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Research paper

Explicitly-correlated double ionization potentials and double electron attachment equation-of-motion coupled cluster methods



CHEMICA PHYSIC

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ABSTRACT

Double ionization and double electron attachment equation-of-motion methods, based on linearly approximated explicitly correlated coupled-cluster singles and doubles [CCSD(F12)] are formulated and implemented. An extension of double electron attachment operator is introduced for proper account of short-range correlation effects in states with two additional electrons. Numerical tests for set of doubly ionized and doubly electron attached states of several molecules have shown a good agreement between obtained explicitly-correlated results and the corresponding complete basis set limit values already at double- ζ level.

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1. Introduction

Computational methods, based on the equation-of-motion coupled-cluster methods (EOM-CC) provide a very convenient way to calculate quantities related to differential energies, such as ionization potentials (IP-EOM-CC) [1], electron affinities (EA-EOM-CC) [2], excitation energies (EE-EOM-CC) [3], double ionization potentials (DIP-EOM-CC) [4], double electron attachment (DEA-EOM-CC) [5] and some related properties [6]. These methods are related to the Fock-space coupled-cluster (FS-CC) formalism whose solutions for the S(p,h) sectors of the effective hamiltonian $\overline{H} = e^{-\widehat{T}} \widehat{H} e^{\widehat{T}}$, S(0,1) and S(1,0), are equivalent to those of IP-EOM-CC and EA-EOM-CC. The former are obtained from a more complicated computational procedure, so that today, the EOM route is preferred. The correspondence, however, ensures exact extensivity and intensivity of target ionization potentials and electron affinities [7–9], despite the linear CI-like operator for the target state in EOM-CC, because the Fock space operator is formally an exponential, like in the CC ground. In the case of the S(0,2) and S(2,0), sectors the results are slightly different between Fock-space coupled-cluster and DIP/DEA-EOM-CCSD methods. All the EOM-CC wave functions are pure in spin when based upon a closed shell reference state, enabling \overline{H} to be readily described in terms of spinfree cluster amplitudes. Both FS-CC and DIP/DEA-EOM-CC are widely used for treatment of multireference problems, like bond breaking and calculation of excitation energies of systems with open-shell ground states [10-12]. Also, the calculation of double ionization potentials are immediately useful to interpret Auger spectra. Yet another application of DIP-EOM-CC is to the ionization spectra of doublet radicals, where a closed-shell anion can be used as a reference state [12]. The excitation spectra of open-shell systems can be obtained from DEA-EOM-CC calculations using the corresponding doubly ionized closed-shell reference in the underlying CC step [12]. The computational cost of such highly applicable DIP-EOM-CCSD and DEA-EOM-CCSD methods is proportional to nocc³nvirt and nvirt³nocc, while the underlying CCSD scheme scales like nvirt⁴nocc², where nocc and nvirt are numbers of occupied and virtual orbitals in the system. Previous studies for excitation energies, electron affinities and ionization potentials have shown a strong dependence of target quantities upon the quality of used basis sets [13–16]. In the case of the addition and removal of two electrons from the system, the 'differential' correlation energies are very large, and the dependence of target double ionization potentials and double electron affinities upon choice of bases can be even larger than that for IPs and EAs. Indeed, in all standard basis methods the difference between the calculated correlation energy and the corresponding complete basis set (CBS) value is proportional to $(L_{max} + 1)^{-3}$ [17], where L_{max} is the highest angular momentum involved in the partial wave expansion. Thus, obtaining highly-accurate converged results might be computationally costly.

The use of an explicitly-correlated approach can be an attractive alternative. After the introduction of even simple linear- r_{12} [18] geminals the convergence of the correlation energy goes as $(L_{max} + 1)^{-7}$ [19]. Consequently, the explicitly correlated coupled-cluster method developed by Kutzelnigg and Noga [20] has become an efficient and convenient approach for the calculation of



