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Linked-cluster theorem in open shell coupled-cluster theory for mp-mh model space determinants

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Abstract. In this paper we have demonstrated the following aspects of the open-shell coupled cluster (CC) theory when the model space consists of *mp-mh* determinants: (i) If no other subsidiary conditions (besides the 'minimality' requirement $PSP = 0$) on the normalization of the wave functions are imposed, then the demand that the waveoperator admits of the core-valence separation of energy is inconsistent with the assumption of intermediate normalization. Thus all the discussions on the appearance of unlinked diagrams based on the implicit use of intermediate normalization are invalid. (ii) The open-shell CC developments of Mukherjee *et al* are independent of the normalization of the wavefunctions and the linked cluster theorems and the core-valence separation derived by them are valid for *mp-mh* model space functions. In particular it has been shown that there are two different cluster ansatz for which the aspect (ii) above is valid. For a valence-universal wave operator Ω admitting of a core-valence separation, it has been proved that the CC equations are linked as a consequence of the multicommutator nature of the expressions. There is a choice between two alternative schemes: one in which S operators connecting all the *kp-kh* determinants with $k < m$ and $k > m$ are retained, and another in which transitions for $k < m$ are ignored. For a normal ordered cluster ansatz for Ω, one has a linked expression if the subsystem embedding condition (SEC) is adhered to. Here coupling of all the *kp-kh* determinants to the model space has to be retained if we wish to decouple the various valence sectors of the Hilbert space.

Keywords. Many-body theory; open-shell theory; coupled-cluster theory.

1. Introduction

There has been extensive development of the open-shell coupled cluster theory over the last decade as a viable method for treating electron correlation, and it now appears that it may finally become competitive in its range of applicability with the configuration interaction technique without, however, the limitation of size-inconsistency (see e.g., Dykstra 1984). In so far as one may view the coupled-cluster (CC) approach as a complement of perturbation theory, involving summation of classes of terms up to infinite order, it seems worthwhile to analyse the efficacies of the coupled-cluster approach vis-a-vis the perturbation theory. Both the open-shell coupled cluster theory and the open-shell perturbation theory start with the partition of the N-electron Hilbert space into a model space (characterized by the projector P) and the virtual space complement (characterized by the projector Q), and develop expansion of a set of the exact eigenfunctions around starting functions in the model space. The coupling between the model space and the virtual space is taken care of in a nonperturbative or perturbative manner and the effect of the coupling is included through the modification

Dedicated to Professor Sadhan Basu on the occasion of his 65th birth anniversary.

of the Hamiltonian to generate an effective Hamiltonian H_{eff} which acts only on the model space and furnishes the exact eigenvalues. It is generally believed that one needs a 'complete' valence model space—amounting to inclusion of the determinants corresponding to all possible ways of allocating electrons in the valence orbitals, to prove the linked cluster theorem for energy. Thus, Brandow (1967) and Lindgren (1974) discuss the consequences of choosing a complete valence model space in generating the linked diagram expansion of energy in the framework of the open-shell perturbation theory. Lindgren (1978) and Jeziorski and Monkhorst (1981), base their proof of the linked cluster theorem in the context of open-shell coupled cluster theory quite essentially on a choice of complete valence model space. In contrast, the development of the coupled cluster theory of Mukherjee and coworkers (Mukherjee *et al* 1975, 1977a, b; Mukherjee 1979; Haque and Mukherjee 1984a) uses model spaces that are somewhat more general than those considered above and the proof of the linked-cluster theorem rests on either a hierarchical generation of the wave-operator for various m valence model spaces, starting at the zero valence level (called the 'subsystem embedding condition' (SEC) (Mukherjee, 1979; Haque and Mukherjee 1984a), or a Lie-algebraic structure of the CC equations, or a combination of both.

