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A variational coupled cluster theory for closed shells using a propagator modification procedure

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A general partial summation method for including arbitrary classes of diagrams to all orders in the coupled cluster based size consistent energy functional for closed shell states is developed. Since the various reduced density matrices which appear in the energy functional are essentially the time-independent analogues of the corresponding many body Green functions, it is possible to derive Dyson-like equations for these quantities. By expanding the associated "proper" self energy parts in terms of the T-amplitudes, one can carry out partial summations in the reduced density matrices and thus in energy. At a higher level, higher order terms in a "proper" self energy can also be generated by renormalizing the internal propagators in it, and considering only the "*irreducible*" self-energy terms.

Key words: Many body theory — Coupled cluster theory — Propagators

1. Introduction

Our understanding of the role of electron correlation in many-electron systems has evolved in rapid strides over the past two decades. As a consequence, the importance of treating electron correlation in a compact and tractable manner is now increasingly being felt. One has now come to believe that a cluster

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expansion representation of a many-electron wave-function possesses the potentiality of describing electron correlation in a manner superior to what is achieved in a linear variation method as in a CI or a simple, order by order, perturbation theory.

The Ursell-Meyer exponential cluster expansion ansatz for a closed-shell many-fermion ground state was first used in nuclear physics by Coester and Kummel [1], and it was later successfully transcribed to atomic and molecular physics by Čižek and Paldus [2] and others [3]. The importance of such an exponential ansatz was also noted by Primas [4] who emphasized the usefulness of this ansatz to guarantee the size-consistency of the extensive properties like energy. This aspect has received its due importance in recent years [5, 6]. Since this initiation, the coupled cluster method has been extensively utilized for treating ground state electron correlation energy and describing the geometries of potential surfaces [5–7].

In the closed-shell coupled cluster development, the ground state wave-function Ψ_{gr} is written as a cluster expansion around the Hartree-Fock (H-F) reference function as

$$|\Psi_{gr}\rangle = \exp(T)|\Phi_{HF}\rangle. \tag{1}$$

It has been noted by several authors [1–3, 6–8] that the desired property of preserving size-consistency of energy stems essentially from the non-variational formulation of the theory: the energy is calculated from an expression

$$E_{gr} = \langle\Phi_{HF}|\exp(-T)H\exp(T)|\Phi_{HF}\rangle \tag{2}$$

which generally differs from the ground state expectation value formula

$$E_{gr} = \frac{\langle\Psi_{gr}|H|\Psi_{gr}\rangle}{\langle\Psi_{gr}|\Psi_{gr}\rangle} = \frac{\langle\Phi_{HF}|\exp(T^{+})H\exp(T)|\Phi_{HF}\rangle}{\langle\Phi_{HF}|\exp(T^{+})\exp(T)|\Phi_{HF}\rangle} \tag{3}$$

unless the exact ground state is used for calculating E_{gr}. Eq. (2) involves an operator $\tilde{H} = \exp(-T)H\exp(T)$ which contains connected terms only, as guaranteed by the Hausdorff formula involving multicommutator expansion of $\tilde{H}$. This property is retained even if the series is truncated. In contrast, Eq. (3) involves a ratio of numerator and denominator, none of which is connected in general, and hence the size-consistency cannot be maintained in a truncated expansion. In special cases of the choice of the exponential cluster operator, the definitions Eqs. (2) and (3) agree, as for example when a unitary cluster operator of an exponential form is chosen, much in the same spirit as the Van Vleck-Kemble transformation [9]. Thus, for example, Kutzelnigg [8] has advocated the use of the following unitary operator W_u:

$$W_u = \exp(\sigma) \tag{4}$$

with

$$\sigma = T - T^{+} \tag{5}$$

where T involves hole-particle excitations only. As $\sigma^+ = -\sigma$, the formulae Eqs. (2) and (3) agree, the denominator in Eq. (3) becomes unity and the numerator coincides with the expression of Eq. (2). A less trivial case of a size-consistent energy functional using the original nonunitary cluster ansatz exp (T) was recently studied by us for closed-shell systems [10] where the numerator in Eq. (3) was shown to factorize into a connected series involving connected operators with T, T^+ and H contracted together and the denominator itself. With the cancellation of the denominator, the resulting expression becomes size-consistent, and this property is retained even in a truncated expression

$$E_{gr} = \langle \Phi_{\mathrm{HF}} | \exp(T^+) H \exp(T) | \Phi_{\mathrm{HF}} \rangle_{conn}. \tag{6}$$

The cluster amplitudes are then determined by invoking a Euler-type variational principle for E_{gr} and solving the resultant Euler equations. The unitary and the nonunitary approaches to variational theories of electron correlations have also been generalized recently to encompass open-shell states [11, 12].

For practical applications, the connected infinite series in Eq. (6) involving the cluster amplitudes of T has to be truncated to a finite power. The strict upper bound property of E_{gr} is thereby lost. The variational principle for solving the cluster amplitudes is then more akin in spirit to the "Varied Portion Approach" (VPA) of Sinanoğlu [13] than a Rayleigh-Ritz variational principle. The loss of the upper bound property as a result of truncation in cluster expansion in nuclear matter calculations is known as the "Emery Difficulty" [14]. However, if the dominant terms in the expansion in Eq. (6) are retained, this difficulty will not be severe, as has been demonstrated by us in model calculations [10]. Nevertheless one feels that one ought to have a general method of summing up at least the physically important terms to infinite order. This will improve the results and the loss of upper bound property will also be annulled, making the results approach the corresponding variational bound.

