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Direct evaluation of one-electron properties in coupled cluster methods

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Summary. An analysis of a method for approximate calculations of expectation values for one-electron operators from available coupled cluster amplitudes is presented and illustrated numerically for the polarizability of the Be atom. The one-particle density matrix resulting from the present approach is accurate through the fourth order in the electron correlation perturbation. It has been found that, in order to obtain quantitative agreement between the energy derivative results and the approximate expectation value formalism, the third order $T_1 T_2 |\Phi^{(0)}\rangle$ wave function term must be included into the calculation of the one-particle density matrix. The present method is also considered as a promising tool for calculations of higher-order atomic and molecular properties from high level correlated wave functions.

Key words: Expectation value—Hellmann–Feynman theorem—Coupled cluster method—One-electron properties—Polarizabilities

1. Introduction

Suppose that a many-electron system with (unperturbed) Hamiltonian H^0 is embedded in some perturbing field, so that

$$H^0 \to H(\lambda) = H^0 + \lambda V \tag{1}$$

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where V is the appropriate perturbation operator and λ defines its strength. Then, for the perturbed Hamiltonian $H(\lambda)$, the k-th order property, $Q^{(k)}$, of the given system is defined [1] as a quantity proportional to the k-th order derivative of the λ-dependent energy $E(\lambda)$:

$$Q^{(k)} \sim E^{(k)} = \frac{1}{k!}\left(\frac{\partial^k E(\lambda)}{\partial \lambda^k}\right)_{\lambda=0}, \tag{2}$$

where

$$E(\lambda) = \langle \Psi(\lambda) | H(\lambda) | \Psi(\lambda) \rangle \tag{3}$$

and $\Psi(\lambda)$ is the normalized (approximate or exact) solution of the perturbed Schrödinger equation for the given value of λ. Equations (2) and (3) give the most general and the only correct definition [1–3] of $Q^{(k)}$. They amount to assuming that both the field-independent and field-dependent problems are treated in exactly the same way. The use of (2) to define $Q^{(k)}$ was advocated long ago [2, 3] and seems to have been generally accepted [4] in calculations of atomic and molecular properties.

One should mention, however, that the definition of $Q^{(k)}$ in terms of the λ-dependent energy (3) may lead to some formal problems for unbound perturbation operators. Though the energy (3) may not be well defined in such cases, each term in its perturbation expansion can be calculated. Hence, Eq. (2) should be understood as a definition of $Q^{(k)}$ in terms of *a complete* k-th order perturbed energy formula compatible with the given form of the approximate wave function.

A direct differentiation of (3) shows that in general the evaluation of $Q^{(k)}$ requires the knowledge of all derivatives of $\Psi(\lambda)$ up to and including the k-th. The well known [5] $2n + 1$ rule which says that the evaluation of the $(2n + 1)$th order energy requires that the wave function is known to n-th order only, makes some assumptions that are rarely satisfied. This rule requires that all perturbed equations up to the n-th order are exactly solved. A weaker condition is sufficient for variationally determined wave functions; the $2n + 1$ rule is satisfied provided all parameters for Ψ which might be affected by the perturbation λV are freely varied. For first-order properties this result is known as the Hellmann–Feynman theorem [6].

The Hellmann–Feynman theorem, and its consequences for higher than the first-order properties [1, 3], provides a useful and convenient computational tool which is frequently applied beyond the range of its validity [7]. If the given wave-function satisfies the Hellmann–Feynman theorem then

$$Q^{(1)}_{HFT} \sim E^{(1)}_{HFT} = \langle \Psi^{(0)} | V | \Psi^{(0)} \rangle \tag{4}$$

where $\Psi^0 = \Psi(0)$. The higher-order properties can then be calculated as derivatives of the λ-dependent values of the first-order energy (4), i.e.

$$Q^{(k)}_{HFT} \sim \left(\frac{\partial^{k-1}}{\partial \lambda^{k-1}} E^{(1)}_{HFT}(\lambda)\right)_{\lambda=0} \tag{5}$$

where

$$E^{(1)}_{HFT}(\lambda) = \langle \Psi(\lambda) | V | \Psi(\lambda) \rangle \tag{6}$$

and $E^{(1)}_{HFT}(0)$ is given by Eq. (4). In particular in the case of $k = 2$, which is considered in the present paper, one obtains from (5)

$$Q^{(2)}_{HFT} \sim \langle \Psi^{(1)} | V | \Psi^{(0)} \rangle + c.c. \tag{7a}$$