Recently Brandow (1983) pointed out that the linked-cluster theorem breaks down in the context of perturbation theory when there are both valence holes and valence particles in the model space and one intuitively takes the space spanned by all the *mp-nh* determinants with m valence particles and n valence holes as constituting the model space. For $m = n$, the situation is tricky: Brandow, in particular, discusses a disturbing situation where one takes all the *h-p* determinants in the model space and finds that there are unlinked terms in H_{eff} coming through a coupling of these determinants with the vacuum Φ_{HF} even at the second order. Thus the vacuum interacts with the model space functions and there is a breakdown of the apparently well-established 'core-valence separation' (Brandow 1967). Ways to overcome this difficulty within the framework of open-shell perturbation theory are (i) to use either incomplete model spaces (taking, for example, the function Φ_{HF} itself in the model space) as done by Haque and Mukherjee (1984b) or (ii) to use an expanded model space which involves determinants corresponding to all possible occupancies of *electrons* (rather than hole-particle occupancies) in the valence orbitals. In the choice (i), there are usually disconnected diagrams (Hose and Kaldor 1979, 1980; Haque and Mukherjee, 1984b) and the choice (ii) utilizes a very large model space which may be computationally cumbersome and is also potentially ill-conditioned because of the intruder state problem (Schucan and Weidenmüller 1972, 1973). This situation persists in the open-shell coupled cluster development of Lindgren (1978) and Jeziorski and Monkhorst (1981). The purpose of this paper is to show that this problem is nonexistent for the approaches of Mukherjee *et al* (1975, 1977a, b) and Haque and Mukherjee (1984a). In particular, we shall prove, utilizing two different cluster ansatze, that one can completely separate the calculation of the vacuum energy from the open-shell calculations in a linked manner, and there is always a core-valence separation, even in the case of *mh-mp* determinants as constituting the model space. Thus the energy differences form a linked series. The development is particularly simple when a valence-universal wave-operator of the form $\exp(S)$ is used for all the *mp-mh* sectors of the Hilbert space (Mukherjee *et al* 1975, 1977a, b). When a normal ordered ansatz $\{\exp(S)\}$ of the wave-operator is used, the situation is somewhat more subtle, and one may show that the intermediate normalization breaks down in this case, although H_{eff} is still

linked. It appears that the manipulations of the Bloch (1958) equation by Lindgren and Jeziorski and Monkhorst implicitly assumed the intermediate normalization condition even for the incomplete model space, and this is the reason behind their arriving at an unlinked series. In contrast, the treatment of Mukherjee and coworkers does not depend on this assumption, though it should be said in all fairness that this aspect had not been recognized by them earlier.

2. Core valence separation for model spaces containing valence holes and valence particles

2.1 *General consideration*

Let us assume that we have a set of model space functions comprised of the complete set of *mp-nh* determinants obtained by assigning m particle and n hole occupancies among the active particle and hole orbitals. As the Hamiltonian H does not conserve the number of hole or particle occupancies separately, this model space couples generally with all the other $m'p$-$n'h$ determinants satisfying the relation m-$n = m'$-n'. The additional complication for valence holes arises precisely due to the presence of this coupling.

In particular, when $m = n$, all the $m'p$-$m'h$ determinants are coupled together, *including the vacuum function* Φ_{HF} *itself* ($m' = 0$), and the demand of core-valence separation presupposes that the wave-operator Ω must contain all possible excitations out of Φ_{HF} itself quite independent of other operators. Thus we have the curious situation that an Ω satisfying core valence separation must have not only the regular excitations for *mp-mh* determinants in the model space to virtual space functions including Φ_{HF}, but also the *reverse* excitation from Φ_{HF} to the model space functions themselves. The combined effect of these two types of excitations will then, in general, lead to terms in Ω which cause scattering within the model space and the assumption of intermediate normalization breaks down! As, in the usual development of open-shell many body theories, the intermediate normalization convention is almost always made use of, many workers start out with expressions valid for intermediate normalization which ceases to be true when *mp-mh* determinants constitute the model space and conclude that there are unlinked terms in this case.

