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A variational method to calculate static electronic properties

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Using a coupled cluster form of the wave function, a variational method is formulated for calculation of static properties of any order. Corresponding to an appropriate perturbed hamiltonian $H(\lambda)$ including the relevant static property, a size consistent functional is set up. In a hierarchical fashion, properties of different orders may be found out using a variational method.

Key words: Size consistency—variational method—atoms and molecules—coupled-cluster wave function

1. Introduction

Coupled Cluster Methods (CCM) have been successful tools to obtaining electron correlation energies for atomic and molecular systems [1–10]. They have been applied extensively to the closed shell systems in particular. CCM, in its pair approximation known as Coupled Pair Many Electron Theory (CPMET), takes into account the major part of the quadruply excited contributions through the unlinked cluster terms of the wave function. Inclusion of single excitation variables as well as triple and higher excitation parameters have also been made. Although, traditionally a nonvariational method has been applied to calculate correlation energies using Coupled Cluster (CC) wave function [1, 2], variational methods have also been envisaged in recent years [5, 6]. The attractive feature of CCM is that it guarantees the separability criterion for many electron systems [11] and consequently the desirable property of size consistency of energy is retained [12]. Despite the attractive physical features of CC wave function and the success of such an ansatz in the calculation of correlation energies, there

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have been fewer attempts at obtaining the other electronic properties using a CC wave function. This note presents a variational method to calculate the first and second order static properties with the use of a CC wave function.

A CC wave function ψ for closed shells is defined as,

$$\psi = e^{T}\Phi_0 \tag{1a}$$

with

$$T = T_1 + T_2 + T_3 + \cdots, \tag{1b}$$

where each T_n operator is a n-body hole-particle excitation operator. Φ_0 is a closed shell Hartree–Fock (HF) determinant. The ansatz was initially proposed by Coester and Kummel [13–14] and later adopted by Cizek [1, 2] in the correlation energy calculations for atomic and molecular systems. Originally Cizek calculated the energy and T-parameters using the nonvariational mode of solution. Subsequently, the variational methods have been applied to find the T-parameters as well as the energies by other authors [5, 6].

However, as mentioned earlier, there have been fewer developments at calculating the other electronic properties using CC wavefunction. One of the earlier methods is to calculate the expectation value $\langle\hat{O}\rangle$ of the first order static property $\hat{O}$ of interest for a state function which is close to the exact function. In the framework of a CC wave function the expectation value $\langle\hat{O}\rangle$ may be given by

$$\langle\hat{O}\rangle = \frac{\langle\Phi_0|e^{T^+}\hat{O}\,e^{T}|\Phi_0\rangle}{\langle\Phi_0|e^{T^+}\,e^{T}|\Phi_0\rangle}. \tag{2}$$

The expression reduces to a sum of linked terms and was investigated by Cizek [2] and Fink [15]. T-parameters may be chosen to be of the values generated for correlation energy calculation in nonvariational CCM or variational methods. However, one significant method to calculate the first and second order static properties as well as the dynamic properties using CC wave function was developed by Monkhorst [16]. Using Hellmann–Feynmann theorem, the framework of CCM has been conveniently used by Monkhorst for the calculation of static properties. The method developed by Monkhorst is, as is traditional for CCM applied to correlation energy calculation, nonvariational in nature. In this paper we present a method where the ansatz is similar to the one proposed by Monkhorst, but which is completely variational in nature.

In Sect. 2, we briefly review Monkhorst's approach highlighting its features. Then in Sect. 3 we present the method to be reported here with a brief summary in Sect. 4. We will restrict ourselves to the problem of determination of static properties here for closed shell systems.

2. Background

In this section a brief review of Monkhorst's approach [16] to calculate the static properties using the CCM is presented. He considered a perturbed Hamiltonian

$H(\lambda)$ as,

$$H(\lambda)=H+\lambda\hat{O}. \tag{3}$$

The wavefunction $\psi(\lambda)$ is defined as

$$\psi(\lambda)=e^{T(\lambda)}\Phi_0. \tag{4}$$

The Schrödinger equation for the perturbed Hamiltonian is,

$$H(\lambda)\, e^{T(\lambda)}\Phi_0=E(\lambda)\, e^{T(\lambda)}\Phi_0 \tag{5}$$

utilizing the CC form of a wave function.

