Theoret. Chim. Acta (Berl.) 52, 93–101 (1979)

THEORETICA CHIMICA ACTA

Many-Orbital Cluster Expansion for the Exchange-Repulsion Energy in the Interaction of Closed-Shell Systems

The Neon-Neon Interaction

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The energy of exchange repulsion between two closed-shell systems described by determinantal wave functions has been represented as a sum of contributions arising from the interaction of two, three and four orbitals at a time. These contributions have been calculated for the interaction of two neon atoms. It has been found that in the van der Waals minimum region the two-orbital components are of secondary importance and that about 90% of the total exchange energy originates from the three-orbital interactions of *L*-shell electrons. The four-orbital as well as the double-exchange terms have been found negligible. The approximate algorithms for evaluation of the exchange repulsion energy have been tested and discussed.

Key words: Closed-shell systems – Neon-neon interaction

1. Introduction

Since the pioneering works of Heitler, London and Slater [1–3] it has been known that the net force acting between atoms and molecules is a result of a balance of two physically different effects: the long-range attraction and the short-range repulsion. The former effect can be given more or less classical interpretation and its contribution to the interaction energy can easily be related to molecular properties such as dipole and higher multipole moments, static and dynamic polarizabilities, hyperpolarizabilities, etc. [4]. Presently, the theory of the long-range interactions is well advanced and, with a proper use of experimental information, can be effectively applied to study interactions of large polyatomic molecules [5]. On

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* This work was partly supported by the Polish Academy of Sciences within the project MR-I.9.

the contrary, the energy of the short-range repulsion, as a purely quantum mechanical exchange effect, cannot be related to any experimentally known property of the interacting molecules and a reliable information about this energy can be obtained only from *ab initio* quantum mechanical calculations. As a consequence, very little is known about the actual magnitude of the exchange repulsion between large and medium size molecules.

In practice, the repulsive effect is usually obtained either variationally, using supermolecular LCAO MO or SCF methods, or within the symmetry-adapted perturbation treatment as the first-order exchange correction, evaluated using SCF wave functions for isolated systems. The supermolecular SCF approach might be considered advantageous since it automatically allows for deformation of orbitals, resulting from induction interaction, the effect which appears in the second and higher orders of the perturbation theory. However, for larger systems it is really difficult to get accurate energies in this way[1] because of the basis set superposition error, which may be sometimes larger than the interaction energy itself [6]. Moreover, the supermolecular SCF method as a rather brute-force approach cannot be effectively applied to large polyatomic molecules. From this point of view, the perturbation theory approach seems to be superior, since it permits the introduction of simple and well defined approximate algorithms for the exchange energy, which can be extended to larger systems. Recently, Murrell and Varandas [10] proposed such a simplified method for the calculation of the first-order exchange repulsion energy. This method consists in using properly selected maximum overlap hybrids rather than all occupied orbitals. In the present paper we propose another method of simplifying calculations of the first-order exchange energy for the interaction of closed-shell systems. The method employs the idea of the many-orbital cluster expansion set forth in Ref. [11]. The advantage of the cluster representation results from the fact that it offers a possibility of computing the exchange energy as a sum of two- three-, and four-orbital contributions. Neglecting the many-orbital contributions resulting from the interaction of weakly overlapping orbitals we obtain well defined and well controlled approximations to the exchange repulsion energy. In the present paper we test these possibilities in the case of the Ne–Ne interaction.

