

# CID and CEPA calculations with linear $r_{12}$ terms

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Inclusion of linear  $r_{12}$ -dependent terms into many-electron wavefunctions considerably speeds up the convergence to the limit of a complete basis. Here, first results of MP3-R12, CID-R12, and CEPA-R12 calculations are presented. They demonstrate that the philosophy that led to the rather successful MP2-R12-scheme is similarly effective in treatments of electron correlation beyond second-order Møller–Plesset perturbation theory. For the atoms He, Be, Ne, Ar, and the molecules LiH, HF, H<sub>2</sub>O, and N<sub>2</sub>, correlation energies are obtained that are supposed to differ by at most a few percent from the basis set limits for the respective methods.

## 1. Introduction

Any many-electron wavefunction can, in principle, be expanded as a linear combination of all Slater determinants constructable from a given set of one-particle functions (spin-orbitals). The convergence, with increasing size of the spin-orbital basis, to the exact solution of the Schrödinger equation is, however, frustratingly slow. If, for an atom, we successively saturate the spin-orbital basis for increasing values of the angular quantum number  $l$ , the truncation error goes as  $\sim (L+1)^{-3}$ , if  $L$  is the highest  $l$  contained in the basis [1–3]. This slow convergence is related to the inability of a finite linear combination of Slater determinants to describe the correlation cusp [4] correctly. It has been shown, that if linear terms in the interelectronic coordinates  $r_{ij}$ , which allow one to account for the correlation cusp, are included in the wavefunction, the convergence is considerably speeded up. In typical cases – at least in the framework of second-order perturbation theory – the truncation error then goes as  $(L+1)^{-7}$  [5,6] rather than as  $(L+1)^{-3}$ , which allows one to achieve much higher accuracy than without  $r_{ij}$ -dependent terms. For the special case of two-electron systems like He or H<sub>2</sub>, the power of explicitly  $r_{12}$ -dependent wavefunctions has been exploited much earlier [7–10], but the generalization to arbitrary

systems has been inhibited by the occurrence of “difficult integrals”.

After a pilot study on He-like atoms [5], we have developed a method [11–15] applicable to arbitrary closed-shell atoms or molecules in the framework of Møller–Plesset perturbation theory (i.e. many-body perturbation theory with Hartree–Fock as reference) to second order with explicitly linear  $r_{12}$ -dependent terms (MP2-R12) and applied this method to a wealth of atoms [13] and molecules [10–12,14] and even to problems of structural chemistry like the comparison of competitive structures of carbonium ions [15].

In order to make our method practicable, some tricks are necessary [6,11,15]. The main philosophy is that some “difficult integrals” are simplified by completeness insertions, in such a way that (a) these simplifications become exact in the limit of a complete one-electron basis and (b) that the truncation errors introduced by these completeness insertions decrease as higher powers of  $L+1$  than the basis incompleteness error in conventional MP2 calculations. We have, in fact, introduced two variants of MP2-R12, referred to as approximations A and B [6,15], such that the error in approximation A goes as  $(L+1)^{-5}$  and in approximation B as  $(L+1)^{-7}$ .

Recently our MP2-R12 method in approximation A has been studied by Handy and co-workers [16] especially as far as the convergence with increasing

basis is concerned. These authors have also described the evaluation of the necessary integrals in terms of Cartesian Gaussians.

We now want to report on preliminary results with our method beyond MP2-R12. On one hand, we have generalized the Møller–Plesset treatment to include the third-order energy (MP3), on the other hand (this did not require additional matrix elements), we have implemented the configuration–interaction method limited to doubly excited configurations, CID, with linear  $r_{12}$  terms, i.e. CID-R12 and various coupled-electron-pair (CEPA) variants, again with linear  $r_{12}$  terms.