A power series expansion for $T(\lambda)$ may be introduced i.e.

$$T(\lambda)=T+\lambda T^{(1)}+\lambda^2 T^{(2)}+\cdots. \tag{6}$$

Similarly, a suitable power series expansion for $E(\lambda)$ may also be introduced

$$E(\lambda)=E+\lambda E^{(1)}+\lambda^2 E^{(2)}+\cdots. \tag{7}$$

In the nonvariational method of solving the Schrödinger Eq. (5), $E(\lambda)$ is given by,

$$E(\lambda)=\langle\Phi_0|\, e^{-T(\lambda)}H(\lambda)\, e^{T(\lambda)}|\Phi_0\rangle. \tag{8}$$

It is known that for the exact state where all possible clusters are taken in defining $T(\lambda)$ (in Eq. 6) the expectation value of a first order static property $\langle\hat{O}\rangle$ is given by

$$\langle\hat{O}\rangle=\left.\frac{\partial E(\lambda)}{\partial\lambda}\right|_{\lambda=0}=E^{(1)} \tag{9}$$

with $E(\lambda)$ as defined in Eq. (8). However for the approximate function where only suitable clusters are included in defining $\psi(\lambda)$ (i.e. Eq. 4), the equality (9) does not hold good. But assuming that the important clusters have been taken in the anasatz, the equality (9) is nearly strict. Monkhorst pointed out that in such approximate cases, $E^{(1)}$ is closer to the exact answer. Monkhorst derived the expression for $E^{(1)}$ and the necessary additional cluster parameters $T^{(1)}$ for first order properties using a nonvariational method. Putting the power series expansion for $T(\lambda)$ in the usual nonvariational equations determining cluster parameters and energy, the equations as derived by Monkhorst for $E^{(1)}$ and $T^{(1)}$ parameters are of the following form:

$$E^{(1)}=\langle\Phi_0|\, e^{-T}\{\hat{O}+[H,T^{(1)}]\}\, e^{T}|\Phi_0\rangle \tag{10a}$$

$$\langle\Phi^*|\, e^{-T}\{\hat{O}+[H,T^{(1)}]\}e^{T}|\Phi_0\rangle=0, \tag{10b}$$

Φ^*'s are the relevant excited states. The nonvariational mode of solution automatically leads to linked energies. $T^{(1)}$ parameters can be obtained from (10b) with T parameters substituted from the solution of usual Cizek's equation (cf. Ref. [1]). One can see that $T^{(1)}$ parameters are sufficient for the first order properties. $T^{(1)}$ can be expanded as,

$$T^{(1)}=\sum_m T_m^{(1)} \tag{11a}$$

with

$$T_1^{(1)} = \sum_{p,\alpha} \langle p|t_1^1|\alpha\rangle a_p^+ a_\alpha \tag{11b}$$

$$T_2^{(1)} = \sum_{\substack{p,q\\ \alpha,\beta}} \langle pq|t_2^1|\alpha\beta\rangle a_p^+ a_q^+ a_\beta a_\alpha \tag{11c}$$

and so on. Greek letter α, β indicate hole orbitals, whereas as p, q, etc. indicate particle/virtual orbitals. $\langle p|t_1^1|\alpha\rangle$, $\langle pq|t_2^1|\alpha\beta\rangle$ are matrix elements of different ranks of $T^{(1)}$'s. Suitable rank of T's and $T^{(1)}$'s have to be chosen for tests and actual applications. Similar equations have been derived by Monkhorst for the calculation of second order property $E^{(2)}$

$$E^{(2)} = \frac{1}{2}\frac{\partial^2 E(\lambda)}{\partial\lambda^2}\bigg|_{\lambda=0}. \tag{12}$$

Explicit knowledge of $T^{(2)}$ parameters are necessary for obtaining $E^{(2)}$. Expressions similar to Eqs. (11b) and (11c) may be written for different ranks of $T^{(2)}$ operators. The solution of $T^{(2)}$ parameters requires in turn the knowledge of $T^{(1)}$ parameters which can again be found from Eq. (10b) with $\hat{O}$ an appropriate property operator. In the next section the variational method for the determination of first and second order static properties with the help of CC wave function is presented.

3. Variational method of determining the static properties

As in Monkhorst's approach [16] we consider the perturbed Hamiltonian $H(\lambda)$ defined by Eq. (3). The ansatz and the pertinent expansion of $T(\lambda)$ parameters are very similar to Eqs. (4) and (6) respectively. But, instead of the nonvariational method, a variational prescription is followed quite in spirit to our method of calculating the correlation energy quoted in Ref. [6].

Let us consider the perturbed expectations value $E(\lambda)$.

$$E(\lambda) = \frac{\langle\psi(\lambda)|H(\lambda)|\psi(\lambda)\rangle}{\langle\psi(\lambda)|H(\lambda)\rangle}. \tag{13}$$

Although the energy functional, which is a function of the perturbation parameter λ, is a ratio of numerator and denominator, it can be shown to be the sum of only linked diagrams. The arguments are very similar to the ones presented by us [6] and others [1, 2] in the context of cancellation of the denominator of the energy functional.