With this motivation in mind, we would like to investigate in this paper a method which has the potentiality of summing up general classes of terms involving T^+/T amplitudes to all orders. The basic idea behind our approach can be succinctly summarized as follows. The energy series in Eq. (6) can always be written as

$$E_{gr} = E_{\mathrm{HF}} + \mathrm{Tr}\, f\rho_1^C + \mathrm{Tr}\, v\rho_2^C \tag{7}$$

where f and v stand for the matrices of the H-F operator and the two-body interaction in the H-F orbital basis, and ρ_1^C and ρ_2^C are the correlation corrections to the one- and two-electron reduced density matrices respectively. ρ_1^C and ρ_2^C are both infinite series in T/T^+ cluster amplitudes, so that what we are after is to find out a general scheme of summing the infinite series for ρ_1^C and ρ_2^C in the cluster amplitudes. This will be achieved by a procedure conceptually analogous to the propagator renormalization method [15] of Green function theory - as applied to the many body perturbation theory for the ground state [16, 17]. That such a procedure will be useful is not entirely unanticipated, because the reduced density matrices are nothing but the time-independent analogues of the appropriate Green functions.

Once we identify certain basic terms as dominant in E_{gr}, their repeated appearances in the energy series are taken care of to all orders by solving certain implicit equations having renormalized Dyson equation-like structure. Just as in the case of propagator renormalization, the methodology and the practical manipulations in this procedure are best described in terms of Green function terminology, using a diagrammatic language, which we shall introduce in Sect. 2. In Sect. 3 we shall make certain pertinent observations regarding important terms in the ground state correlation problems and include the relevant discussions. In Sect. 4 we shall introduce the concept of irreducible self-energy insertions to compactify the development. In Sect. 5 we summarize the main features of our theory.

2. Use of modified propagators in a variational coupled cluster method

In what follows, we shall describe the development of our method in terms of the concrete approximations pertinent to the closed shell situation. Generalization of our method to incorporate the terms left out of our consideration is fairly straightforward.

Following Čižek and others [2, 3], we only retain the two-body cluster operator T_2 in T, corresponding to the retention of pair and higher order pair interactions. Collecting all the T^+/T amplitudes in rows/columns t^+/t, the infinite series in Eq. (6) may be written as [10]

$$E_{gr} = E_{\mathrm{HF}} + \sum_{\substack{m,n \\ m+n=1,\infty}} [t^+ \otimes t^+ \otimes \cdots m \text{ terms } A^{m,n} t \otimes t \otimes \cdots n \text{ terms}] \tag{8}$$

where $A^{m,n}$ is the matrix of coefficients associated with m-th and n-th total power of T^+ and T amplitudes respectively. $A^{m,n}$ involves matrix-elements of f and v. Comparing Eq. (8) with Eq. (7), we observe that for the f-containing terms of $A^{m,n}$, the series in t^+ and t constitute ρ_1^C and, similarly, the v containing terms, the t^+/t series constitute ρ_2^C. Diagrammatically, Eq. (7) (or the whole series, Eq. (8)) may be represented as shown in Fig. 1. The hatched portion of each diagram represents the part of ρ_1^C or ρ_2^C, as the case may be, and the vertices with a circle with two or four lines represent the f or v matrix-element. As concrete examples, the lowest order terms for each of the shapes of ρ_1^C and ρ_2^C are shown in Fig. 2 with $T = T_2$ approximation. The vertices with filled circles and squares stand for

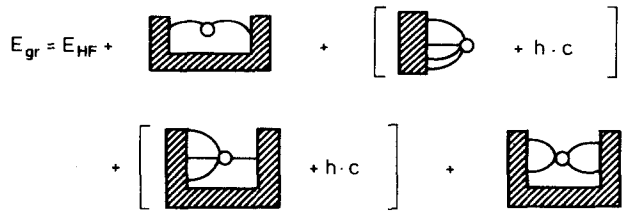

Fig. 1. Diagrammatic representation of Eq. (7). The hatched portion of each diagram represents the concerned reduced density matrices ρ_1^C and ρ_2^C. Open circles represent the Hamiltonian