These extensions are straightforward as soon as one knows how to evaluate the necessary matrix elements [6]. We shall give a brief outline of CID-R12 and CEPA( $k$ )-R12 in section 2. We then describe applications to the atoms He, Be, Ne, Ar and the molecules LiH, HF, H<sub>2</sub>O, and N<sub>2</sub> in section 3.

For some small systems studied here (He, Be, Ne, LiH), results from the Gaussian–geminal method [17–20] are available and agree rather well with our results. In this method, a linear combination of functions of the type  $\exp(-\gamma r_{12}^2)$  is taken instead of a linear  $r_{12}$  term. This allows the closed evaluation of all integrals, but requires a somewhat tedious optimization of non-linear parameters.

## 2. The basic ideas of CID-R12 and CEPA( $k$ )-R12

As in standard CI calculations, we define some one-electron basis and start by performing a single-configuration SCF calculation in this basis. The SCF wavefunction  $\phi$  is then taken as reference. Let the spin-orbitals  $\psi_i, \psi_j$ , etc. be occupied in  $\phi$  and let  $\psi_a, \psi_b$ , etc. be unoccupied, such that the  $\psi_i$  together with the  $\psi_a$  form an orthogonal set. Let  $Q$  be the projector onto this one-electron basis,

$$Q = \sum_i |\psi_i\rangle\langle\psi_i| + \sum_a |\psi_a\rangle\langle\psi_a|. \quad (1)$$

We then construct two types of “doubly excited” configurations, (a) those expressible in the spin-orbital basis,

$$\phi_{ij}^{ab} = a_{ij}^{ab}\phi = a_a^\dagger a_b^\dagger a_j a_i \phi \quad (2)$$

and (b) additional double excitations  $\phi_{ij}$  that are not

expressible in the given basis and which describe the cusp behaviour for small  $r_{12}$ . The  $\phi_{ij}$  can be formally written (implying the Einstein summation convention [21]) as [6]

$$\phi_{ij} = \frac{1}{2} r_{\alpha\beta}^{ij} a_{ij}^{\alpha\beta} \phi, \quad (3)$$

$$r_{\alpha\beta}^{ij} = \langle \psi_\alpha(1)\psi_\beta(2) | r_{12} | \psi_i(1)\psi_j(2) \rangle, \quad (4)$$

where  $\psi_\alpha, \psi_\beta$  are unoccupied spin-orbitals, that (unlike the  $\psi_a, \psi_b$ ) together with the  $\psi_i, \psi_j$  form a complete set. In a pictorial description, one can say that  $\phi_{ij}$  is obtained from  $\phi$  in replacing the spin-orbital pair

$$[ij] = 1/\sqrt{2}[\psi_i(1)\psi_j(2) - \psi_j(1)\psi_i(2)] \quad (5)$$

by

$$w_{ij}(1, 2) = \frac{1}{2} r_{12} [ij]. \quad (6)$$

It has turned out to be convenient not to use the  $\phi_{ij}$  as such, but to orthogonalize them to the  $\phi_{ij}^{ab}$ . The orthogonalized functions  $\tilde{\phi}_{ij}$  can formally be written as (with  $N_{ij}$  a normalization factor)

$$\tilde{\phi}_{ij} = \frac{1}{2} N_{ij} (r_{\alpha\beta}^{ij} a_{ij}^{\alpha\beta} - r_{ab}^{ij} a_{ij}^{ab}) \phi. \quad (7)$$

They can be obtained from  $\phi$  in replacing  $[ij]$  by

$$\tilde{w}_{ij}(1, 2) = [1 - Q(1)][1 - Q(2)] w_{ij}. \quad (8)$$

The CID-R12 wavefunction is of the form

$$\Psi = \phi + \sum_{i < j} \tilde{c}_{ij} \tilde{\phi}_{ij} + \sum_{i < j} \sum_{a < b} c_{ab}^{ij} \phi_{ij}^{ab} \quad (9)$$

and both the  $\tilde{c}_{ij}$  and the  $c_{ab}^{ij}$  are treated as variational parameters.