while Eqs. (2) and (3) give

$$\begin{aligned} Q^{(2)} \sim {} & \langle \Psi^{(2)} | H^{(0)} - E^{(0)} | \Psi^{(0)} \rangle + \langle \Psi^{(0)} | H^{(0)} - E^{(0)} | \Psi^{(2)} \rangle \\ & + \langle \Psi^{(1)} | H^{(0)} - E^{(0)} | \Psi^{(1)} \rangle + \langle \Psi^{(1)} | \mathrm{V} | \Psi^{(0)} \rangle \\ & + \langle \Psi^{(0)} | V | \Psi^{(1)} \rangle \end{aligned} \tag{7b}$$

The two formulae give the same result if either

(i) the zero-th and first-order perturbed equations are exactly solved, or

(ii) $\Psi^{(0)}$ and $\Psi^{(1)}$ are determined variationally from the expansion of the energy functional (3).

Obviously with the approximate solutions of the Schrödinger equation approaching the exact ones, the difference between (7a) and (7b) becomes negligible. The same might be expected if $\Psi^{(0)}$ is determined variationally and $\Psi^{(1)}$ follows from some incomplete variational treatment in which the λ-dependence of some parameters is neglected in a justifiable way.

Since the evaluation of properties directly from Eq. (5) using approximate-high-quality wave functions is easier than the explicit calculation of derivatives (2), the differences between the numerical results from Eqs. (7a) and (7b) deserve a careful analysis. In the present paper this problem is studied for wave functions obtained within the coupled-cluster (CC) approach [8–10]. This is a continuation and extension of our recent study of approximate methods for the evaluation of expectation values of one-electron operators with CC wave functions [11].

2. The expectation value of one-electron operators for CC wave functions

For the purpose of the further analysis, we assume that V is a sum of one-electron operators. This assumption covers most of the physically interesting perturbations [12]. The unperturbed many electron Hamiltonian is partitioned according to the single-particle approximation into its Hartree-Fock (HF) and its correlation components:

$$H^{(0)} = H^{(0)}_{HF} + \nu W^{(0)}, \tag{8a}$$

where ν is a formal expansion parameter. According to the CC formalism [8–10] the solution $\Psi^{(0)}$ of the Schrödinger equation with the Hamiltonian (8a) can be generated from the reference HF determinant $\Phi^{(0)}_{HF}$:

$$\Psi^{(0)} = \exp(T^{(0)})\Phi^{(0)}_{HF}, \tag{9a}$$

where

$$T^{(0)} = T_1^{(0)} + T_2^{(0)} + \cdots \tag{10a}$$

is the cluster operator [8–10] for the unperturbed system. As long as the $T^{(0)}$ operator for an n-electron system contains all terms $T_1^{(0)} \cdots T_n^{(0)}$, the Hellmann–Feynman theorem is satisfied and

$$Q^{(1)} = Q_{HFT}^{(1)} = \langle \Phi_{HF}^{(0)} | \exp(T^{(0)+}) V \exp(T^{(0)}) | \Phi_{HF}^{(0)} \rangle_c, \tag{11}$$

where the subscript c means that only the connected [8, 9] terms are retained in the diagrammatic representation of (11).

Alternatively, the one-electron approximation and the respective partition of the total Hamiltonian can be introduced at the level of the λ-perturbed system [1, 13, 14] leading to

$$H = H_{HF}(\lambda) + vW(\lambda) \tag{8b}$$

$$\Psi(\lambda) = \exp\{T(\lambda)\}\Phi_{HF}(\lambda), \tag{9b}$$

and

$$T(\lambda) = T_1(\lambda) + T_2(\lambda) + \cdots + T_n(\lambda), \tag{10b}$$

where $\Phi_{HF}(\lambda)$ is the λ-dependent HF determinant which is built from the HF spinorbitals determined in the presence of the perturbation λV. The cluster operator depends on λ through its amplitudes. Each term in Eqs. (8b)–(10b) can be expanded into an infinite series in λ:

$$H_{HF}(\lambda) = H_{HF}^{(0)} + \lambda H_{HF}^{(1)} + \lambda^2 H_{HF}^{(2)} + \cdots \tag{12}$$

$$W(\lambda) = W^{(0)} + \lambda W^{(1)} + \lambda^2 W^{(2)} + \cdots \tag{13}$$

$$T_k(\lambda) = T_k^{(0)} + \lambda T_k^{(1)} + \lambda^2 T_k^{(2)} + \cdots \tag{14}$$

and the CC energy formula [8–10] reads:

$$E(\lambda) = E_{HF}(\lambda) + \langle \Phi_{HF}(\lambda) | W(\lambda)\{T_1(\lambda) + \tfrac{1}{2}T_1^2(\lambda) + T_2(\lambda)\} | \Phi_{HF}(\lambda) \rangle \tag{15}$$