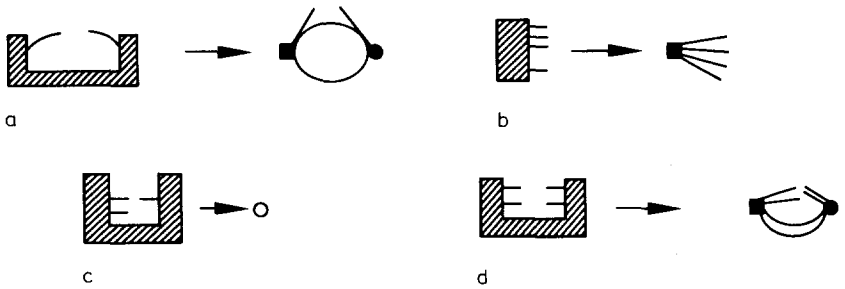

Fig. 2. Diagrammatic representation of some typical terms in ρ_1^C (a) and ρ_2^C (b-d) in the pair ($T = T_2$) approximation. Note that the (*pp, ph*) matrix elements of ρ_2^C (c) are identically zero in this approximation. Filled squares and circles represent T^+ and T vertices respectively

the T and T^+ amplitudes respectively. The higher order terms contributing the various shapes of ρ_1^C and ρ_2^C are obtained by dissecting one or more lines of the lowest order diagram for each shape and attaching an appropriate composite skeleton having as many open lines obtained from T^+/T contractions. As an example, consider a higher order term contributing to the ρ_1^C diagram, Fig. 2a. In Fig. 3a we have traced its genesis from Eq. (7) and have shown that by suitably

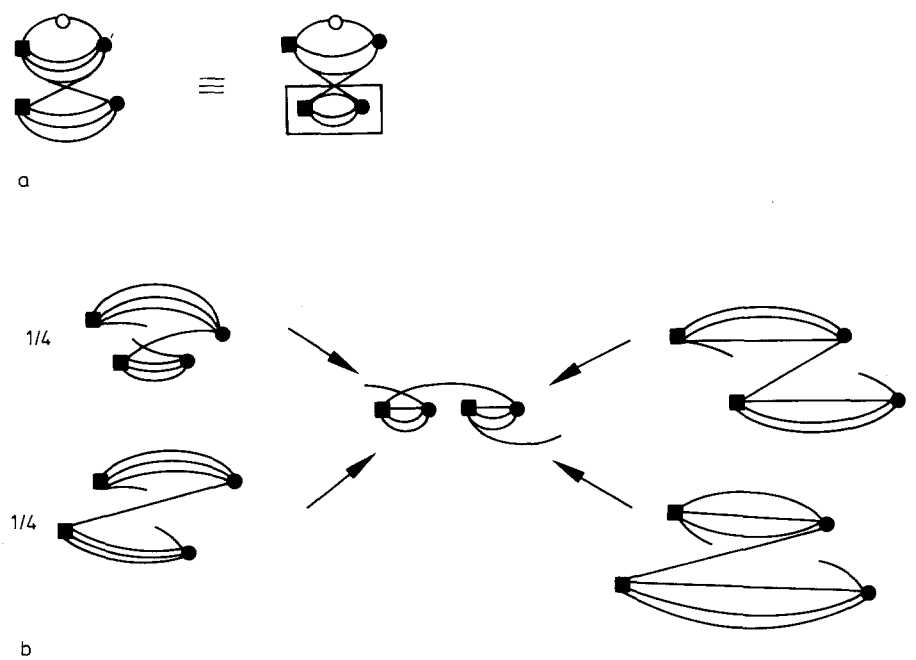

Fig. 3. Higher order terms of ρ_1^C and ρ_2^C can be generated by skeletal insertions on the lines of basic diagrams of lower order. The generation of such a fourth order term of ρ_1^C is depicted in (a). Various possible orderings of T and T^+ vertices will sum up to cancel the weight factor of such terms. This is illustrated in (b)

juggling the components of the energy diagram, we can make it look like an insertion on a single line to the lowest order diagram of ρ_1^C. The portion inserted is shown inside a box. Clearly, a repeated insertion of the skeleton of the box onto a single line is going to generate an infinite series. It is easy to show, that for n such insertions on a line, there are $n!^2$ ways of keeping the inserted T^+/T vertices with respect to each other in various ways. The weight of any insertion for a particular term is $1/n!^2$, each $1/n!$ coming from the exponential on either side of H in Eq. (6). These diagrams are all topologically equivalent, so that it suffices to stretch all the diagrams to make them look like successive insertions and consider only one of them and multiply by a factor $n!^2$ to take care of all of them. The overall contribution of n insertions on a line is thus effectively only one insertion without additional weights. This aspect is illustrated diagrammatically in Fig. 3b for $n=2$. Thus, if we look upon the successive insertions of the skeleton of the box of Fig. 3a as a kind of propagator modification of a particular internal line of the lowest order diagram Fig. 2a, then we may include the effect of the successive insertions by redefining the value of the contraction corresponding to a single internal line through evaluating a series of the form

$$\nu_{1ii'} = \nu^0_{1ii'} + \sum_{jk} \nu^0_{1ij} x_{jk} \nu^0_{1ki'} + \sum_{jklm} \nu^0_{1ij} x_{jk} \nu^0_{1kl} x_{lm} \nu^0_{1mi'} + \cdots \tag{9}$$

where $\nu_{1ii'}$ is the modified value of the contraction and $\nu^0_{1ii'}$ etc. are unmodified values of the contraction. x_{ij} etc. the contributions from a single insertion. Clearly, using time independent Wick's theorem, we have

$$\nu^0_{1ij} = (\text{sign})\delta_{ij} \tag{10}$$

where sign $= \pm 1$ for particles/holes. For all the choice of orbital labels, we have the matrix equation

$$\boldsymbol{\nu}_1 = \boldsymbol{\nu}^0_1 + \boldsymbol{\nu}^0_1 \mathbf{x} \boldsymbol{\nu}^0_1 + \boldsymbol{\nu}^0_1 \mathbf{x} \boldsymbol{\nu}^0_1 \mathbf{x} \boldsymbol{\nu}^0_1 + \cdots = \nu^0_1 + \nu^0_1 \boldsymbol{x} \nu_1. \tag{11}$$