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molecular systems. Modern implementations of CC-F12 methods use Kato's cusp conditions for the definition of geminal amplitudes (the so-called SP-Ansatz) [21] and utilize short-range Slater geminals, introduced by Ten-no [22]. A linearly approximated F12 coupled cluster singles and doubles method known as CCSD(F12) that retains only linear-F12 terms [23], is computationally less expensive than full CC-F12, but provides similar accuracy for target correlation energies. Explicitly-correlated EOM-CCSD schemes have been presented in the literature for IPs, EAs and excitation energies, the latter by Köhn [24] in the linear response framework. Also, the explicitly-correlated treatment of response properties has been reported recently [25-27]. For the case of excited and electronattached states an extended XSP-Ansatz was introduced in order to describe short-range correlation effects of promoted or attached electrons [24]. Similarly, if two electrons are attached it is necessarv to extend the DEA-EOM-CCSD(F12) attachment operator for the proper description of the state with two additional electrons. In this letter we report on the formulation and implementation of explicitly-correlated DIP and DEA-EOM-CCSD(F12) methods. In order to estimate the accuracy of the methods developed, test calculations are conducted for DIPs and DEAs of several molecules.

2. Theory

Henceforth, we denote occupied, virtual, virtuals from the complete basis set and general orbitals in a given basis set as $ij, ..., ab, ..., \alpha, \beta, ...$ and pq, ..., respectively.

2.1. CCSD(F12) model for the neutral state

Within the coupled-cluster (CC) theory the ground-state wave function of a neutral system has the form

$$\Psi_0 = e^{(T_1 + T_2 + ...)} \Phi_0, \tag{1}$$

where \hat{T}_n are regular cluster operators and Φ_0 – any single determinant reference, but frequently the ground-state Hartree-Fock determinant. The details of CC theory with the corresponding working equations have been presented in numerous articles and textbooks. In this work the coupled cluster singles and doubles (CCSD) neutral-state wave function will be used:

$$\Psi_0(CCSD) = e^{(T_1 + T_2)} \Phi_0.$$
(2)

The linearly approximated explicitly-correlated extension of CCSD, known as CCSD(F12) [23] includes an additional operator, \hat{T}'_{2} which takes care of short-range correlation effects:

$$\Psi_0(CCSD(F12)) = e^{(\widehat{T}_1 + \widehat{T}_2 + \widehat{T}'_2)} \Phi_0, \tag{3}$$

The \hat{T}'_2 operator has the form:

$$\hat{T}'_{2} = \frac{1}{2} \sum_{ijkl} t'^{ij}_{kl} \left(\sum_{\alpha\beta} \langle \alpha\beta | f_{12} | kl \rangle \hat{E}_{\alpha i} \hat{E}_{\beta j} - \sum_{ab} \langle ab | f_{12} | kl \rangle \hat{E}_{a i} \hat{E}_{b j} \right).$$
(4)

Here \hat{E}_{pq} denote unitary group generators,

$$E_{pq} = a_{p\uparrow}^+ a_{q\uparrow} + a_{p\downarrow}^+ a_{q\downarrow}.$$
⁽⁵⁾

and f_{12} are Slater-type geminals[22]:

$$f_{12} = -\frac{1}{\gamma} \exp(-\gamma r_{12}).$$
 (6)

Geminal amplitudes are defined according to Kato's cusp conditions[21]: $t_{ij}^{\prime ij} = \frac{3}{8}, t_{ji}^{\prime ij} = \frac{1}{8}, t_{ii}^{\prime ii} = \frac{1}{2}$, while all the remaining $t_{kl}^{\prime ij}$ amplitudes are set equal to zero.

2.2. DIP and DEA-EOM-CCSD(F12) methods

Within the DIP-EOM-CCSD(F12) approach the wave function of a doubly-ionized state has the form:

$$\Psi^{2+} = \widehat{R}^{2+} \Psi_0(\operatorname{CCSD}(F12)), \tag{7}$$

where \widehat{R}^{2+} can be presented as:

$$\widehat{R}^{2+} = \widehat{R}_1^{2+} + \widehat{R}_2^{2+}, \tag{8}$$

$$\widehat{R}_{1}^{2+} = \frac{1}{2} \sum_{i,i} r_{ij} \{ a_{j} a_{i} \}, \tag{9}$$

$$\widehat{R}_2^{2+} = \frac{1}{6} \sum_{i,j,k,a} r^a_{ijk} \{ a^{\dagger}_a a_k a_j a_i \}.$$

$$\tag{10}$$

Working equations for the DIP-EOM-CCSD(F12) method can be obtained by the projection of \overline{H} onto the proper excitation manifolds:

$$\langle \Phi_{ij} | [\overline{H}, \widehat{R}^{2+}(k)] | \Phi_0 \rangle = \omega_k \langle \Phi_{ij} | \widehat{R}^{2+}(k) | \Phi_0 \rangle, \tag{11}$$

$$\langle \Phi^a_{ijk} | [\overline{H}, \widehat{R}^{2+}(k)] | \Phi_0 \rangle = \omega_k \langle \Phi^a_{ijk} | \widehat{R}^{2+}(k) | \Phi_0 \rangle, \tag{12}$$

where Φ_{ij} and Φ^a_{ijk} are doubly-ionized Slater determinants, index k stands for numbering of doubly-ionized states and ω_k is the corresponding double ionization potential. Detailed diagrammatic representation of these equations can found in Ref. [10]. The explicitly-correlated version of the Eqs. (11) and (12) has the same form, but the elements of \overline{H} will be augmented by terms originating from geminals[13].There is no contribution of F(12) to the R-equations for the DIP problem.

The DEA-EOM-CCSD wave function of the target doubly electron attached state assumes the following form:

$$\Psi^{2-} = \widehat{R}^{2-} \Psi_0(CCSD(F12)), \tag{13}$$

and the \widehat{R}^{2-} operator can be written as:

$$\widehat{R}^{2-} = \widehat{R}_1^{2-} + \widehat{R}_2^{2-} + \widehat{R}_2^{\prime 2-}, \tag{14}$$

$$\widehat{R}_{1}^{2-} = \frac{1}{2} \sum_{a,b} r^{ab} \{ a_{a}^{\dagger} a_{b}^{\dagger} \},$$
(15)

$$\widehat{R}_2^{2-} = \frac{1}{6} \sum_{a,b,c,i} r_i^{abc} \{ a_a^{\dagger} a_b^{\dagger} a_c^{\dagger} a_i \},$$
(16)

$$\begin{aligned} \hat{R}_{2}^{2-} &= \frac{1}{2} \sum_{i,k,c,d,f} (r^{fc}) t_{id}^{\prime kc} \left(\sum_{\alpha,\beta} \langle \alpha\beta | f_{12} | dk \rangle \{ a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\beta}^{\dagger} a_{i}^{\dagger} \} - \sum_{a,b} \langle ab | f_{12} | dk \rangle \{ a_{a}^{\dagger} a_{b}^{\dagger} a_{f}^{\dagger} a_{i} \} \right) + \\ &+ \frac{1}{2} \sum_{i,k,c,d,f} (r^{fc}) t_{dk}^{\prime ic} \left(\sum_{\alpha,\beta} \langle \alpha\beta | f_{12} | kd \rangle \{ a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{f}^{\dagger} a_{i} \} - \sum_{a,b} \langle ab | f_{12} | kd \rangle \{ a_{a}^{\dagger} a_{b}^{\dagger} a_{f}^{\dagger} a_{i} \} \right). \end{aligned}$$

$$(17)$$

Geminal amplitudes in the Eq. (17) are fixed using the known cusp conditions:

$$t_{ia}^{\prime ia} = \frac{3}{8}, t_{ai}^{\prime ia} = \frac{1}{8}, \tag{18}$$

while all the remaining t_{jb}^{ia} and t_{bj}^{ia} amplitudes are set equal to zero. The working equations for r^{ab} and r_i^{abc} amplitudes have form:

$$\langle \Phi^{ab} | [\overline{H}, \widehat{R}^{2-}(k)] | \Phi_0 \rangle = \omega_k \langle \Phi^{ab} | \widehat{R}^{2-}(k) | \Phi_0 \rangle, \tag{19}$$

$$\langle \Phi_i^{abc} | [\overline{H}, \widehat{R}^{2-}(k)] | \Phi_0 \rangle = \omega_k \langle \Phi_i^{abc} | \widehat{R}^{2-}(k) | \Phi_0 \rangle, \tag{20}$$

where Φ^{ab} and Φ^{abc}_i are Slater determinants with two extra electrons and ω_k is the corresponding two-electron affinity. Detailed

expressions for the regular version of the DEA-EOM-CCSD equations is presented elsewhere[5,11]. In the Eqs. (19) and (20) \overline{H} will contain contributions from Slater geminal in the reference state plus extra terms, which originate from the \hat{R}_2^{2-} operator. The contribution of \hat{R}_2^{2-} to the elements of \overline{H} in Eq. (19) can be presented as:



while the Eq. (20) will contain the following extra terms:





Table 1

where Reg stands for the regular CCSD terms and the referencestate geminal contributions to the corresponding elements of effective hamiltonian. The addition of the \hat{R}_2^{2-} term provides a balanced treatment of ground and doubly electron attached states when the DEA-EOM method is based on CCSD(F12) wave functions. Algebraic expressions for used diagrams are available at Electronic Supplementary Material.