2. Many-Orbital Cluster Expansion of the First-Order Exchange Energy

Let us consider the interaction of two closed-shell systems, A and B, and let Φ_A and Φ_B denote the determinantal wave functions of these systems. The first-order energy in the symmetry-adapted perturbation theory is defined:

$$E_{\text{int}}^{(1)} = \frac{\langle \Phi_A \Phi_B | \mathscr{A} V | \Phi_A \Phi_B \rangle}{\langle \Phi_A \Phi_B | \mathscr{A} | \Phi_A \Phi_B \rangle}, \tag{1}$$

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[1] In fact, even for the relatively small Ne_2 system, three values of the SCF interaction energy at $R = 6$ a.u. (van der Waals minimum region) pretend to be in error by a few percent: 0.44 (-4) [7], 0.56 (-4) [8] and 0.63 (-4) a.u. [9].

where $\mathscr{A}$ is the antisymmetrizer for all electrons in the complex AB and V is the operator of intermolecular interaction. V can be conveniently expressed in the form

$$V = \sum_{s\in A} \sum_{t\in B} v(st), \tag{2}$$

where $v(st)$ is a generalized two-electron potential [11]. For the interaction of two neutral atoms it is defined

$$v(st) = R^{-1} - r_{At}^{-1} - r_{Bs}^{-1} + r_{st}^{-1}$$

where R is the internuclear separation and r_{At}, r_{Bs} and r_{st} are distances between the nuclei and electrons specified by the subscripts A, B, t and s.

The first-order energy (1) is usually represented as a sum of Coulomb and exchange contributions

$$E_{\text{int}}^{(1)} = Q + E_{\text{exch}}^{(1)}, \tag{3}$$

where $Q = \langle \Phi_A \Phi_B | V | \Phi_A \Phi_B \rangle$ and the first-order exchange, $E_{\text{exch}}^{(1)}$, is defined essentially as a difference $E_{\text{int}}^{(1)} - Q$. The main, single exchange part of $E_{\text{exch}}^{(1)}$ is given by

$$E_{\text{exch}} = \langle \Phi_A \Phi_B | V(\mathscr{P} - \langle \mathscr{P} \rangle) | \Phi_A \Phi_B \rangle, \tag{4}$$

where

$$\mathscr{P} = -\sum_{s\in A} \sum_{t\in B} P_{st} \tag{5}$$

is the sum of permutation operators P_{st} interchanging the coordinates of sth and tth electrons, and $\langle \mathscr{P} \rangle$ is calculated with $\Phi_A \cdot \Phi_B$ [11]. The explicit expression for the difference between $E_{\text{exch}}^{(1)}$ and E_{exch} can be found in Ref. [12]. The first who expressed E_{exch} in terms of orbitals were Williams, Schaad and Murrell [13]. Their result can be written in the form of a cluster expansion which is transparent and simple to interpret:

$$E_{\text{exch}} = \sum_{i\in A} \sum_{j\in B} \varepsilon(i \mid j) + \sum_{\substack{i,k\in A \\ i<k}} \sum_{j\in B} \varepsilon(ik \mid j) + \sum_{i\in A} \sum_{\substack{j,l\in B \\ j<l}} \varepsilon(i \mid jl) + \sum_{\substack{i,k\in A \\ i<k}} \sum_{\substack{j,l\in B \\ j<l}} \varepsilon(ik \mid jl), \tag{6}$$

where, for instance, the symbol $\varepsilon(ik \mid j)$ indicates that the corresponding three-orbital contribution depends only on the ith and kth orbitals of system A and jth orbital of system B. The contributions $\varepsilon(ik \mid j)$, $\varepsilon(i \mid jl)$ and $\varepsilon(ik \mid jl)$ are defined to be symmetric with respect to the interchange of indices i and k or l and j and can be obtained by a symmetrization of the "primitive" quantities $\tilde{\varepsilon}(ik \mid j)$, $\tilde{\varepsilon}(i \mid jl)$ and $\tilde{\varepsilon}(ik \mid jl)$:

$$\varepsilon(ik \mid j) = \tilde{\varepsilon}(ik \mid j) + \tilde{\varepsilon}(ki \mid j) \tag{7}$$

or

$$\varepsilon(ik \mid jl) = \tilde{\varepsilon}(ik \mid jl) + \tilde{\varepsilon}(ki \mid jl) + \tilde{\varepsilon}(ik \mid lj) + \tilde{\varepsilon}(ki \mid lj). \tag{8}$$