Hence we obtain

$$\begin{aligned} E(\lambda) &= \frac{\langle\psi(\lambda)|H(\lambda)|\psi(\lambda)\rangle}{\langle\psi(\lambda)|\psi(\lambda)\rangle} \\ &= \frac{\langle\Phi_0|\, e^{T(\lambda)^+} H(\lambda)\, e^{T(\lambda)}|\Phi_0\rangle}{\langle\Phi_0|\, e^{T(\lambda)^+}\, e^{T(\lambda)}|\Phi_0\rangle} \\ &= \langle\Phi_0|N[e^{T(\lambda)^+} H(\lambda)\, e^{T(\lambda)}]|\Phi_0\rangle_{\text{Linked}}. \end{aligned} \tag{14}$$

Subscript ‘Linked’ denotes that only linked or connected diagrams need be considered. $N[\ ]$ denotes normal ordering of the operator product contained in the bracket. The last equality in Eq. (14) is obtained by the expansion of numerator and denominator using Generalised Wick’s Theorem (GWT) [6]. $E(\lambda)$ can now be expanded as in Eq. (7) as a power series of λ. A variational recipe is now prescribed for calculation of T, $T^{(1)}$, $T^{(2)}$ etc. matrix elements in spirit to the variational determination of T matrix elements by Euler variation of $\langle\Phi_0|N[e^{T^+}He^T]|\Phi_0\rangle_{\text{linked}}$ followed in the first citation of Ref. 6. However, as we set up the equations for T, $T^{(1)}$, etc. matrix elements explicitly, we will see that some interesting features are encountered because of the appearance of the $T^{(i)}$ matrix elements corresponding to different orders of the parameters λ. Equating different powers of λ, E, $E^{(1)}$, $E^{(2)}$, etc. can then be obtained from the various matrix elements.

It may be noted that $T^{(1)}$, $T^{(2)}$ etc. operators are of the form (11b), (11c) as discussed in the previous section. Eq. (14) contains contractions of various powers of T^+, T, $T^{(1)+}$, $T^{(1)}$, $T^{(2)+}$, $T^{(2)}$ etc. with f and v vertices in normal order. The number of variables are the number of matrix elements of the type $\langle pqr---|t_n^{(i)}|\alpha\beta\gamma---\rangle$. n denotes the rank of operator i.e. that the corresponding cluster refers to the n-body linked excitation. i denotes the operator corresponding to λ^i in the expansion of $T(\lambda)$ in Eq. (6).

As is obvious from the Eq. (14), the first order static property $E^{(1)}$ only needs the knowledge of matrix elements of operators upto the level of $T^{(1)}$.

$$E^{(1)} = \langle\Phi_0|N[e^{T^+}\{\hat{O} + T^{(1)+}H + HT^{(1)}\}\, e^T]|\Phi_0\rangle_L. \tag{15}$$

L stands for ‘linked’. The equation determining $E^{(1)}$ is linear in $T^{(1)}$, though nonlinear in T-matrix elements. Similarly, $E^{(2)}$ involves the knowledge of $T^{(2)}$ upto the linear level, a total of quadratic power of $T^{(1)}$, and, in principle, all possible powers of T-matrix elements. So, for the determination of higher order static properties a hierarchical scheme of solution must be followed. This will be made clear in what follows where the scheme for the solution of different $T^{(i)}$ matrix elements by variation method is discussed.

Before discussing variational method to be envisaged in this paper, it must be noted that the perturbed energy functional (Eq. 14) does not terminate after finite powers. For simplicity we discuss the Eqs. for T and $T^{(1)}$ matrix elements needed for first order static properties. Similarly, upto a given order the equations can be generated to solve $T^{(2)}$ matrix elements needed for second order properties. The nature of the equations are discussed in the approximation $T \sim T_2$, $T^{(1)} \sim T_2^{(1)}$. However, the operators corresponding to other linked excitations can also be systematically introduced. In the discussion we remain in the framework of these approximations *only for simplicity.*

The necessary equations for calculation of first order properties are of the following form.

$$\frac{\partial E(\lambda)}{\partial\{\langle\alpha\beta|t_2^+|pq\rangle\}} = 0 \tag{16a}$$

$$\frac{\partial E(\lambda)}{\partial\{\langle pq|t_2|\alpha\beta\rangle\}}=0 \tag{16b}$$

$$\frac{\partial E(\lambda)}{\partial\{\langle\alpha\beta|t_2^{(1)^+}|pq\rangle\}}=0 \tag{16c}$$

$$\frac{\partial E(\lambda)}{\partial\{\langle pq|t_2^{(1)}|\alpha\beta\rangle\}}=0 \tag{16d}$$