The starting point in all the developments of open-shell many-body theories is the so-called Bloch equation (Bloch 1958):

$$H\Omega P = \Omega H_{\text{eff}} P. \tag{1}$$

If intermediate normalization (i.e. $P\Omega P = P$) is assumed, then

$$QH\Omega P = Q\Omega P H_{\text{eff}} P \tag{2}$$

and

$$PH\Omega P = PH_{\text{eff}} P. \tag{3}$$

As the foregoing argument demonstrated, for *mp-mh* model space functions, the Ω satisfying core-valence separation does not satisfy $P\Omega P = P$, and, consequently, instead of (3) we have the expression

$$PH\Omega P = P\Omega P H_{\text{eff}} P. \tag{4}$$

We want to prove that with *mp-mh* determinants in the model space there are no unlinked terms in H_{eff} when (4) is used to generate H_{eff}. The unlinked terms discussed by Brandow (1983) originated from the use of (3) for H_{eff}.

Let us assume that we consider in addition to the functions in the model space, all other $m'p$-$n'h$ (with $m', n' \leqslant m$) functions as constituting lower valence rank model spaces. We want to consider all these model spaces simultaneously (Mukherjee *et al* 1977a, b; Haque and Mukherjee 1984a), because only by considering all these model spaces together can we get around the 'redundancy problem' associated with the cluster amplitudes of Ω (Mukherjee *et al* 1977a, b; Haque and Mukherjee 1984a; Pal *et al* 1984). According to Kutzelnigg (1982, 1984) and Kutzelnigg and Koch (1983) this is a 'Fock space formulation'. The core-valence separation will now be proved for two different choices of the cluster-ansatz for Ω. We shall show that there are two distinct ways of achieving this, each appropriate for one particular choice of Ω.

2.2 *Use of valence-universal Ω with core-valence separation*

We assume that our wave-operator Ω is of the form (Mukherjee *et al* 1977b; Mukhopadhyay *et al* 1979):

$$\Omega = \exp(T)\exp(S), \tag{5}$$

acting on the starting functions $\Psi_{0I}^{mp\text{-}mh}$, where T corresponds to the cluster-amplitudes of the vacuum problem:

$$\psi_{gr} = \exp(T)\Phi_{\text{HF}} \tag{6}$$

We also assume that these T amplitudes have been solved. The Schrödinger equation for the *mp-mh* model space problem may be written as

$$H\psi_I^{mp\text{-}mh} = E_I^{(m)}\ \Psi_I^{mp\text{-}mh} \tag{7}$$

Introducing the "dressed" Hamiltonian $\bar{H}$ through

$$\bar{H} = \exp(-T)H\exp(T) \tag{8}$$

and separating the ground state energy E_{gr} from $\bar{H}$ as

$$\bar{H} = \tilde{H} + E_{gr} = \tilde{H} + \langle \Phi_{\text{HF}} | \bar{H} | \Phi_{\text{HF}} \rangle, \tag{9}$$

we have

$$\begin{aligned} \tilde{H}\exp(S)\Psi_{0I}^{mp\text{-}mh} &= (E_I^{(m)} - E_{gr})\exp(S)\,\Psi_{0I}^{mp\text{-}mh} \\ &= (\Delta E_I^{(m)})\exp(S)\,\Psi_{0I}^{mp\text{-}mh} \end{aligned} \tag{10}$$

Thus, provided we are interested only in "energy differences' ΔE_I, core-valence separation is guaranteed through the multiple cluster ansatz (5) for Ω.

If we impose in addition the condition that Ω is valence-universal in the sense that it correlates also all the lower valence $m'p$-$n'h$ (with $m', n' < m$) sectors of the Hilbert space, then there is no redundancy problem, and we may solve for the S cluster-amplitudes by solving the set of equations

$$\langle \Phi_I^{kp\text{-}lh} | \exp(-S)\tilde{H}\exp(S) | \Phi_I^{m'p\text{-}n'h} \rangle = 0 \tag{11}$$

with

$$1 \leqslant m'n' \leqslant m \text{ and } 1 \leqslant k', l' \neq m'n' \leqslant m$$