Equation (11) is an implicit equation in ν_1, and is strongly reminiscent of the Dyson equation of Green function theory [15, 18]. If we depict the single line contractions ν_1 by heavy lines and ν^0_1 by thin lines, then all the single insertions of Fig. 2a will be automatically accounted for if we replace the thin lines by heavy lines. This is illustrated in Fig. 4a. The corresponding single line modifications on Figs. 2b, d, etc. will likewise sum similar single line insertions to all orders. Modification of 2a will improve ρ_1^C, those of 2b and 2d will improve ρ_2^C. As an example of ρ_2^C modification, the type of terms generated by single line modification Fig. 2b are shown in Fig. 4b.

Before proceeding further it seems appropriate here to introduce the terminology used extensively in the Green function literature to classify the various diagrams – both the lowest order terms and the ones with insertions. The insertions we introduce will be called self energy insertions from now on. If they are one-body operators, we call such insertions one body self energy. We shall call an n-body self energy insertion a proper n-body self energy if the insertion cannot be disconnected by cutting just n internal lines. Thus, the insertion in the box of Fig. 3a is a proper self-energy, while all those in the multiple insertions (as for

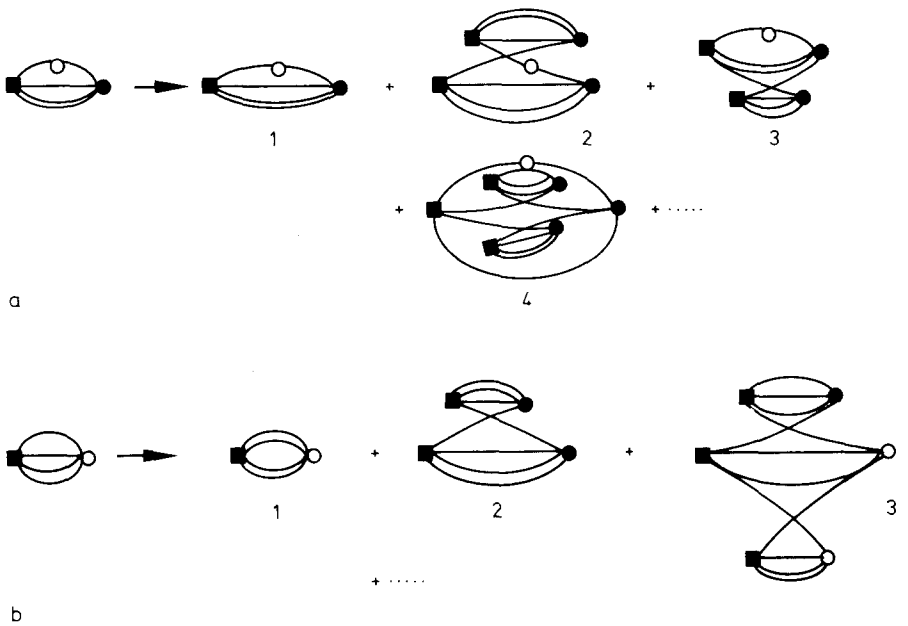

Fig. 4. (a) Terms in the energy series summed by renormalizing the internal contractions (ν_1). Heavy and light lines represent renormalized and bare contractions respectively. Filled squares and circles represent T^+ and T vertices respectively and Hamiltonian is represented by open circle. (b) Terms summed up by renormalizing ν_2 in the energy series. Diagrammatic notation is as before

example in Figs. 3b) are not. Calling contributions of all the proper self-energies as Σ_1, the exact single particle contraction ν_1^{ex} may be written as

$$\boldsymbol{\nu}_1^{ex} = \boldsymbol{\nu}_1^0 + \boldsymbol{\nu}_1^0 \boldsymbol{\Sigma}_1 \boldsymbol{\nu}_1^{ex}. \tag{12}$$

Some examples of higher order $\boldsymbol{\Sigma}_1$ diagrams are shown in Fig. 5. The paper self energy of Fig. 2a is the lowest order term of $\boldsymbol{\Sigma}_1$.

We are now in a position to concretely describe the procedure we are going to advocate for incorporating classes of diagrams to all orders, once the important classes are identified. We first look for the lowest order diagram, insertions onto