3. Details of implementation

The derived DIP-EOM-CCSD(F12) and DEA-EOM-CCSD(F12) methods are implemented in the ACES III quantum chemistry software package [28]. The underlying CCSD(F12) method uses the B-approximation according to Ref. [29]. The necessary Slater and Yukawa integrals are evaluated using a Rys quadrature technique [30]. Many-electron integrals are computed with numerical quadratures, using the Becke fuzzy cell method [31]. The atomic grids used for the calculation of the many-electron integrals are constructed using 50-point radial grids, and for angular integration, 194-point Lebedev-Laikov grids [32]. All two- and threeelectron integrals with the dipole moment operator are calculated with numerical quadratures. For the implementation of F12 contributions from the Eqs. (21) and (22) following intermediates are used:

$$V_{ie}^{pq} = \left\langle pq \left| \frac{f_{12}}{r_{12}} \right| ie \right\rangle + \sum_{k,l} \langle ie|f_{12}|kl\rangle \langle kl|pq\rangle - \sum_{a,b} \langle ie|f_{12}|ab\rangle \langle ab|pq\rangle - \sum_{k} (\langle iek| \frac{f_{12}}{r_{23}} |kqp\rangle + (\langle eik| \frac{f_{12}}{r_{23}} |kpq\rangle)$$
(23)

4. Results and discussion

Numerical tests of the new DIP and DEA-EOM-CCSD(F12) methods are conducted for several molecules using aug-cc-pVXZ basis sets with X = D, T, and Q[33–35]. We use the Slater exponent γ = 1.5 for all F12 calculations. Double ionization potentials are calculated for molecules using their equilibrium geometries, available online [36]. The values in complete basis set limit are obtained using the two-point scheme of Helgaker [37] and for our purpose (45) extrapolation is done for all considered molecules. Results for double ionization potentials, obtained with regular and explicitly-correlated DIP-EOM-CCSD methods are given in Table 1.

Double ionization potentials (in eV), calculated with regular(Reg.) and explicitly-correlated (F12) DIP-EOM-CCSD method.

					, ,				
	AUG-CC-PVDZ		AUG-CC-PVTZ		AUG-CC-PVQZ		AUG-CC-PV5Z	CBS	Exp.
	Reg.	F12	Reg.	F12	Reg	F12			
H ₂ O									
¹ A ₁	41.668	42.386	42.093	42.425	42.256	42.410	42.319	42.385	41.3
¹ B ₁	43.141	43.832	43.500	43.817	43.649	43.796	43.707	43.768	42.0
СО									
$^{1}\Sigma^{+}$	41.715	42.163	42.046	42.371	42.188	42.349	42.248	42.311	41.7
$^{1}\Pi$	42.526	43.177	42.854	43.170	42.995	43.150	43.053	43.114	42.2
C ₂ H ₂									
${}^{1}\Delta_{g}$	33.561	34.001	33.829	34.035	33.938	34.035	33.981	34.026	33.0
${}^{1}\Pi_{u}$	38.883	39.349	39.167	39.385	39.282	39.383	39.326	39.375	37.6
C₂H₄									
${}^{1}A_{g}$	30.913	31.273	31.218	31.382	31.316	31.392	31.357	31.378	30.1
${}^{1}A_{g}$	32.571	32.939	32.847	33.011	32.942	33.016	32.975	32.992	32.2
${}^{1}B_{3u}$	35.321	35.090	35.611	35.806	35.716	35.804	35.754	35.773	34.0
CH ₂ O									
¹ A ₁	33.328	33.943	33.756	34.038	33.904	34.034	33.959	33.986	
¹ A ₂	37.190	37.773	37.532	37.801	37.668	37.742	37.721	37.797	
¹ B ₁	39.116	39.764	39.444	39.749	39.590	39.732	39.647	39.675	
MAE	0.554	0.110	0.224	0.034	0.095	0.031	0.044		