Equation (11) clearly shows that for a particular model space characterized by m', other kp-kh determinants with $k \neq m'$ constitute the virtual space, so that each set of $m'p$-$m'h$ determinants acts both as virtual space functions and model space functions depending on what model space we have in mind. As the vacuum function is already decoupled from the rest of the functions through the condition

$$\langle \Phi_1^{kp\text{-}kh} | \tilde{H} | \Phi_{\mathrm{HF}} \rangle = 0 \quad \text{for all } k > 0, \tag{12}$$

the modified Schrödinger equation (10) guarantees that eigenvalues of $\tilde{H}$ may be obtained *without considering* Φ_{HF} in the Hilbert space. The multicommutator nature of the operator $\exp(-S)\tilde{H}\ \exp(S)$ appearing in (11) indicates that the equations determining the cluster amplitudes of S are linked. Also, by projecting on to functions $\Phi_j^{(m'p\text{-}m'h)}$ we have

$$\sum_j \langle \Phi_i^{m'p\text{-}m'h} | \exp(-S)\tilde{H} \exp(S) | \Phi_j^{m'p\text{-}m'h} \rangle C_{jl}^{m'} = \Delta E_l^{(m')} C_{il}^{(m')}, \tag{13}$$

where

$$\Psi_{0l}^{m'p\text{-}m'h} = \sum_j \Phi_j^{m'p\text{-}m'h} C_{jl}^{(m')}. \tag{14}$$

The results discussed above are formally exact, but for connectivity some other additional considerations have been found to be fruitful. Thus, for a transition from a $\Phi_i^{m'p\text{-}m'h}$ to another $\Phi_j^{kp\text{-}kh}$ which involves an *odd* number of 'spectator valence lines', it becomes necessary to introduce S amplitudes corresponding to excitations from $(N \pm 1)$-electron determinants as well, where N corresponds to number of electrons in Φ_{HF}. For example, for an excitation of the types $\alpha p \rightarrow \alpha\beta rs$ ($\alpha,\beta \in_{\mathrm{HF}}$; $p, q, r, s \notin_{\mathrm{HF}}$), (11) will look like

$$G_{\alpha p}^{\alpha\beta rs} + G_p^{\beta rs} = 0 \tag{15}$$

where $G_p^{\alpha\beta rs}$ consists of all the connected diagrams involving all the outgoing lines ($\alpha\beta rs$) and incoming lines (αp) in the scattering process, and $G_p^{\beta rs}$ contains all the diagrams in which the open line α does not figure at all. Clearly, if we include in S, operators of the form $\langle rs|s|p\beta \rangle \{a_r^+ a_s^+ a_\beta a_p\}$ (with $\{\ \}$ as normal ordering) corresponding to shake-up operators for $(N+1)$-electron model spaces $a_p^+ \Phi_{\mathrm{HF}}$, and demand that $G_p^{prs} = 0$ separately, then electron affinities can also be simultaneously obtained with excitation energies. Symmetrically, if all operators of the form $\langle \alpha\beta|s|\gamma p \rangle \{a_\alpha^+ a_\beta^+ a_p a_\gamma\}$ are also included, then ionization potentials may also be obtained. In that case, for practical purposes, one may use the approximation that higher rank S operators with spectator lines are zero, as for example the operator $\langle \alpha rs|s|\alpha p\beta \rangle \{a_\alpha^+ a_r^+ a_s^+ a_\beta a_p a_\alpha\}$, and omit the $G_{\alpha p}^{\alpha\beta rs}$ term altogether in (15). In other words, we may use a truncation scheme where S amplitudes for $(N+1)$-electron problems are used to simulate scattering processes for N-electron problems having a greater number of spectator labels through product operator of the form $(1/n!)S^n$ arising from Ω. Pilot numerical applications of the theory for mp-mh model spaces utilized this version (Mukhopadhyay *et al* 1979), where there are three sets of model space functions (a) $0p$-$1h$ determinants $\{a_{\alpha\ \mathrm{HF}}\}$; (b) $1p$-$0h$ determinants $\{a_p^+ \Phi_{\mathrm{HF}}\}$ and $1p$-$1h$ determinants $\{a_p^+ a_\alpha \Phi_{\mathrm{HF}}\}$, so that $m = 1$.