The necessary matrix elements of the Hamiltonian have been derived elsewhere [6] and they will not be repeated here. Note that the secular matrix of the CID-R12 method contains the conventional CID block as the dominant one.

As in our MP2-R12 calculations, we assume that the Hartree–Fock equations are satisfied exactly and that a generalized as well as an extended Brillouin-theorem hold, i.e. that [6]

$$\begin{aligned} \langle \phi_i | F | \phi_a \rangle &= 0, & \langle \phi_i | F | \phi_\alpha \rangle &= 0, \\ \langle \phi_a | F | \phi_\alpha \rangle &= 0, \end{aligned} \quad (10)$$

where  $F$  is the Fock-operator. We further evaluate three- and four-electron integrals formally by means of completeness insertions, as mentioned in the in-

roduction. While for MP2-R12 calculations [13,14], both approximations A and B turned out to be acceptable, our experience with CI calculations has so far been that only the more sophisticated approximation B gives good results. All results reported here were obtained on this level.

The final CI equations are effectively solved by means of the matrix-oriented direct CI approach, where the recent reformulation of Pulay et al. [22] has been implemented.

CEPA-type methods are formally very similar to CID, but they remedy one defect of CID, namely that CID is not extensive, i.e. does not scale with the

number of particles. We have considered the three most-used CEPA-variants, namely CEPA(0) (also called L-CPMET or L-CCD), CEPA(1), and CEPA(2). For details on their definition, see, e.g. refs. [23–25]. We have also implemented the CPFD-method [26] with a CEPA(1) type energy denominator. As required by a formal analysis [27], CPFD and CEPA(1) are not identical, but numerically almost indistinguishable. The results of CEPA-calculations, especially CEPA(1), are usually quite close to those obtained by the coupled-cluster-with-doubles (CCD) method. For a recent review on the latter, see ref. [28].

Table 1  
Results of R12 calculations on closed-shell atoms <sup>a)</sup>. Energies in mhartree

	He	Be	Ne	Ar
SCF	-2861.68	-14573.02	-128546.70	-526816.84
reference SCF <sup>b)</sup>	-2861.68	-14573.02	-128547.10	-526817.51
MP2	-36.46	-73.40	-350.75	-605.57
MP2-R12	-37.36	-75.86	-384.14	-687.83
reference MP2	-37.36 <sup>d)</sup>	-76.36 <sup>e)</sup>	-387.8 <sup>b)</sup>	-706 <sup>k)</sup>
MP3	-4.11	-10.90	-0.01	-14.69
MP3-R12	-3.63	-9.54	4.39	-12.19
reference MP3	-3.63 <sup>e)</sup>	-8.87 <sup>e)</sup>	≈4–5 <sup>l)</sup>	
CID	-41.53	-88.28	-341.95	-584.44
CID-R12	-42.00	-89.52	-369.47	-655.38
CEPA(0)	-41.87	-97.19	-353.70	-626.00
CEPA(0)-R12	-42.34	-98.49	-382.45	-705.21
CEPA(2)		-92.14	-352.95	-624.53
CEPA(2)-R12		-93.47	-381.61	-703.46
CPFD		-91.87	-350.92	-620.15
CPFD-R12		-93.17	-379.36	-698.19
reference CCD		-92.96 <sup>o)</sup>	-381 <sup>l)</sup>	
reference $E(\text{corr})$	-42.04 <sup>f)</sup>	-94.31 <sup>g)</sup>	-389 <sup>k)</sup>	-732 <sup>m)</sup>
single excitations <sup>e)</sup>	-0.03	-0.7	-1.6	-0.9

<sup>a)</sup> GTO basis sets: [16.10.6.3] for He and Be, [16.10.7.3] for Ne, and [17.13.7.3] for Ar.

<sup>b)</sup> As quoted in ref. [29]. <sup>c)</sup> From CEPA-PNO [30] calculations with the same basis set.