The equivalence of Eq. (11) and the first-order derivative of $E(\lambda)$:

$$\begin{aligned} E^{(1)} = Q^{(1)} = E_{HF}^{(1)} &+ \langle \Phi_{HF}^{(0)} | W^{(0)}\{T_1^{(1)} + \tfrac{1}{2}T_1^{(1)}T_1^{(0)} + \tfrac{1}{2}T_1^{(0)}T_1^{(1)} + T_2^{(1)}\} \\ &+ W^{(1)}\{T_1^{(0)} + T_1^{(0)2} + T_2^{(0)}\} | \Phi_{HF}^{(0)} \rangle \{\langle \Phi_{HF}^{(1)} | W^{(0)} \\ &\times \{T_1^{(0)} + T_1^{(0)2} + T_2^{(0)}\} | \Phi_{HF}^{(0)} \rangle + c.c.\} \end{aligned} \tag{16}$$

in the complete CC limit, shows that the relaxation terms [1, 13, 14] which enter explicitly Eq. (16) must be contained in the operator

$$[\exp\{T^{(0)+}\} V \exp\{T^{(0)}\}]_c = V + T^{(0)+}V + VT^{(0)} + T^{(0)+}VT^{(0)} + \cdots \tag{17}$$

We recall that terms like $(T^{(0)+})^2 V, V(T^{(0)})^2$, etc cannot form connected contributions when V is a first order one electron operator and thus do not contribute to the expansion (17).

For a truncated form of the T operator, Eqs. (11) and (16) are no longer equivalent. One might expect, however, that the most important terms would be retained when T is truncated at a relatively low level, e.g. including only the first two or three terms of the cluster expansion (10a). Indeed, it has been shown by Bartlett et al. [15] that the CC model with the $T^{(0)}$ operator approximated (CCSD approximation [9, 10]) as

$$T^{(0)} \cong T_1^{(0)} + T_2^{(0)} \tag{18a}$$

is able to include most of the orbital relaxation effects for first- and second-order properties. This important result opens new possibilities [11, 15] for the evaluation of atomic and molecular properties by using the Hellmann–Feynman theorem (6) combined with Eq. (11).

It should be noted, however, that in molecules where triple excitations are important, the operator $T_3^{(0)}$ must also be included into the CC wave function, since its presence may have a significant effect on the amplitudes of the $T_1^{(0)}$ and $T_2^{(0)}$ operators. This has been demonstrated numerically and explained theoretically [11], on the basis of the relation between $T_3^{(0)}$ and the order to which the Hellmann–Feynman theorem is satisfied.

While evaluating (11) the infinite expansion (17) has to be truncated. In the previous paper [11] this truncation has been achieved by considering the formal orders of $T_n^{(0)}$ with respect to the perturbation $\nu W^{(0)}$. If the $T^{(0)}$ operator is approximated by

$$T^{(0)} \cong T_1^{(0)} + T_2^{(0)} + T_3^{(0)} \tag{18b}$$

(CCSDT approximation [9, 10, 16, 17]), the formula for the evaluation of $Q^{(1)}$ proposed in our previous paper [11] becomes

$$\begin{aligned} Q^{(1)} = \langle \Phi_{HF}^{(0)} | (1 + T_1^{(0)} + T_2^{(0)} + T_3^{(0)} + \tfrac{1}{2} T_2^{(0)} T_2^{(0)})^{+} \\ \times V(1 + T_1^{(0)} + T_2^{(0)} + T_3^{(0)} + \tfrac{1}{2} T_2^{(0)} T_2^{(0)}) | \Phi_{HF}^{(0)} \rangle_c . \end{aligned} \tag{19}$$

In the CCSD approximation (18a) the $T_3^{(0)}$ operators are removed from (19).