Eqs. (16a) and (16b) are hermitian conjugates to each other. Similarly, (16c) and (16d) are hermitian conjugates to each other. Hence it is necessary to solve only Eqs. (16a) and (16c). But as may be seen, Eq. (16a) itself generates many equations, corresponding to various powers of λ. For the specific case of calculation of first order properties two equations – one independent of λ and the other linear in λ are relevant. In a hierarchical fashion, corresponding to higher powers of λ, Eqs. for $T^{(2)}$, $T^{(3)}$ etc. necessary for higher order properties may be generated. Similarly, Eq. (16c) would generate many equations corresponding to different powers of λ (starting from the linear term in λ). For first order properties, there will be two relevant Eqs. from (16c) one linear in λ the other corresponding to quadratic terms in λ. So, apparently there are more equations than the number of variables. If there N-number of T_2 and $T_2^{(1)}$ variables each, we have from (16a) and (16c) $4N$-number of pertinent equations. However, it will be shown in the following that if we include in the approximation of $T\sim T_2$, $T^{(1)}\sim T_2^{(1)}$ etc. all terms containing T_2, $T_2^{(1)}$ etc. consistent with the expansion of $[T^+(\lambda)]^n$ and/or $[T(\lambda)]^m$ for suitable m and n, the Eqs. (16a) are identical to the Eqs. (16c). The system of equations corresponding to nth power of λ obtained from (16a) would be identical to the system of equations corresponding to $(n+1)$th power of λ obtained from (16c). Diagrammatically also this can be easily visualised. Similarly, if we include $T_2^{(2)}$ for calculation of second order properties consistent upto a given power of $[T^+(\lambda)]$ and $[T(\lambda)]$ first three equations of (16a) corresponding to λ^0, λ^1, λ^2 terms respectively will be identical to the first three equations generated from (16c) corresponding to λ^1, λ^2 and λ^3. These, in turn, will be identical to the first three equations of

$$\frac{\partial E(\lambda)}{\partial\{\langle\alpha\beta|t_2^{(2)^+}|pq\rangle\}}=0 \tag{17}$$

corresponding λ^2, λ^3, λ^4 respectively.

In the following the two relevant equations of (16a) and (16c) are shown to be same for first order properties by taking all the necessary terms involving only T_2, $T_2^{(1)}$ obtained from the expansion of $[T^+(\lambda)]$ and $[T(\lambda)]$ in the energy functional (14).

Energy functional, in such a case, may be written as,

$$\begin{aligned}E(\lambda)=&\langle\Phi_0|H|\Phi_0\rangle+\lambda\langle\Phi_0|\hat{O}|\Phi_0\rangle+\langle\Phi_0|T_2^+H|\Phi_0\rangle+\langle\Phi_0|HT_2|\Phi_0\rangle\\&+\lambda\langle\Phi_0|T_2^{(1)^+}H|\Phi_0\rangle+\lambda\langle\Phi_0|HT_2^{(1)}|\Phi_0\rangle+\lambda\langle\Phi_0|T_2^+\hat{O}|\Phi_0\rangle\end{aligned}$$

$$+\lambda\langle\Phi_0|\hat{O}T_2|\Phi_0\rangle+\lambda^2\langle\Phi_0|T_2^{(1)+}\hat{O}|\Phi_0\rangle+\lambda^2\langle\Phi_0|\hat{O}T_2^{(1)}|\Phi_0\rangle$$
$$+\langle\Phi_0|T_2^+HT_2|\Phi_0\rangle+\lambda\langle\Phi_0|T_2^+\hat{O}T_2|\Phi_0\rangle+\lambda\langle\Phi_0|T_2^{(1)+}HT_2|\Phi_0\rangle$$
$$+\lambda^2\langle\Phi_0|T_2^{(1)+}\hat{O}T_2|\Phi_0\rangle+\lambda\langle\Phi_0|T_2^+HT_2^{(1)}|\Phi_0\rangle+\lambda^2\langle\Phi_0|T_2^+\hat{O}T_2^{(1)}|\Phi_0\rangle$$
$$+\lambda^2\langle\Phi_0|T_2^{(1)+}HT_2^{(1)}|\Phi_0\rangle+\lambda^3\langle\Phi_0|T_2^{(1)+}\hat{O}T_2^{(1)}|\Phi_0\rangle.$$