The explicit expressions for the many-orbital contributions to E_{exch} are as follows:

$$\begin{aligned}\varepsilon(i \mid j) = {} & -2\langle a_i b_j|v_{12}|b_j a_i\rangle + 6\langle a_i b_j|v_{12}|a_i b_j\rangle S_{ij}^2 \\ & - 2\langle a_i b_j|v_{12}|b_j b_j\rangle S_{ij} - 2\langle a_i b_j|v_{12}|a_i a_i\rangle S_{ij},\end{aligned} \tag{9}$$

$$\begin{aligned}\tilde{\varepsilon}(ik \mid j) = {} & 2\langle a_i b_j|v_{12}(1 - 2P_{12})|a_k a_l\rangle S_{kj} \\ & + 2\langle a_i b_j|v_{12}|a_k b_j\rangle S_{kj} S_{ij} + 4\langle a_i b_j|v_{12}|a_i b_j\rangle S_{kj}^2,\end{aligned} \tag{10}$$

$$\begin{aligned}\tilde{\varepsilon}(ik \mid jl) = {} & -2\langle a_i b_j|v_{12}|a_k b_l\rangle S_{il} S_{kj} \\ & + 4\langle a_i b_j|v_{12}|a_i b_l\rangle S_{kl} S_{kj} + 4\langle a_i b_j|v_{12}|a_k b_j\rangle S_{kl} S_{il},\end{aligned} \tag{11}$$

where the occupied orbitals of systems A and B are denoted by a_i, a_k and b_j, b_l respectively, $S_{ij} = \langle a_i \mid b_j\rangle$, $v_{12} \equiv v(12)$ and the expression for $\tilde{\varepsilon}(i \mid jl)$ can easily be obtained from (10) by substituting b_l for a_k, v_{21} for v_{12} and interchanging a_i and b_j.

In a similar way the Coulomb energy may be written as

$$Q = \sum_{i \in A} \sum_{j \in B} q(i \mid j), \tag{12}$$

where $q(i \mid j) = \langle a_i b_j|v_{12}|a_i b_j\rangle$.

It should be stressed that the expression for $\varepsilon(i \mid j)$ is identical with the expression for E_{exch} in the interaction of two helium-like systems. Therefore the contribution $\varepsilon(i \mid j)$ can be interpreted as the result of the exchange interaction between the orbital a_i of system A and the orbital b_j of system B. The last three terms in Eq. (6) are reponsible for the pair-wise orbital nonadditivity of E_{exch}. The contribution $\varepsilon(ik \mid j)$, for instance, can be defined as a three-orbital pair-wise nonadditive part of the exchange energy in the interaction between a beryllium-like system, with orbitals a_i and a_k, and a helium-like system, described by an orbital b_j. Similarly, $\varepsilon(ik \mid jl)$ is defined as a four-orbital contribution to the exchange interaction of two beryllium-like systems with orbitals a_i, a_k and b_j, b_l.

It is important to note here, that the expressions (6) and (12) are quite general and enable us to expand E_{exch} and Q also in terms of shells or other subgroups of orbitals. Many-shell contributions can be built up of many-orbital components using the method given in Ref. [11].

3. Numerical Example: Interaction of Two Neon Atoms

In our calculations of the first-order energy and its many-orbital components for Ne_2 system we have used Clementi's SCF orbitals for the Ne atom [14]. Their radial parts were approximated in the form of Gaussian expansion

$$\varphi(r) \simeq r^l \sum_{k=1}^{N} c_k e^{-\alpha_k r^2}, \tag{13}$$

where l is the angular quantum number. The nonlinear parameters α_k and linear ones c_k have been optimized to obtain the least square fit [15] to $\varphi(r)$. This ensures a faithful representation of HF function at large distances from the nucleus which

Table 1. Parameters of Gaussian representations (14) of Clementi's Hartree–Fock orbitals [14]. The mean square deviation δ is defined by Eq. (15)