<sup>d)</sup> Malinowski et al. [31] have extrapolated a second-order energy of  $-37.364 mE_h$ , which compares well with the STO-MP2-R12 result of  $-37.359 mE_h$  [13]. The Gaussian-geminal method yields  $-37.372 mE_h$  [17].

<sup>e)</sup> Extrapolated value of ref. [32]. The Gaussian-geminal result is  $-3.62 mE_h$  [18]. <sup>f)</sup> Pekeris' result [33].

<sup>g)</sup> From a recent paper of Salomonson and Öster [34], where earlier calculations with STOs and Gaussian-geminals are compared and the full CI limit is discussed. An extrapolation from the STO-MP2-R12 method gives  $E^{(2)} = -76.32 mE_h$  [13].

<sup>h)</sup> Recommended value of ref. [13].

<sup>i)</sup> Three values are available for comparison:  $3.5 mE_h$  from a numerical approach [35],  $4.4 mE_h$  from STO-MP3 calculations [36], and  $4.63 mE_h$  from the Gaussian-geminal method [19].

<sup>j)</sup> See refs. [35] and [19]. <sup>k)</sup> As estimated by Lee et al. [37]. Others predict  $-385 \pm 8$  [38] and  $-390$  [39]  $mE_h$ .

<sup>l)</sup> From ref. [40]. <sup>m)</sup> Ref. [39]. See also ref. [40].

The basis sets in our calculations were of GTO-type, with p, d, f functions constructed from Gaussian lobes. They are indicated in the respective tables. [16.10.6.3], e.g. means a basis of 16s, 10p, 6d, and 3f AOs. They are usually taken uncontracted. The basis sets used here are in most cases identical to basis sets described in detail in refs. [13,14].

### 3. Discussion of the results

In table 1, results for He, Be, Ne, and Ar are shown. The entire correlation energy (including inner shells) is always taken care of. The MP2-R12 values are essentially those of ref. [13] and they need not be further discussed. Note that we have only considered results from approximation B and that the STO results (with larger basis sets) are usually superior to the GTO results (but that GTOs can be used for molecules as well). The error of the MP2-R12 values with respect to the estimated basis set limit is of the order of 1% or less (except for Ar, where it is almost 3%; here a somewhat larger basis ought to be used).

For the third-order energy MP3, there are no reliable basis set limits available. Estimates are very difficult since rather large positive and negative terms, which cancel in part, contribute to the MP3-energy. The change from MP3 to MP3-R12 is therefore more spectacular than the corresponding change on MP2 level. A more detailed discussion of the third-order energies, including also STO results, will be given elsewhere.

Among the CEPA-variants usually CEPA(1) – which is in this context, i.e. without single excitations, practically equivalent to CPDF – is regarded as best, i.e. closest to full CI. Our CPDF results are supposed to be close to the basis set limit of CCD, and this is confirmed by the values which are available. The difference from the exact correlation energies must be attributed mainly to the contributions of single and triple excitations, which have so far been neglected in our calculations.

In table 2, we compare the contributions of the various pairs to the CID correlation energy of Ne with and without  $r_{12}$  terms, and a recent conventional calculation with a large STO basis set [41]. The agreement between CID-R12 and the results of ref. [41] (IRR in table 2) is surprisingly good.

Table 2

Comparison of CID and CID-R12 pair energies (in millihartree) of the Ne atom with pair energies from a recent calculation <sup>a)</sup> by Iwański, Rutkowska and Rutkowski (IRR) [41]