All operator products are in normal order. Eqs. (16a) or (16c) would generate diagrams which have blocks with open 2 particle and 2 hole lines at the left of the block. The block is schematically depicted in Fig. 1. Under the approximation in which the functional (14) has been truncated to linear power in $T^+(\lambda)$ and $T(\lambda)$, the two systems of equations generated from (16a) by differentiation of a T_2^+ vertex corresponding to terms independent of λ and linear in λ may be written in diagrammatic language as,

diagrams (having the shape of Fig. 1) generated from

$$[H+\overline{HT}_2]=0 \tag{19a}$$

diagrams (having the shape of Fig. 1) generated from

$$[\hat{O}+\overline{\hat{O}T}_2+\overline{HT}{}_2^{(1)}]=0. \tag{19b}$$

Symbol ‘$\ulcorner\urcorner$’ denotes the contraction between the operators which have been capped by this symbol. In a similar language Eq. (16c) may be written in the following as two relevant systems of Eqs. (20a) and (20b) which correspond to linear and quadratic terms in λ respectively.

Diagrams (having the shape of Fig. 1) generated from

$$[H+\overline{HT}_2]=0 \tag{20a}$$

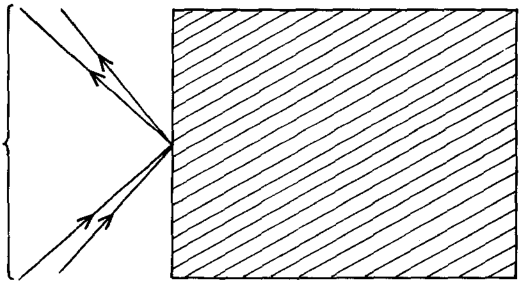
Diagrams (having the shape of Fig. 1) generated from

$$[\hat{O}+\overline{\hat{O}T}_2+\overline{HT}{}_2^{(1)}]=0 \tag{20b}$$

Clearly the equations are identical, so that one may consider only one set of equations.

When we write the equation (16a) corresponding to terms proportional to λ^2 for determination of $T_2^{(2)}$ matrix elements, we must also include the diagrams arising

Fig. 1. Schematic depiction of the diagrams generated by the differentiation of the energy functional (14) with respect to a $T_2^+/T_2^{(1)+}$ etc. vertex. Hole lines are indicated by right going arrows and particle lines are indicated by left going arrows



from contractions involving $T_2^{(2)}$ operators. From the discussions presented before it is clear that in such a two body approximation for the $T^{(i)}$ operators, for any order property calculation, only one set e.g. the set (16a) is sufficient to calculate all matrix elements. It is to be noted that the first system of equation in any set obtained from the stationarity condition of the functional $\langle\Phi_0|N[\{T_2^+(\lambda)\}^m H(\lambda)\{T_2(\lambda)\}^n]|\Phi_0\rangle_L$ with respect to variation of $T^{(i)}$ parameters is (for example, the equation for λ-independent term from (16a) or equation corresponding to linear terms in λ from (16c) etc.) identical to the system of equations obtained by making the energy functional $\langle\Phi_0|N[T_2^{+m}HT_2^n]|\Phi_0\rangle_L$ stationary with respect to variation of T-parameters in the correlation energy calculation of work related to the first citation of the Ref. [6].

In a similar spirit, operators of other n-body excitations (ranks) can be introduced into the calculation. As long as we include all the operators $T^{(i)}$ upto the same rank we will continue to have a similar structure of identical equation. In such a case

$$\frac{\partial E(\lambda)}{\partial T_n^{(i)+}}=0 \qquad i=0,1,2,\ldots \tag{21}$$

will produce identical system of equations for all i. Here i denotes the cluster parameter corresponding to λ^i in the expansion (6). Here corresponding to $i=0$, $T_n^{(0)}$ is the T_n parameter referred to earlier so that again the set of equations obtained by variation with respect to only T_n^+ parameters is sufficient for any n.

4. Summary

As we see the first equation in the system of equations obtained by making the functional (14) stationary with respect to variations of $T^{(i)}$ parameters for any i is identical to the stationary condition of the functional $\langle\Phi_0|e^{T^+}He^T|\Phi_0\rangle_L$ with respect to the variation of T-parameters. But with the introduction of $T^{(1)}$ parameters, in case, e.g. of first order static properties, $E^{(1)}$ is quite different from the simple expectation value of the operator. In contrast with Monkhorst's nonvariational approach, the functional is not a finite power series of T. But if dominant terms are taken into consideration, the effect of truncation may not be serious.

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