For model spaces involving $2p$-$2h$ determinants etc., i.e. $m > 1$, the above procedure may be modified leading to a drastic reduction in the number of amplitudes to be used. Denoting by $p^{(m')}$ the projector for the $m'p$-$m'h$ determinantal model space, the

transformation (11) indicates that H_{eff} has the following structure:

$$P^{(k)} H_{\text{eff}} P^{(m')} = 0 \text{ for } k \neq m'. \tag{16}$$

Thus H_{eff} is block-diagonal for both $k < m'$ and $k > m'$. This complete block-diagonal form is, however, not essential to guarantee that $\Delta E_I^{(m')}$'s are the corresponding energy differences. A simpler, but equivalent, condition can be that

$$P^{(k)} H_{\text{eff}} P^{(m')} = 0 \text{ for } k > m' \tag{17}$$

which gives H_{eff} in a form that is block-diagonal only along the lower part of the diagonal. Equation (17) implies that we need not include in our S operator excitations out of the $m'p$-$m'h$ model space to lower valence kp-kh model spaces $k < m'$, but then we have a fewer number of equations like (11) with conditions $1 \leqslant m' \leqslant m$ and $k > m'$. We note, however, that Ω is then not a wave-operator because it furnishes energies and not wave-functions.

2.3 *Use of Ω in normal order*

We now consider the other form of Ω, which is written in normal order. Lindgren (1978) developed his version of the open-shell CC theory using this ansatz for the complete model spaces involving valence particles only. As Lindgren's coupled-cluster equations are well-defined only when one assumes that the same Ω correlates all the lower valence sectors of the Hilbert space (Haque and Mukherjee 1984a; Haque and Mukherjee, to be published), a situation similar to the one considered in §2.2 holds good for a normal ordered ansatz for Ω involving valence holes and valence particles. Clearly, to maintain the core-valence separation for mp-mh model space determinants we should include in Ω operators inducing excitation from Φ_{HF}, and as this spells a break-down of the intermediate normalization, Lindgren's working equation will be invalid (compare the discussion of the corresponding perturbative situation by Brandow 1983). Mukherjee (1979) and Haque and Mukherjee (1984a) discussed an alternative mode of development where intermediate normalization is not used, but instead of solving (2) and (3), one solves

$$Q\Omega^{-1} H \Omega P = 0 \tag{18}$$

and

$$\Omega P^{-1} H \Omega P = P H_{\text{eff}} P. \tag{19}$$

Clearly, (19) is valid independent of the normalization of Ω. Using the condition that Ω correlates all the $m'p$-$m'h$ sectors of the Hilbert space, and also that Ω involves amplitudes corresponding to excitations from $(N \pm 1)$-electron determinants (similar to what was done in §2.2), one may show (Mukherjee 1979; Haque and Mukherjee 1984a) that we have equations

$$Q^{(M)}[\Omega^{(M)^{-1}} \tilde{H} \Omega^{(M)}] P^{(M)} = 0, \text{ for all } M, \tag{20}$$

and

$$P^{(M)}[\Omega(M)^{-1} \tilde{H} \Omega^{(M)}] P^{(M)} = P^{(M)} H_{\text{eff}}^{(M)} P^{(M)}, \tag{21}$$

where $\Omega^{(M)}$ is defined by

$$\Omega^{(M)} P^{(M)} = \Omega P^{(M)}, \tag{22}$$

and diagonalization of $H_{\text{eff}}^{(M)}$ in the M valence model space furnishes the energy differences $\Delta E_I^{(M)}$. The valence rank M is defined by all the possible $n'p$-$m'h$ model space functions with $n' = (m' \pm 1)$, and m' etc.