	CID <sup>b)</sup>	CID-R12 <sup>b)</sup>	IRR <sup>a)</sup>
1s <sup>2</sup> ( <sup>1</sup> S)	-38.88	-40.94	-40.74
1s2s ( <sup>1</sup> S)	-3.84	-4.01	-3.97
( <sup>3</sup> S)	-1.55	-1.59	-1.58
2s <sup>2</sup> ( <sup>1</sup> S)	-10.92	-11.90	-11.85
1s2p ( <sup>1</sup> P)	-7.43	-8.10	-8.22
( <sup>3</sup> P)	-13.55	-13.73	-13.76
2s2p ( <sup>1</sup> P)	-52.40	-60.84	-61.04
( <sup>3</sup> P)	-22.30	-23.26	-23.66 <sup>d)</sup>
2p <sup>2</sup> ( <sup>1</sup> D)	-74.39	-84.89	-84.25
( <sup>1</sup> S)	-41.09	-43.29	-43.09
( <sup>3</sup> P)	-75.58	-76.93	-77.57
total	-341.95	-369.47	-369.36
$E(\Psi^{(0)} + \lambda \Psi^{(1)})$ <sup>e)</sup>	-338.8	-366.6	-368.4 <sup>e)</sup>

<sup>a)</sup> The method used may be regarded as a symmetry-adapted version of Siegbahn's pair-contracted CI [42]. An STO basis set with  $l \leq 9$  was used.

<sup>b)</sup> GTO basis set: [16.10.7.3].

<sup>c)</sup> Minimum of the expectation value of a two-term function.

<sup>d)</sup> In table 1 of ref. [41], a pair energy of  $-23.66 mE_h$  is reported. This value is clearly not the product of the numbers 0.874 and  $-26.61$  also printed in table 1 as it should be and is not consistent with the total correlation energy. We therefore assume a misprint and suppose the correct pair energy to be  $-23.26 mE_h$ .

<sup>e)</sup> See also ref. [43], where the accuracy of first-order wavefunctions for ten-electron atomic systems is discussed.

The results for the molecules LiH, HF, H<sub>2</sub>O, and N<sub>2</sub> are displayed in table 3. The general pattern is similar to that in table 1. Again, there are only few reliable reference values available. As before, the difference between our CEPA(1)-R12 correlation energies and the estimated exact correlation energies comes mainly from the neglect of singly and triply substituted configurations. Note that in N<sub>2</sub>, only the valence-shell correlation energy was considered.

In table 4, we finally report on an application of our method to the evaluation of spectroscopic constants, namely in the case of N<sub>2</sub>. For this example, the changes due to inclusion of linear  $r_{12}$  terms are small. The equilibrium distance is consistently reduced by 0.003 Å, while the harmonic frequency is increased by  $\approx 15 \text{ cm}^{-1}$ . Compared with experi-

Table 3  
Results of R12 calculations on closed-shell molecules <sup>a)</sup>. Energies in mhartree

	LiH	HF	H <sub>2</sub> O	N <sub>2</sub> <sup>b)</sup>
SCF	-7987.30	-100070.22	-76065.75	-108991.33
reference SCF <sup>b)</sup>	-7987.35	-100070.81		
MP2	-69.43	-346.14	-323.98	-377.73
MP2-R12	-72.16	-378.78	-356.74	-409.28
reference MP2	-72.78 <sup>d)</sup> -70.88 <sup>b)</sup>	-367.9 <sup>b)</sup>		
MP3	-8.85	1.64	-3.38	11.01
MP3-R12	-7.65	4.61	0.10	8.84
reference MP3	-6.89 <sup>e)</sup> -8.35 <sup>b)</sup>	2.05 <sup>b)</sup>		
CID	-79.66	-332.98	-313.78	-343.92
CID-R12	-81.31	-360.58	-340.71	-373.51
CEPA(0)	-82.28	-349.44	-333.66	-382.65
CEPA(0)-R12	-83.99	-378.78	-362.59	-418.08
CEPA(2)	-81.03	-348.31	-332.27	-379.81
CEPA(2)-R12	-82.73	-377.54	-361.07	-414.80
CPFD	-80.96	-345.41	-328.69	-372.28
CPFD-R12	-82.64	-374.31	-357.14	-406.06
reference CCD	-82.7 <sup>d)</sup> -81.5 <sup>b)</sup>			
reference <i>E</i> (corr) single excitations <sup>c)</sup>	-83.2 <sup>f)</sup> -0.25	-381 <sup>f)</sup> -2.5		
			-2.2	