Function (4/4/4)		Function (6/8/8)	
α_k	c_k	α_k	c_k
1*s* ($\delta = 11.0\%$)		1*s* ($\delta = 5.0\%$)	
0.159277	−0.000021	0.027167	−2.4 (−8)
0.772291	0.001079	0.168719	−0.000025
5.175634	0.341560	0.728456	0.000887
23.578653	7.243614	4.136383	0.132252
		13.292992	2.982685
		125.741670	13.657932
2*s* ($\delta = 8.5\%$)		2*s* ($\delta = 1.0\%$)	
0.115314	0.000701	0.097661	0.000164
0.254129	0.033829	0.166164	0.004112
0.793608	0.500741	0.287921	0.027941
39.123468	−3.092994	0.443377	0.051872
		0.681464	0.194150
		1.549567	0.484850
		17.926980	−1.722855
		141.993370	−2.879560
2*p* ($\delta = 9.6\%$)		2*p* ($\delta = 0.5\%$)	
0.087504	0.001320	0.060449	0.000038
0.210580	0.052411	0.104132	0.001254
0.744971	1.056962	0.192142	0.014033
5.363038	10.726426	0.411053	0.113568
		1.031536	0.586092
		3.194203	2.230887
		13.118573	4.581282
		138.453810	6.081587

has been shown to be very important to obtain an accurate value of exchange energy [6, 16].

Two representations of the HF wave function were used in practical calculations: the (6/8/8) fit (1*s* expanded into 6, 2*s* into 8 and 2*p* into 8 Gaussian functions) and the (4/4/4) fit. The (6/8/8) function has been used to provide accurate values for many-orbital contributions, while the (4/4/4) function to test usefulness of short representations (14). The latter is important from the point of view of practical computations for larger systems. The parameters α_k and c_k of both functions have been listed in Table 1. To demonstrate the aptness of Gaussian expansions, the mean square deviation from the exact orbitals, defined as

$$\delta = \left(\frac{1}{R} \int_0^R \frac{|\varphi(r) - r^l \sum_k c_k e^{-\alpha_k r^2}|^2}{\varphi(r)^2} \, dr \right)^{1/2}, \tag{14}$$

has been also reported in Table 1. For particular orbitals the range of integration R has been chosen so as $|\varphi(r)| < 10^{-8}$ for $r > R$.

Table 2. A comparison of the values of the exchange energy $E_{\mathrm{exch}}^{(1)}$ obtained with $(6/4)_{\mathrm{STO}}$ Clementi's wave function and its (4/4/4) and (6/8/8) Gaussian representations. The energy and the internuclear distance R are expressed in atomic units

R	(4/4/4)	(6/8/8)	$(6/4)_{\mathrm{STO}}$ [17]	$(E_{\mathrm{exch}}^{(1)} - E_{\mathrm{exch}})^{\mathrm{a}}$
4.0	1.1609 (−2)	1.1734 (−2)	1.2367 (−2)	1.53 (−4)
5.0	1.1397 (−3)	1.0161 (−3)	1.0650 (−3)	8.60 (−6)
5.5	3.2773 (−4)	3.0282 (−4)	3.1670 (−4)	2.29 (−6)
6.0	9.1057 (−5)	8.9851 (−5)	9.4360 (−5)	6.20 (−7)
7.0	7.3927 (−6)	7.7907 (−6)	8.3211 (−6)	4.67 (−8)

[a] Results obtained with (6/8/8) function.