The disadvantage with the normal ordered ansatz is that there is no multi-commutator Hausdorff expansion, so that the linked cluster theorem has to be proved in a much more involved manner. The advantage is that the form of Ω is more compact than the ordinary exponential. For model spaces not containing valence holes, this automatically leads to the decoupling of the equations for S amplitudes for various M valence sectors of the Hilbert space (Haque and Mukherjee 1984a). If such a procedure is applied for $m'p$-$m'h$ model space determinants, then it follows from (20) that we introduce various different transformations to $\tilde{H}$ for getting $H_{\text{eff}}^{(M)}$'s, unlike a single transformation, (11) as in §2.2. Thus, the simplification afforded by modified conditions (16) and (17) are not possible. This is compensated for by the decoupling of the equations for cluster amplitudes for $n'p$-$m'h$ model spaces with $n' = m' \pm 1$, and m'. This procedure has been followed to generate ionization potential, electron affinity and excitation energy for prototypal π-electron systems by Haque and Mukherjee (1984a).

An alternative procedure, which avoids introduction of scattering amplitudes from $m'p$-$m'h$ model spaces to the kp-kh determinants with $k < m'$ is to use a single transformation

$$Q^{(M)}\Omega^{-1}\tilde{H}\Omega P^{(M)} = Q^{(M)}\Omega^{-1}\tilde{H}^{(M)}P^{(M)} = 0, \tag{23}$$

rather than (20). This, however, will *couple* the various M-valence sectors in general and one of the advantages of using the normal order ansatz will be lost.

2.4 *SEC And Lindgren's cc equation for mp-mh model spaces*

It is instructive to indicate here how SEC can be invoked to generate a linked diagram expansion for energy in Lindgren's formalism in the case of *mp-mh* model spaces. This will demonstrate two things: (a) the modification necessary to arrive at the linked cluster theorem when valence holes are present and (b) the decoupling between the various $n'p$-$m'h$ sectors through SEC, which is essential for arriving at a connected series for H_{eff}.

We start out from (1), and find generally, using the normal ordered ansatz that

$$Q\{\overbrace{H\Omega\Omega}\} P = Q\{\Omega\overbrace{\Omega H_{\text{eff}}}\} P. \tag{24}$$

If we consider a particular M valence sector, then it follows that

$$Q^{(M)}\{\overbrace{H\Omega\Omega}\}_M P^{(M)} = Q^{(M)}\{\Omega\overbrace{\Omega H_{\text{eff}}}\}_M P^{(M)}, \tag{25}$$

where $\{\ \}$ denotes normal ordering and $\{\ \}_M$ denotes that the total valence rank of the operator is M. Equation (25) implies that

$$\sum_{i=0}^{M} Q^{(M)}\{(\overbrace{H\Omega})_{M-i}\Omega_i\}_M P^{(M)} = \sum_{i=0}^{M} Q^{(M)}\{\Omega_i(\overbrace{\Omega H_{\text{eff}}})_{M-i}\}_M P^{(M)}, \tag{26}$$

where Ω_i is the i-valence part of Ω. If we invoke SEC, and demand that

$$(\overbrace{H\Omega})_{M-i} = (\overbrace{\Omega H_{\text{eff}}})_{M-i}, \tag{27}$$

then it follows that

$$(\overbrace{H\Omega})_{M'} = (\overbrace{\Omega H_{\text{eff}}})_{M'}, \text{ for all } M' \leqslant M. \tag{28}$$

Clearly, to satisfy this for all $M' \leqslant M$, we must have S operators which induce transitions from all the M' model spaces to the corresponding virtual spaces. Thus, when M corresponds to *mp-mh* model spaces, all other *kp-kh* determinants with $k < m$ and $k > m$ are part of virtual spaces, and all such transitions must be incorporated to have connected equations like (28). The various M' valence sectors are necessarily decoupled, however, and (28) is equivalent to (20) derived by Haque and Mukherjee (1984a). Again, as Ω involves excitations from one *m'p-m'h* space to another *kp-kh* space and vice-versa, $P\Omega P \neq P$, and instead of (3), we have an analogue of (4):

$$P^{(M)}\{\overbrace{H\Omega\Omega}\}_M P^{(M)} = P^{(M)}\{\Omega\Omega\overbrace{H_{\text{eff}}}\}_M P^{(M)}. \tag{29}$$

Using SEC, we show quite generally that

$$P^{(M')}\{\overbrace{H\Omega}\}_{M'} P^{(M')} = P^{(M')}\{H_{\text{eff}}\}_{M'} P^{(M')} + P^{(M')}\{\overbrace{\Omega' H_{\text{eff}}}\}_{M'} P^{(M)},$$
$$\text{for all } M' \leqslant M \tag{30}$$

and the linked nature of $\{H_{\text{eff}}\}_{M'}$ can be proved by iteration. Here $\Omega' = 1-\Omega$.