<sup>a)</sup> GTO basis sets and geometries: LiH: [14.7.4.1/11.7.4.1] for Li and [12.6.3.1/9.6.3.1] for H,  $R_c=3.015 a_0$ ; HF: [15.10.5.2] for F and [10.4.1/7.4.1] for H,  $R_c=1.7328 a_0$ ; H<sub>2</sub>O: [12.7.4.1/9.7.4.1] for O and [10.4.1/7.4.1] for H,  $R_c=1.80885 a_0$  and  $\alpha=104.52^\circ$ ; N<sub>2</sub>: [14.10.4.1],  $R_c=2.07 a_0$ .

<sup>b)</sup> Results from the semi-numerical McCullough method. See ref. [44] and references therein.

<sup>c)</sup> As in table 1. <sup>d)</sup> Obtained with the Gaussian-geminal method [20].

<sup>e)</sup> From the Gaussian-geminal method [18]. The corresponding second-order energy from this calculation is  $-72.18 mE_h$ .

<sup>f)</sup> See ref. [44]. <sup>b)</sup> Valence-shell correlation only.

ment, all CEPA variants predict a too-short  $r_e$  and too-large  $\omega_e$ . Curiously enough, CEPA(0) without  $r_{12}$  terms is closest to experiment. For this example, the inclusion of single and triple substitutions is obviously more important than the correct description of the short-range correlation.

#### 4. Conclusions

This paper clearly shows that the concept of describing the correlation cusp by means of linear  $r_{12}$  terms in the wavefunction to speed up the convergence of a many-electron wavefunction in an orbital

basis, is not limited to Møller-Plesset perturbation theory, but generally applicable on any level of many-electron theory.

It appears now possible to get about 99% of the basis set limit in MP2, or CID, or CEPA type calculations. The next step must be to combine a full coupled-cluster approach including single and, hopefully, triple substitutions with the linear  $r_{12}$  method to obtain results close to the exact correlation energies.

Table 4

Equilibrium distance  $r_e$ , harmonic vibration frequency  $\omega_e$ , anharmonicity  $\omega_e x_e$  and minimum energy  $E_{\min}$  for  $N_2$  in different approximations <sup>a)</sup>

	$r_e$ (Å)	$\omega_e$ (cm <sup>-1</sup> )	$\omega_e x_e$ (cm <sup>-1</sup> )	$E_{\min}$ (hartree)
SCF	1.066	2730	10	-108.9889
MP2	1.113	2194	19	-109.3648
MP2-R12	1.109	2217	19	-109.3825
MP3	1.089	2531	10	-109.3564
MP3-R12	1.086	2546	10	-109.3751
CID	1.086	2528	12	-109.3329
CID-R12	1.083	2545	12	-109.3489
CEPA(0)	1.099	2383	15	-109.3719
CEPA(0)-R12	1.096	2397	15	-109.3911
CEPA(2)	1.097	2404	14	-109.3690
CEPA(2)-R12	1.094	2419	14	-109.3880
CPFD	1.094	2440	13	-109.3614
CPFD-R12	1.091	2456	13	-109.3797
other theory <sup>b)</sup>	1.100	2353		
experiment <sup>c)</sup>	1.0977	2358.6	14.3	

<sup>a)</sup> GTO basis set: [10.6.2.1/6.4.2.1], taken from ref. [45]. Ten electrons are correlated in all approximations.

<sup>b)</sup> From the work of Almlöf et al. [46]. The computed spectroscopic constants were obtained from a CAS(6act)/MR-CI+Q calculation with a [18.13.6.5.4.3/6.5.4.3.2.1] GTO basis set.

<sup>c)</sup> Ref. [47].

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