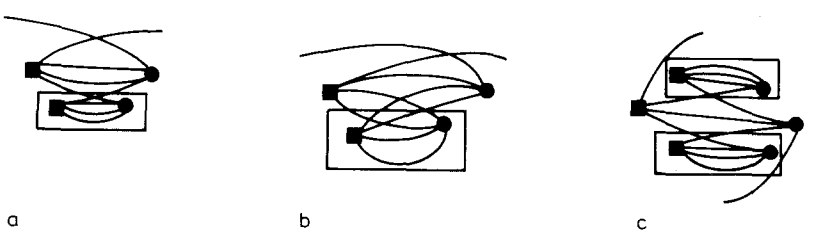

Fig. 5. Some higher order terms of the proper self energy part Σ_1. The parts enclosed in the box are skeletal insertions onto a basic skeleton and can be generated by renormalizing ν_1 and ν_2 within Σ_1

the external lines of which will generate the terms deemed as important. We then classify the insertions as various n-body self energy insertions and pick out from them only the proper n-body self-energy skeletons. If we agree to keep up to m-body self energy terms then calling the collection of all the m-body self energy skeletons as $\mathbf{\Sigma}_m$, the modifications of a bunch of m-internal line contractions may be written as

$$\boldsymbol{\nu}_m^{ex} = \boldsymbol{\nu}_m^0 + \boldsymbol{\nu}_m^0 \mathbf{\Sigma}_m \boldsymbol{\nu}_m^{ex} \tag{13}$$

where $\boldsymbol{\nu}_m^0$ is an appropriate product of functions of the lower rank $\boldsymbol{\nu}_k$'s defined recursively:

$$\boldsymbol{\nu}_2^0 = \boldsymbol{\nu}_1 \otimes \boldsymbol{\nu}_1 \tag{14a}$$

$$\boldsymbol{\nu}_3^0 = \boldsymbol{\nu}_1 \otimes \boldsymbol{\nu}_1 \otimes \boldsymbol{\nu}_1 + \boldsymbol{\nu}_1 \otimes \boldsymbol{\nu}_2^0 \mathbf{\Sigma}_2 \boldsymbol{\nu}_2 \tag{14b}$$

and so on. Clearly $\boldsymbol{\nu}_m^{ex}$ satisfies an implicit equation analogous to Bethe–Salpeter equation of Green function theory [18].

We illustrate this procedure by taking $m = 2$. We first identify the one body proper self energies contributing to $\mathbf{\Sigma}_1$ and evaluate $\boldsymbol{\nu}_1^{ex}$ from Eq. (12). Next we identify the proper two-body self energy insertions and call them $\mathbf{\Sigma}_2$. The modification of a bunch of two internal lines may then be evaluated by solving Eq. (13) for $m = 2$. The procedure becomes clear from the Fig. 6. Some illustrative diagrams of $\mathbf{\Sigma}_2$ are shown in Fig. 7.

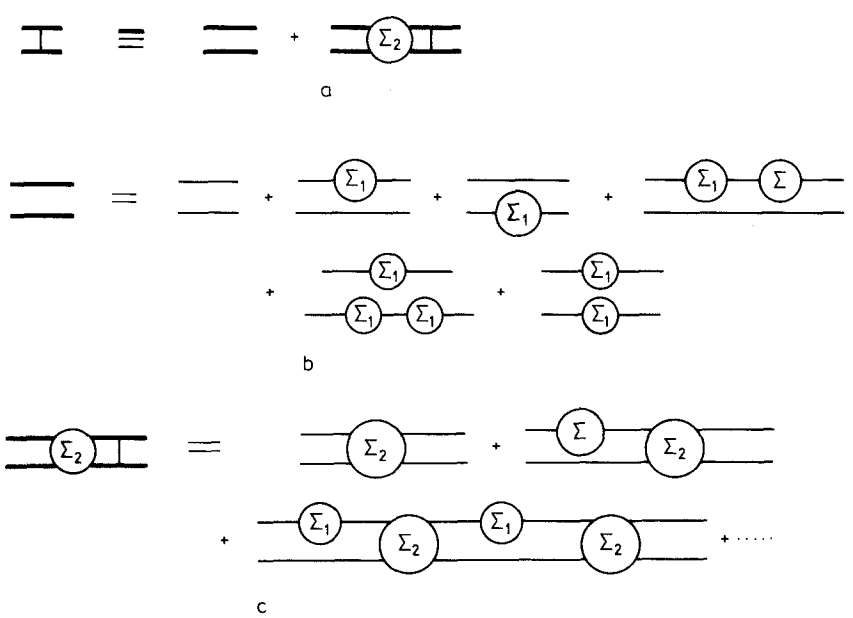

Fig. 6. (a) Diagrammatic representation of Eq. (13). Heavy and light lines represent the renormalized and bare ν_1 lines. (b) Since renormalized ν_1 is used to define ν_2^0 it consists of the infinite series shown here. (c) The full series for ν_2

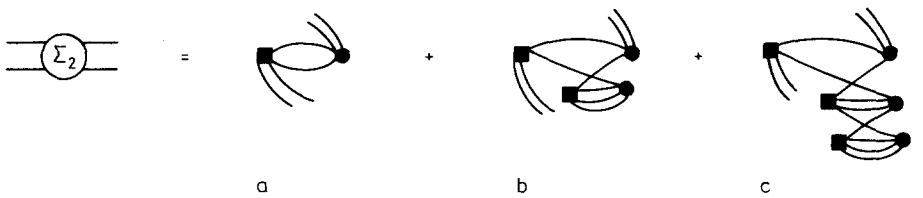

Fig. 7. Diagrammatic representation of some of the low order terms in Σ_2. Diagrammatic notation is as before

3. The one- and two-body Σ insertions for the closed shell problem

As a concrete application of the procedure described above, we now enumerate certain representative and important diagrams of Eq. (6) yielding E_{gr}, and demonstrate by working out the appropriate equations how the scheme should be carried out in practice.