3. Summary of the main results and concluding remarks

In this paper, we have shown the following things: (a) the demand that one has core-valence separation when the model space functions are a complete set of *mp-mh* determinants is incompatible with the intermediate normalization conditions unless other extra constraints are imposed, so that discussions of the linked nature of H_{eff} based on expressions derived using tacit assumption of intermediate normalization are invalid; (b) the open-shell coupled cluster theories developed by Mukherjee *et al* are independent of the normalization of the wave-functions and the linked cluster theorems derived by them are valid even for *mp-mh* model space determinants; (c) using a valence-universal wave-operator Ω admitting of the core-valence separation, it has been shown that coupled-cluster equations can be written down which are automatically linked because of the Hausdorff formula; there is a choice between two alternative schemes: (i) one in which S amplitudes connecting all the *kp-kh* determinants with *m'p-m'h* determinants with $k \neq m'$ are taken and (ii) the S amplitudes for $k < m'$ are ignored; (d) using a normal ordered cluster ansatz for Ω and SEC, connected expressions for S determining equations and H_{eff} are obtained; if one insists on a decoupling of the various M valence sectors, then coupling of *all kp-kh* determinants with $k < m'$ and $k > m'$ are essential.

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Adjoinder

Lindgren has recently developed a cc-theory for a class of restricted model spaces (Lindgren 1985a). A closer look at his formulation, however, reveals that it will involve disconnected diagrams when valence holes are present and when spectator lines are not used to define the cluster-amplitudes (Lindgren 1985b). It can again be shown that the disconnected diagrams do not appear if an intermediate normalization condition is not used.

The strategy that one can use for a general incomplete model space is the following: (1) We define an m-valence incomplete model space with projector $P^{(m)}$ as consisting of m-valence determinants which are somewhat separated energetically from the other determinants constituting the virtual space $Q^{(m)}$; (2) We introduce m-valence operators $\tilde{S}^{(m)}$ which causes transitions from $P^{(m)}$ to $Q^{(m)}$ space; (3) We invoke *SEC and demand that the wave-operator* $\Omega = \{\exp(\tilde{S})\}$ correlates all the lower valence model spaces as well. These lower k-valence model spaces ($0 \leqslant k < m$) are spanned by k-valence determinants obtained by deleting $(m-k)$-valence lines from the m-valence model space functions. (4) We introduce $\tilde{S}^{(k)}$ operators obtained by deleting $(m-k)$ spectator valence lines from $\tilde{S}^{(m)}$ systematically. They are of two kinds: the set $\tilde{S}^{(k)}_{\text{op}}$ causes transitions from $P^{(k)}$ to $Q^{(k)}$; the set $\tilde{S}^{(k)}_{\text{cl}}$cause transitions within $P^{(k)}$. The $\tilde{S}^{(k)}_{\text{op}}$ amplitudes are determined from the conditions that $Q^{(k)} H^{(k)}_{\text{eff}} P^{(k)} = 0$, which also determines $\tilde{S}^{(m)} = \tilde{S}^{(m)}_{\text{op}}$; the $\tilde{S}^{(k)}_{\text{cl}}$are determined from the condition that the corresponding $P^{(k)} - P^{(k)}$ matrix-elements of H_{eff}, for which $\tilde{S}^{(k)}_{\text{cl}}$'s exist, are zero. As there are operators causing transitions within the model space, Ω does not support intermediate normalization. More detailed analysis will appear in forthcoming publications (Mukherjee 1986; Mukherjee *et al* 1986).

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