The calculations of $E_{\mathrm{int}}^{(1)}$ and its components have been performed for internuclear distances ranging from 4 a.u. to 7 a.u., i.e. in the region close to the van der Waals minimum. In Tables 2 and 3, E_{exch} and Q, computed with the both wave functions, are compared with the results of Conway and Murrell [17], obtained with the exact Clementi's orbitals. At first, we would like to point to the aptness of the (4/4/4) function which yields the results being less than 10% in error in the region considered. Secondly, we notice that the results obtained with the function (6/8/8) are uniformly lower than the Conway and Murrell values by about 5%. Since the values of δ for $2s$ and $2p$ orbitals are in this case not higher than 1%, this discrepancy can be attributed only in part to the fact that the approximate orbitals have been used. However, we should note that the formulae used in Ref. [17] to calculate E_{exch} and Q differ from those used in the present paper by terms due to more than single exchanges. We have investigated the effect of multipole exchanges and we have found that $E_{\mathrm{exch}}^{(1)} - E_{\mathrm{exch}}$ amounts to from 1.3% at $R = 4$ a.u. to 0.6% at $R = 7$ a.u. of the exchange energy (see Table 2).[2] Finally, it is plausible that the results of Conway and Murrell may not be highly accurate because of well-known problems with very accurate calculations of two-electron integrals over Slater-type orbitals.

Table 3. A comparison of the values of the Coulomb energy obtained with $(6/4)_{\mathrm{STO}}$ Clementi's wave function and its (4/4/4) and (6/8/8) Gaussian representations. The energy and the interatomic distance R are expressed in atomic units

R	(4/4/4)	(6/8/8)	$(6/4)_{\mathrm{STO}}$ [17]
4.0	−3.328 (−3)	−3.186 (−3)	−3.360 (−3)
5.0	−2.832 (−4)	−2.531 (−4)	−2.649 (−4)
5.5	−7.848 (−5)	−7.186 (−5)	−7.530 (−5)
6.0	−2.150 (−5)	−2.036 (−5)	−2.148 (−5)
7.0	−1.691 (−6)	−1.627 (−6)	−1.744 (−6)

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[2] This result contradicts the recent assessment of the role of double exchanges in the Ne_2 system made by Gerratt [18], who found them accounting for 18% of exchange energy at $R = 5.7$ a.u.

Table 4. A comparison of the largest individual inter-shell contributions to Coulomb and exchange energies (for the (6/8/8) wave function). The interatomic distance R is expressed in atomic units, all other quantities in percent

R	4.0	5.0	5.5	6.0	7.0
$(Q^{AB}_{KL} + Q^{AB}_{LK})/Q$	0.34	0.14	0.11	0.10	0.08
Q^{AB}_{LL}/Q	99.66	99.86	99.89	99.90	99.92
$(E^{AB}_{KL} + E^{AB}_{LK})/E_{\text{exch}}$	0.48	0.36	0.31	0.27	0.22
$E^{AB}_{LL}/E_{\text{exch}}$	96.17	97.19	97.58	97.90	98.36
$(E^{AAB}_{KLL} + E^{ABB}_{LKL})/E_{\text{exch}}$	3.35	2.45	2.11	1.83	1.42

In Table 4 we report the multi-shell partitioning of E_{exch} and Q. The symbols used to denote the particular multi-shell components are constructed in the same way as in Ref. [11]. Since the contributions E^{AB}_{KK}, E^{AAB}_{KLK}, E^{ABB}_{KLK}, E^{AABB}_{KLKL} and Q^{AB}_{KK} amount to less than 0.1% of E_{exch} and Q respectively, they are omitted in Table 4. Our results show that for all distances considered, both the exchange and Coulomb parts of the first-order energy may be approximated with the accuracy greater than 95% by the interaction of outer shells only. Inclusion of *KL-L* type terms leads to 99% accuracy.

Since the L-shell consists of four orbitals ($2s$, $2p_x$, $2p_y$, $2p_z$ – z denotes axis joining A and B) we have made an orbital analysis of E^{AB}_{LL} term decomposing it into components originating from two-, three- and four-orbital constributions