We consider first the one-body insertions, and assume that only the lowest order term in $\boldsymbol{\Sigma}_1$, viz that of Fig. 2a is the important one. In that case Eq. (12) with $\boldsymbol{\Sigma}_1$ approximated as $\tilde{\boldsymbol{\Sigma}}_1$ corresponding to Fig. 2a will yield an approximate $\boldsymbol{\nu}_1$. Evaluating the value of the insertion using standard diagram rules, we find using Eq. (12)

$$\nu_{1\alpha\beta} = [\boldsymbol{\nu}_1^0 - \tilde{\boldsymbol{\Sigma}}_1]^{-1}_{\alpha\beta} \tag{15a}$$

$$\nu_{1pq} = [\boldsymbol{\nu}_1^0 - \tilde{\boldsymbol{\Sigma}}_1]^{-1}_{pq} \tag{15b}$$

for hole labels $\alpha, \beta, \ldots$ and particle labels p, q, etc. $\boldsymbol{\nu}_0$ is defined in Eq. (10). $\tilde{\boldsymbol{\Sigma}}_{\alpha\beta}$ and $\tilde{\boldsymbol{\Sigma}}_{pq}$ are given by

$$\tilde{\boldsymbol{\Sigma}}_{\alpha\beta} = \tfrac{1}{4} \sum_{\sigma pq\gamma} \{pq|t|\gamma\beta\}_\sigma \{pq|t|\gamma\alpha\}_\sigma (2\sigma+1) \tag{16a}$$

$$\tilde{\boldsymbol{\Sigma}}_{pq} = \frac{-1}{4} \sum_{\sigma\gamma\delta r} \{qr|t|\gamma\delta\}_\sigma \{pr|t|\gamma\delta\}_\sigma (2\sigma+1) \tag{16b}$$

where $\{ab|t|cd\}_\sigma$ etc. are reduced Hugenholtz matrix elements [10], as used in our earlier work, following earlier works of Mukherjee et al. [19]. Calculation of the $\boldsymbol{\nu}_1$ matrix thus involves inversion of the matrix $[\boldsymbol{\nu}_1^0 - \boldsymbol{\Sigma}_1]^{-1}$.

We consider the two-body insertion next. Let us again assume that only the lowest order basic skeleton as shown in Fig. 7a is the important one. There are in all hole-hole, particle-particle and hole-particle insertions corresponding to various ways of placing the arrows on the skeleton of Fig. 7a. The Bethe-Salpeter equation (13) takes the form

$$\boldsymbol{\nu}_2 = [\boldsymbol{\nu}_2^0 - \boldsymbol{\Sigma}_2]^{-1} \tag{17}$$

The relevant matrix-elements are given by

$$\nu^0_{2\alpha\beta,\gamma\delta} = \nu_{1\alpha\gamma} \cdot \nu_{1\beta\delta}, \tag{18a}$$

$$\nu^0_{2pq,rs} = \nu_{1pr} \cdot \nu_{1qs}, \tag{18b}$$

$$\nu^0_{2p\alpha,q\beta} = \nu_{1pq} \cdot \nu_{1\alpha\beta}, \tag{18c}$$

$$\tilde{\Sigma}_{2\alpha\beta,\gamma\delta\sigma} = \sum_{pq} \{pq|t|\alpha\beta\}_\sigma \{pq|t|\gamma\delta\}_\sigma, \tag{19a}$$

$$\tilde{\Sigma}_{2pq,rs,\sigma} = \sum_{\alpha\beta} \{pq|t|\alpha\beta\}_\sigma \{rs|t|\alpha\beta\}_\sigma, \tag{19b}$$

$$\tilde{\Sigma}_{2p\alpha,q\beta,\sigma} = \sum_{\substack{q\gamma,r \\ \sigma_i\sigma_j}} \{pr|t|\gamma\beta\}_{\sigma_i} \{qr|t|\gamma\alpha\}_{\sigma_j} \begin{Bmatrix} 1/2 & 1/2 & \sigma \\ \sigma_i & 1/2 & 1/2 \\ 1/2 & \sigma_j & 1/2 \end{Bmatrix} (2\sigma_i+1)(2\sigma_j+1). \tag{19c}$$

Here $\begin{Bmatrix} 1/2 & 1/2 & \sigma \\ \sigma_i & 1/2 & 1/2 \\ 1/2 & \sigma_j & 1/2 \end{Bmatrix}$ is a $9-j$ symbol.