Table 2
(in eV), calculated with regular(Reg.) and explicitly-correlated (F12) DEA-EOM-CCSD method

	AUG-CC-PVDZ		AUG-CC-PVTZ		AUG-C	C-PVQZ	AUG-CC-PV5Z	CBS
	Reg.	F12	Reg.	F12	Reg	F12		
F_2 ${}^1\Sigma_g^+$ R(F-F) = 2.25 Å	0.006	0.630	0.271	0.578	0.462	0.614	0.557	0.604
$N_2^{3}\Sigma_u^{-}$ R(N-N) = 1.60 Å	1.476	2.021	1.888	2.157	2.039	2.174	2.096	2.125
$CO^{3}\Sigma_{u}^{-}$ R(C-O) = 2.00 Å	4.009	4.568	4.340	4.621	4.470	4.613	4.521	4.547
O_2^{2+} $^{3}\Sigma_u^{-}$ R(O-O) = 1.1 Å	48.148	49.171	48.674	49.123	48.885	49.109	48.985	49.035
C_2 ${}^3\Sigma_g^+$ R(C-C) = 1.243 Å	1.197	1.425	1.664	1.782	1.915	1.977	2.162	2.285

The corresponding values for the mean absolute error (MAE) indicate significant improvement in the accuracy of obtained DIP results: for the case of the double-¿basis, the introduction of Slater geminals makes the MAE five times smaller then that of the regular DIP-EOM-CCSD method, while in the triple- ζ case even more accurate results are obtained. The errors do not exceed a few hundredth of eV. The regular DIP-EOM-CCSD results converge towards the CBS limit from below, while the explicitly-correlated results approach the CBS limit from above. This phenomena has been studied before for the case of ionization potentials and is related to the fact that correlation and relaxation effects contribute to the overall values of target properties with different signs. At the double-ζlevel some DIP-EOM-CCSD(F12) values show irregular behavior and may be even smaller then those in the better triple- ζ bases. This is related to the balance of correlation and relaxation since those effects are especially strong in this case. Overall, DIP-EOM-CCSD(F12) produces significantly improved results for all considered bases.

In order to assess the efficiency of the derived DEA-EOM-CCSD (F12) approach, double electron affinities are calculated for several molecules using the same bases as in DIP calculations. Normally closed-shell molecules cannot attach two electrons in their equilibrium geometries so we use stretched configurations for our purpose. Results for double electron affinities are presented in Table 2. The DEA-EOM-CCSD(F12) results are always improved compared to the regular DEA-EOM-CCSD approach: observed errors with respect to CBS are usually within several tenths of an eV. for the standard method, while the deviation of the explicitly correlated results from CBS does not exceed several hundredth of eV. Again, relaxation effects can be very strong for the case of doubly electron attached states, so the convergence can be different depending upon the magnitudes of correlation and relaxation in each case. Results for the C₂ molecule show only a little improvement over the regular method, and, on the other hand, the difference between quadruple and quintuple-ζvalues is almost 0.25 eV, that indicates that relaxation effects dominate over correlation and convergence to CBS is not reached. In most cases DEA-EOM-CCSD(F12) brings significant improvement over the regular method and can be a helpful tool for calculation of double electron affinities.

5. Conclusions

In this work the explicitly-correlated equation-of-motion coupled-cluster methods for double ionization potentials and dou-

ble electron affinities has been formulated and implemented. An extended *Ansatz* is offered for the double electron attachment operator that is necessary for a balanced treatment of neutral and double-electron attached states. Numerical results for the DIP and DEA-EOM-CCSD methods indicate slow convergence of the corresponding results with the maximal angular momentum of the basis sets used. The explicitly-correlated methods enables accurate results at the double- ζ level without any significant increase in computational costs, while even more precise values are available for triple- ζ . These facts makes the developed method a helpful tool for the treatment of double ionization and double electron attachment, whose accurate treatment is of significant importance for the current emphasis on core ionization and excitation processes encouraged by attosecond spectroscopy [38] among other new experimental technques.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.cplett.2017.12.040.

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