$$E^{AB}_{LL} = E_{LL}(2) + E_{LL}(3) + E_{LL}(4). \tag{15}$$

The contributions of particular terms to E^{AB}_{LL} have been compared in Table 5. It turns out that the two-orbital contributions account for only about 10% of E^{AB}_{LL} for all distances considered, while the major part of E^{AB}_{LL} (about 90%) results, rather unexpectedly, from the three-orbital interactions. We see that the role of the $E_{LL}(2)$ term slightly increases with increasing R. The above result disposed us to perform a more detailed analysis of $E_{LL}(3)$ contribution. It turned out that the major part of $\varepsilon(ik \mid j)$ (and $\varepsilon(i \mid jl)$) results from the first term in Eq. (10), i.e. from hybrid integrals. Moreover, we have found that the sum of terms arising from the interaction of $2p_z$ orbital localized at the A(B) centre with $2s$ or $2p_z$ orbital localized at the B(A) centre in presence of the third orbital of L-shell at the B(A) centre gives a very reliable approximation to $E_{LL}(3)$ (see the last but one row of Table 6).

Table 5. A comparison of many-orbital contributions to exchange interaction of L-shells (for the (6/8/8) wave function). The interatomic distance R is expressed in atomic units, all other quantities in percent

R	4.0	5.0	5.5	6.0	7.0
$E_{LL}(2)/E^{AB}_{LL}$	8.03	8.65	9.33	9.97	11.08
$E_{LL}(3)/E^{AB}_{LL}$	93.86	92.30	91.36	90.54	89.22
$E_{LL}(4)/E^{AB}_{LL}$	−1.89	−0.95	−0.69	−0.51	−0.30

Table 6. A comparison of various three-orbital contributions to exchange interaction of L-shells and to the exchange energy E_{exch} (for the (6/8/8) wave function). The interatomic distance R is expressed in atomic units, all other quantities in percent

R	4.0	5.0	5.5	6.0	7.0
$4\epsilon(2s2p_x \mid 2p_z)/E_{LL}^{AB}$	27.48	26.04	24.80	23.56	21.12
$4\epsilon(2p_y2p_z \mid 2p_z)/E_{LL}^{AB}$	28.40	33.96	36.28	38.32	41.80
$2\epsilon(2s2p_z \mid 2p_z)/E_{LL}^{AB}$	29.40	31.62	32.32	33.00	33.82
$E_{LL}^{\text{approx}}(3)/E_{LL}^{AB}$	85.28	91.62	93.40	94.88	96.74
$(E_{LL}(2) + E_{LL}^{\text{approx}}(3))/E_{\text{exch}}$	85.10	90.53	92.38	93.88	95.79

Making use of the symmetry of the system considered one can write the approximate formula as follows:

$$E_{LL}^{\text{approx}}(3) = 4\varepsilon(2s2p_x \mid 2p_z) + 4\varepsilon(2p_x2p_z \mid 2p_z) + 2\varepsilon(2s2p_z \mid 2p_z). \tag{16}$$

The importance of the terms included in (16) seems to be a consequence of large integral overlap between $2p_z$ at one centre and $2p_z$ or $2s$ at the other, and large differential overlap of atomic orbitals of the L-shell at the same centre. The relative contributions to E_{LL}^{AB} from individual terms in (16) have been compared in Table 6. In the last row of Table 6 we have tried to reproduce the total exchange energy as the sum $E_{LL}(2) + E_{LL}^{\text{approx}}(3)$. The result is encouraging: the accuracy proves to be better than 85% within the considered region. It is worthwhile to note here that $E_{LL}(2)$ cannot be approximated by the single term $\varepsilon(2p_z \mid 2p_z)$ because the other two-orbital contributions are equally large and of opposite signs.

Concluding the above analysis, we see that on the basis of the cluster expansion (6) it is possible to introduce the following simplifications in calculations of the first-order exchange repulsion:

1) Neglect of higher-order exchange terms.
2) Neglect of contributions comprising inner-shell orbitals.
3) Neglect of four-orbital contributions.
4) Use of the approximate formula of the type given by Eq. (16).
5) Evaluation of some less important terms using shorter expansions (14).

Application of the approximations 2, 3 and 4 may lead for larger systems to a reasonable reduction of the number of integrals over occupied orbitals whereas use of the approximation 5 will decrease the effort needed to calculate some of those integrals.

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Received October 17/December 23, 1978