The iterative solution of the CC equations [9, 10, 16, 17] shows that the $T_2^{(0)}$ operator is at least first-order in $W^{(0)}$ while $T_1^{(0)}$ and $T_3^{(0)}$ are at least second-order in the correlation perturbation if canonical Hartree–Fock reference wave functions are used. Hence, the wave function generated in the CCSDT approximation is accurate to second-order in $W^{(0)}$ and contains several contributions from higher-order terms. Hence, the approximate expression used in [11] will be correct to third-order in $W^{(0)}$. According to Bartlett et al. [15], this expression simultaneously accounts for the majority of the self-consistency terms [13–15] whose contributions are explicitly indicated in Eq. (16).

According to some exploratory calculations presented in our previous paper it appeared to be essential to consider the contributions of $Q^{(1)}$ to (19) accurate to fourth order in $W^{(0)}$. However, on adopting this criterion one finds that Eq. (19) must be augmented by the term which includes the third order wave function component $T_1^{(0)} T_2^{(0)} | \Phi_{HF}^{(0)} \rangle$,

$$\langle \Phi_{HF}^{(0)} | T_1^{(0)} + T_2^{(0)+} V T_2^{(0)} + h.c. | \Phi_{HF}^{(0)} \rangle \tag{20}$$

Provided that the amplitudes are obtained from the full CCSDT method, the one-particle density matrix [11] is accurate to fourth-order in $W^{(0)}$, within the approximation for the CC wave function given by (18b), using the truncation of (17) to the form used in Eq. (19) and adding the contribution (20).

It should be stressed that the main objective of developing an approximate expectation value theory for CC wave functions is to make it competitive with the energy differentiation methods. This pragmatic criterion is used to investigate the validity of different truncated forms of the expansion (17). According to the numerical illustration given in the next section and our previous experience [11], adding the contribution (20) to the approximate expression for $Q^{(1)}$ (Eq. 19) results in a considerable improvement of the calculated expectation values.

The calculation of expectation values of one-particle operators is not extremely cumbersome even when using the energy derivative formulae [4, 15] and is not considered as the final goal of the present study. Once the expectation values can be computed accurately and fast enough from the approximate formulae, the standard finite-field perturbation methods can be used according to Eq. (5) for the calculation of higher-order atomic and molecular properties. This approach is illustrated in the present paper by calculating the dipole polarizability from the induced dipole moment. Values of the induced dipole moment are obtained from the approximate method described in this section.

3. Numerical results, discussion, and conclusions

The validity and numerical accuracy of the approximate eigenvalue expressions discussed in this paper have been investigated at the level of the CCSD and CCSDT models [9, 10, 16, 17]. In the later case only the approximate CCSDT approach known as the CCSDT-1a method [9, 10, 16] has been employed. As an illustrative example, for both the theory and its application to calculations of higher-order properties, we have chosen the evaluation of the induced dipole moment for the Be atom in an external homogeneous electric field. Its value has been obtained from different approximate formulae for $Q^{(1)}$ and then used for the numerical (finite difference) evaluation of the dipole polarizability of Be. Simultaneously, the polarizability values have been calculated numerically as the second-order derivatives of the respective field-dependent CC energies.

The application of the present theory to the calculation of induced dipole moments in Be offers certain advantages in comparison with our previous study of molecular multipole moments [11]. Since the correlation correction to the dipole polarizability of Be is quite large [18], the corresponding corrections to the SCF value of the induced dipole moment will be large as well. Hence, the relative importance of different terms of Eqs. (19) and (20) can be investigated in the range of rather large numbers. Moreover, the previous studies of the dipole polarizability of Be [18] have shown that the convergence of the MBPT correlation perturbation series is quite slow. The fourth-order MBPT result ($\alpha = 38.42$ a.u. [18]) is still considerably different from the estimated accurate value of the dipole polarizability of Be ($\alpha = 35.7$ to 37.7 a.u.). Thus, the higher-order correlation effects which are accounted for in CC models make a non-negligible contribution to the beryllium atom polarizability. However, the contribution due to $T_3^{(0)}$ can be expected to be very small if not negligible and in this case the CCSD model should perform almost as well as the CCSDT-1a approximation.

The numerical results presented in Tables 1 and 2 have been obtained with the [12.8.4] uncontracted GTO basis set employed previously in our MBPT studies of the dipole polarizability of Be [18]. This basis set gives the near-HF value of α at the SCF level and is capable of recovering most of the correlation contribution to the dipole polarizability of Be. The induced dipole moment and field-dependent energies have been computed for the electric field strength equal to 0.002 a.u. and the relevant data are shown in Table 1.