Let us note carefully that we must avoid multiple counting of a diagram in Eq. (6) while using the modified contractions. Thus, single line insertions in the diagram of Fig. 4a generate a diagram (marked 2) which can be deformed in a way such that it appears as a modification of three lines, as shown in Fig. 8. In that case, a simple strategy will be to drop all three-body Σ diagrams as insertions on internal lines connecting T/T^+ of an energy diagram. Let us note that this procedure automatically excludes a double counting of the diagram (2) of Fig. 4b as well. Essentially with $T = T_2$ approximation, basic skeletons are just one and two body self energy terms in the lowest order. Three body Σ's are redundant for one T^+ and one T vertex and four-body Σ's cannot be constructed unless one goes to a quartic term involving two T^+ and two T vertices. Thus, up to quartic terms in E_{gr}, only Σ_1 and Σ_2 suffice. In our earlier communication [10] we considered a simple energy series up to cubic total power of T^+/T amplitudes and the results were encouraging. We thus advocate in this paper use of the modified diagrams as shown in Fig. 9. The meaning of the vertical line cutting

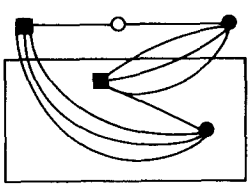

Fig. 8. The second diagram in Fig. 4b can also be viewed as the insertion of renormalized three body density matrix as shown here. Thus simultaneously renormalizing one and three body density matrices can lead to overcounting in the energy

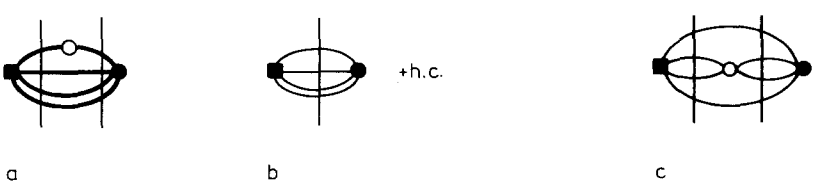

Fig. 9. The three lowest order terms in the renormalized energy series. Heavy lines indicate renormalized contraction. The vertical intersecting line indicates that the global propagator should be evaluated by Bethe-Salpeter equation (13). The resultant series is exact through third order in T/T^+

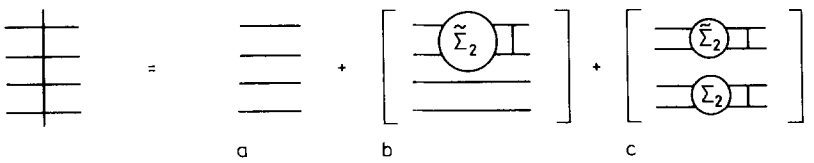

Fig. 10. Diagrammatic representation of Bethe-Salpeter equation for a $2p-2h$ propagator. The heavy lines indicate the renormalized single particle contractions. Σ_2 are the various types of two body irreducible vertex parts

four thick lines of the diagrams is as follows. We have to evaluate the propagation of the four thick lines as being calculated with the Bethe-Salpeter equation (13) using (14) with $\tilde{\Sigma}_1$ and $\tilde{\Sigma}_2$ only.

Diagrammatically this will correspond to Fig. 10. Fig. 10b is actually a symbolic representation of ${}^4C_2=6$ diagrams obtained by joining two lines out of four having the topology shown there. Similarly Fig. 10c is a collection of six diagrams. It is clear from Fig. 10 that an iteration of ν_2 and ν_1 using Eqs. (12), (13) and (14) will generate all possible insertions with $\tilde{\Sigma}_1$ and $\tilde{\Sigma}_2$ as given in Figs. 2a and 7a respectively. Insertion of Σ_3 and Σ_4 can be similarly accomplished.

One wonders at this stage whether it will be possible to incorporate higher order skeletons of Σ_1 and Σ_2 (and Σ_i, $i>2$, in general) in a simpler and more compact manner instead of a brute force enumeration and inclusion of all the skeletons in Σ_1 and Σ_2. This is indeed possible, as we shall show in Sect. 4, by invoking the concept of irreducible self energy in a way analogous to what is done in propagator renormalization in Green function theory [15, 18].

4. Propagator modification through irreducible self-energy insertion

As before, we shall explain our approach by again taking concrete examples. Let us consider the one-body self-energy and try to analyze the topological structures of the few low-order components of Σ_1. The lowest order basic self-energy is, of course, that shown in Fig. 3a. The higher order ones are shown in Fig. 5. Let us note that all these higher order terms in Σ_1 have one feature in common: there is always a part (or parts) which could be looked upon as basic skeleton insertion(s) onto one or several *internal* lines of the Σ_1. Thus, the part inside the square of Fig. 5a is a proper one-body self energy insertion, and similarly the two parts inside the two squares of Fig. 5c are two one-body self energy insertions. The insertion in Fig. 5b is a two-body self energy insertion. Clearly, if we modify the propagators for the internal lines of the proper self energy of Fig. 3a, then all these higher order proper self energies will be automatically accounted for. Thus, if we define a proper self-energy with modified propagators as in Fig. 11a, with a modified three line propagator as defined in Fig. 11b, then all the higher order diagrams of Σ_1 of Fig. 5 and a host of other complicated diagrams will be exhausted. In order to avoid multiple counting, all the proper self-energy terms of Fig. 5 have, of course, to be excluded. Thus, once we decide which parts of

