&\quad+\tfrac{1}{2}\eta^{\tau\upsilon tu}(\theta_{\tau\rho r}{}^\sigma\theta_{\upsilon tu}{}^s-\theta_{\rho rt}{}^s\theta_{\tau\upsilon u}{}^\sigma)-\eta^{\tau\upsilon tu}(\theta_{\rho\tau t}{}^\sigma\theta_{\upsilon ur}{}^s+\tfrac{1}{4}\theta_{\rho tu}{}^s\theta_{\tau\upsilon r}{}^\sigma)\\&=g_{\rho r}{}^{\sigma s}\ .\end{aligned} \tag{17d}$$

The above effective potential is necessary in calculations for excited states of the N-particle system, see Eqs. (I.105b) and (I.106).

It can be checked that Eqs. (16a) and 16(b) and Eq. (17a) are in fact identical with those of the BHF(2) method of Ref. 2. Therefore, that approach may be used as a starting point in the present extended BHF method. It is to be noted that the definition of the BHF operator $\hat{b}$ in Ref. 2 does not require the knowledge of CC amplitudes $\theta_{\rho\sigma r}{}^\xi$ and $\theta_{\rho rs}{}^z$. In the present treatment these amplitudes are determined by solving Eqs. (16c) and (16d), respectively. It is interesting to find that if one substitutes

in these equations [see Eqs. (17b) and 17(c)],

$$\theta_{\rho\sigma r}{}^{\tau}\gamma_{\tau}{}^{\xi}\rightarrow\theta_{\rho\sigma r}{}^{\tau}\eta_{\tau}{}^{\xi}\ , \tag{18a}$$

$$\theta_{prs}{}^{t}\gamma_{t}{}^{z}\rightarrow\theta_{prs}{}^{t}\eta_{t}{}^{z}\ , \tag{18b}$$

the resulting equations will become linear in the unknown amplitudes.

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APPENDIX

Here we derive an analog of formula (I.B18) for a product of three operators:

$$\hat{K}=\hat{B}\hat{C}\hat{D}\ . \tag{A1}$$

It is assumed that operators $\hat{B}$, $\hat{C}$, and $\hat{D}$ belong to subalgebra $\tilde{\mathfrak{F}}$ (even), and are expressed in the form (I.49), with linear parameters $b_X{}^Y$, $c_X{}^Y$, and $d_X{}^Y$, respectively. The same applies to operators $\hat{K}$ and $\hat{\Lambda}=\hat{C}\hat{D}$, where the corresponding parameters are $\kappa_X{}^Y$ and $\lambda_X{}^Y$, respectively. For operator $\hat{K}=\hat{B}\hat{\Lambda}$ formula (I.B18) gives

$$\kappa_X{}^Y=\sum_{X_1}\sum_{X_4}\sum_{Y_1}\sum_{Y_2}\sum_{Z}\delta_X{}^{X_1X_4}b_{X_1}{}^{Y_1Z}\lambda_{ZX_4}{}^{Y_4}\delta_{Y_1Y_4}{}^{Y}\ , \tag{A2}$$

and one can find also that

$$\lambda_{ZX_4}{}^{Y_4}=\sum_{V_2}\sum_{V_3}\sum_{Y_2}\sum_{Y_3}\sum_{Z_{23}}\delta_{ZX_4}{}^{V_2V_3}c_{V_2}{}^{Y_2Z_{23}}d_{Z_{23}V_3}{}^{Y_3}\delta_{Y_2Y_3}{}^{Y_4}\ . \tag{A3}$$

In order to combine formulas (A2) and (A3), it will be useful to express the generalized Kronecker delta $\delta_{ZX_4}{}^{V_2V_3}$ in a different form. We observe that when nonzero it can be written as

$$\delta_{ZX_4}{}^{V_2V_3}=\delta_Z{}^{Z_{12}Z_{13}}\delta_{X_4}{}^{X_2X_3}\delta_{Z_{12}Z_{13}X_2X_3}{}^{Z_{12}X_2Z_{13}X_3}\times\delta_{Z_{12}X_2}{}^{V_2}\delta_{Z_{13}X_3}{}^{V_3}\ , \tag{A4}$$

where strings of indices Z_{12}, Z_{13}, X_2, and X_3 (of unspecified internal ordering) are unequivocally determined by strings Z, X_4, V_2, and V_3. Taking into account that

$$\delta_{Z_{12}Z_{13}X_2X_3}{}^{Z_{12}X_2Z_{13}X_3}=(-1)^{z_{13}x_2}\ , \tag{A5}$$

we can now write

$$\delta_{ZX_4}{}^{V_2V_3}=\sum_{X_2}\sum_{X_3}\sum_{Z_{12}}\sum_{Z_{13}}\delta_Z{}^{Z_{12}Z_{13}}\delta_{X_4}{}^{X_2X_3}\times\delta_{Z_{12}X_2}{}^{V_2}\delta_{Z_{13}X_3}{}^{V_3}(-1)^{z_{13}x_2}\ , \tag{A6}$$

where the restricted summation over strings of indices is performed [see the comments to Eq. (I.49)]. It can be found that Eq. (A6) is valid for any choice of strings Z, X_4, V_2, and V_3. By combining Eqs. (A2), (A3), and (A6), and performing summations

$$\sum_{Y_4}\delta_{Y_2Y_3}{}^{Y_4}\delta_{Y_1Y_4}{}^{Y}=\delta_{Y_1Y_2Y_3}{}^{Y}\ , \tag{A7}$$

$$\sum_{Z}b_{X_1}{}^{Y_1Z}\delta_Z{}^{Z_{12}Z_{13}}=b_{X_1}{}^{Y_1Z_{12}Z_{13}}\ , \tag{A8}$$

etc., we arrive at the desired formula

$$\kappa_X{}^Y=\sum_{X_1}\sum_{X_2}\sum_{X_3}\sum_{Y_1}\sum_{Y_2}\sum_{Y_3}\sum_{Z_{12}}\sum_{Z_{13}}\sum_{Z_{23}}(-1)^{z_{13}x_2}\delta_X{}^{X_1X_2X_3}b_{X_1}{}^{Y_1Z_{12}Z_{13}}c_{Z_{12}X_2}{}^{Y_2Z_{23}}d_{Z_{23}Z_{13}X_3}{}^{Y_3}\delta_{Y_1Y_2Y_3}{}^{Y}\ . \tag{A9}$$

The corresponding formulas for products of four, five, etc., operators can be derived in a similar fashion.

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