The performance of the approximate expectation value formula (19) can be analysed in terms of the calculated dipole polarizabilities. The additional term brought in by Eq. (20) is by no means negligible and constitutes about 10 per cent of the total correlation correction to α. Its inclusion in calculations of the

Table 1. Energies, induced dipole moments, and polarizabilities of Be in different approximations calculated with the [12.8.4] GTO basis set. All values in a. u.

Method[a]	Energy[b]	$\mu_{\mathrm{ind}}^{\mathrm{c}}$	α^{d}	
			A	B
Correlation contributions				
MBPT(2)	−0.066740	—	—	−4.19
MBPT(4)	−0.083795	—	—	−7.21
T(4)	−0.000156	—	—	−0.01
CCSD	−0.087387	−0.01761	−8.81	
		−0.01604	−8.02	−7.98
CCSDT-la	−0.087768	−0.01744	−8.72	
		−0.01586	−7.93	−8.03
Total				
SCF	−14.572845	0.09127	45.63	45.63
SCF + CCSD	−14.660232	0.07366	36.82	
		0.07523	37.61	37.65
SCF + CCSDT-la	−14.660613	0.07383	36.91	
		0.07541	37.70	37.60

[a] MBPT(n) denotes the MBPT correlation contribution through the n-th order. $T(4)$ denotes the 4-th order contribution due to triple excitations. CCSD and CCSDT-la denote the CC methods restricted to T_1 and T_2 or T_1, T_2, and approximate treatment of T_3, respectively. For details see [9, 10]

[b] Calculated for the field strength equal to zero

[c] Induced dipole moment calculated with the electric field strength equal to 0.002 a.u. The first value for each method corresponds to Eq. (19) while the second value includes also the contribution of Eq. (20)

[d] Dipole polarizability calculated as either the induced dipole moment derivative (A) or the second-order derivative of the field dependent energy (B). In column A the first value for each method is obtained from the induced moments calculated according to Eq. (19) and the second value includes the contribution from Eq. (20)

Table 2. Correlation contributions (in a.u.) to the expectation value of the induced dipole moment (μ) of Be for the electric field strength of 0.002 a.u. in the CCSD and CCSDT-la approximations

Operator[a]	μ	
	CCSD	CCSDT-la
$VT_1 + h.c.$	−0.01625	−0.01602
$T_1^+ VT_1$	0.00054	0.00052
$T_2^+ VT_2$	−0.00437	−0.00445
$T_3^+ VT_3$	—	0.00000
$T_2^+ T_2^+ VT_2 T_2$	0.00043	0.00043
Unsymmetric[b]	0.00205	0.00207
$T_1^+ T_2^+ VT_2 + h.c.$[c]	0.00157	0.00158
Total	−0.01604	−0.01586

[a] V denotes the dipole moment operator

[b] All other unsymmetric terms contributing to Eq. (19): $T_1^+ VT_2$ in CCSD and $T_1^+ VT_2$, $T_2^+ VT_3$, and $T_3^+ VT_2 T_2$ in CCSDT, plus their h.c.

[c] Contribution of Eq. (20)

induced dipole moment brings the calculated polarizabilities into almost quantitative agreement with the energy derivative data. As could have been expected from a negligible fourth-order contribution of triple substitutions (T(4), Table 1), there is only an insignificant difference between the CCSD and CCSDT-1a results due to the particular shell structure of the Be atom. The corresponding differences will obviously be much larger for systems with three or more electrons occupying orbitals of similar energy and spatial distribution.

A more detailed analysis of the different contributions to the approximate eigenvalue formula is given in Table 2. Naturally, the major part of the correlation contribution to μ comes from VT_1 and $T_2^+ VT_2^+$, i.e. the lowest order terms.

The present paper offers a relatively simple method to obtain one-particle density matrices from CC wave functions. The present formulae give the exact result to fourth order in the electron correlation perturbation. At the same time the CCSDT approach also guaranties the inclusion of a substantial part of the orbital relaxation. For less accurate wavefunctions, like MBPT(4), the analytic response form has been formulated previously [19].

The most promising application of the approximate method developed in this paper seems to be the calculation of higher order atomic and molecular properties by combining the present analytic formulae with the finite field approach. Another possible application is the calculation of correlation corrections to molecular magnetic properties. By using the present formalism one can at least partly avoid the problems arising from the pure imaginary character of the relevant perturbation operators.

Finally, we note that some methods closely related to the present approach have been proposed by Bartlett and his co-workers [15, 19]. Also, the earlier formulation of the method for the evaluation of different properties devised by Monkhorst [20] has recently been extended by Stolarczyk and Monkhorst [21].

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