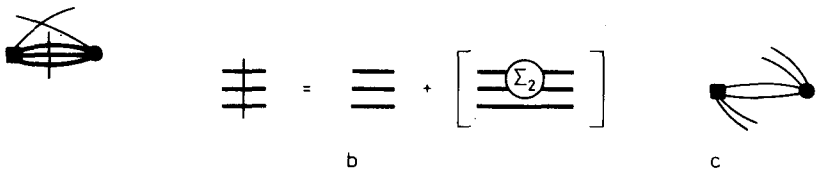

Fig. 11. (a) An example of renormalized self energy term. The three internal lines of this term are renormalized contractions as indicated by the heavy lines. Additionally, the intersecting line on the three internal lines indicates the two body vertex part insertions. The resultant series for the internal propagator is shown in (b). (c) An example of renormalized two body vertex part

the internal line propagators in a term of Σ are going to be modified by sets of selected insertions we must exclude those higher order skeletons of Σ which have one or more of these selected insertions from our consideration. There is a similar procedure for propagator renormalization in Green function theory and, following this analogy, we call the modified proper self energy skeletons "irreducible self energy". The higher order basic skeletons which have to be excluded shall be called "reducible self energy" [18]. The choice of the insertions into the internal lines of an irreducible self energy obviously dictates what will have to be considered as reducible self energy at higher order.

Similarly, if we want to modify the basic two-body term Fig. 7a of Σ_2, the simplest way will be to replace it by a diagram as shown in Fig. 11c. The modified two-line propagator is defined as in Fig. 6a. This will automatically incorporate the higher two-body proper self energy terms like Figs. 7b and 7c and also a host of two-body insertions onto the diagram of Fig. 7a. Thus an optimal choice to include higher order Σ_1 and Σ_2 insertions is to consider only the modified self energies of Figs. 11a and 11c, with insertions modifying the internal lines as defined in Figs. 3a and 7a.

As an example of working the expressions out for actual calculations, below we give the expressions for the renormalised propagator matrix-element $\tilde{\Sigma}^{RN}_{1\alpha\beta}$ and $\tilde{\Sigma}^{RN}_{2\alpha b,\gamma\delta}$ using the approximations discussed in the preceding paragraph.

$$\tilde{\Sigma}^{RN}_{1\alpha\beta} = \tfrac{1}{4}\sum_{\sigma}\sum_{\substack{pp'qq'\\ \gamma\gamma'}} \nu_{3pq\gamma p'q'\gamma'}\{p'q'|t_2|\alpha\gamma'\}_{\sigma}\{pq|t_2|\beta\gamma\}_{\sigma}(2\sigma+1) \tag{20a}$$

$$\tilde{\Sigma}^{RN}_{2\alpha\beta,\gamma\delta\sigma} = \tfrac{1}{2}\sum_{pp'qq'} \nu_{2pq,rs}\{p'q'|t_2|\alpha\beta\}_{\sigma}\{pq|t_2|\gamma\delta\}_{\sigma} \tag{20b}$$

with ν_2 defined through Eqs. (17)-(19), and an analogous formula for ν_3 may be found out by writing the algebraic expression equivalent to Fig. 11b.

For a practical calculation of $\tilde{\boldsymbol{\Sigma}}^{RN}_1$ and $\tilde{\boldsymbol{\Sigma}}^{RN}_2$ an iterative self-consistent procedure has to be followed. One may start out with $\boldsymbol{\nu}^0_2$ and $\boldsymbol{\nu}^0_3$ as the starting $\boldsymbol{\nu}_2$ and $\boldsymbol{\nu}_3$ matrices, get the T-amplitudes through solving the Euler variational equation of E_{gr} and calculate $\boldsymbol{\Sigma}^{(0)}_1$ and $\boldsymbol{\Sigma}^{(0)}_2$ matrices using Eq. (20). With these $\boldsymbol{\Sigma}$'s one goes back to Eq. (17) for $\boldsymbol{\nu}_2$ and the analogue of $\boldsymbol{\nu}_3$ and recalculates $\boldsymbol{\nu}^1_2$ and $\boldsymbol{\nu}^1_3$. With

these new iterates, T-amplitudes are evaluated and $\tilde{\Sigma}_1^{(1)}$ and $\tilde{\Sigma}_2^{(1)}$ are re-calculated. The process is continued till the input and the output v_2 and v_3 matrices coincide.

5. Concluding remarks

In this paper, we have shown how to incorporate the contribution of physically important terms with all powers of T^+/T amplitudes appearing in the size-consistent infinite series of the ground state energy functional. The method is conceptually analogous to the propagator modification method of Green function theory. One first selects a few low order terms of the correlation contribution of one- and two-electron density matrices ρ_1^C and ρ_2^C, and starts incorporating higher order contributions to ρ_1^C and ρ_2^C through the use of modified values of the propagators of the internal lines appearing in the selected low order terms of ρ_1^C and ρ_2^C. This automatically includes in ρ_1^C and ρ_2^C the terms which are generated by inserting one or multiple composites involving T^+/T amplitudes. The insertions are legitimately called proper self energy insertions in a way reminiscent of the proper self energy terms of the Green function theory. Reclassifying the proper self energy insertions into irreducible self energy and reducible self energy in a manner similar to what is used in propagator renormalization in Green function theory [18], one is also able to include, using only few low order n-body self energy insertions, many other higher order n-body self energy contributions. The approach appears completely general, and, once certain T^+/T diagrams are identified as important, affords a recipe of incorporating them to all orders in the size-consistent expression for energy. The method should thus prove useful in removing the loss of an upper bound property of the energy functional [14] as a result of truncation of the functional by systematic inclusion of higher order terms.

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