

Erratum: “Modeling the Pauli Potential in the Pair Density Functional Theory” [J. Chem. Phys. 129, 204108 (2008).]

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After publication of our paper [1], we have noticed that, due to a renormalization of the basis set used for the expansion of the pair density amplitude, the scaling parameter λ introduced in Equation (37) altered the trial pair density in a way not fully described by Equations (47) and (48). We started, in fact, by a Hartree-Fock pair density amplitude written in the following form

$$\chi^{HF} = \sum_{k,l} C_{kl} N_k(\alpha_k) r_1^{p_k} e^{-\alpha_k r_1} N_l(\alpha_l) r_2^{p_l} e^{-\alpha_l r_2} \quad (1)$$

where, with the notation used in Equation (38),

$$\Omega_{kl} = C_{kl} N_k(\alpha_k) N_l(\alpha_l) . \quad (2)$$

At this point, by changing the exponents α_k by $\alpha_k \lambda$, the program altered also the normalization constants $N_k(\alpha_k)$ introduced above. The global change, after scaling,

of the matrix elements Ω_{kl} resulted as follows

$$\bar{\Omega}_{kl} = C_{kl} N_k(\alpha_k \lambda) N_l(\alpha_l \lambda) \lambda^{p_k + p_l} \quad (3)$$

and not simply as written in Equation (47). This modification determines not only the scaling discussed in our work but also a slight deformation of the pair density itself. This fact does not alter the content of our study, which was addressed to the search of a model Pauli potential for a given trial pair density amplitude. A further point concerns data of Tables II-IV. Energies and Pauli kinetic energies of these tables are consistent with the above definition of matrix elements $\bar{\Omega}_{kl}$ but, instead, the moments $\langle r^q \rangle$ have been determined with the really scaled HF intracule density and consequently, for the reason reported in this note, are not consistent with the previous energies. In order to correct this inconsistency, we have recomputed the aforementioned moments according with the real expression of the approximate pair density amplitude used in our work and the new results are reported here in the Tables 1-3. The agreement of these new values with the most accurate from literature, in the spirit of our study, is good.

References

- [1] C. Amovilli and Á. Nagy, J. Chem. Phys. **129**, 204108 (2008).
- [2] F. J. Gálvez, E. Buendía and A. Sarsa, J. Chem. Phys. **111**, 10903 (1999).
- [3] J. Komasa, W. Cencek and J. Rychlewski, Phys. Rev. A **52**, 4500 (1995).

a	λ	E	T_p	$\langle r^{-2} \rangle$	$\langle r^{-1} \rangle$	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle r^3 \rangle$
4	0.9835	-14.660(4)	0.878(3)	9.70	4.369	15.407	53.47	225.6
5	0.9847	-14.669(4)	0.864(3)	9.88	4.405	15.349	53.18	224.2
6	0.9860	-14.669(4)	0.855(3)	10.00	4.428	15.310	52.98	223.2
HF ^(a)		-14.573	1.005	10.536	4.489	15.120	51.956	218.11
corr ^(b)		-14.667	—	9.536	4.337	15.272	52.854	222.48

^(a) In the T_p column is reported the difference $T_{ex} - T_w^{(1)}$ and moments are from refs. [2, 3].

^(b) Moments from [3].

Table 1: Total energy (E), Pauli kinetic energy (T_p) and some moments $\langle r^k \rangle$ for Be atom for different choices of the correlation function parameter a and the scaling constant λ calculated in this work and comparison with HF and correlated literature data. Data are in atomic units.

a	λ	E	T_p	$\langle r^{-2} \rangle$	$\langle r^{-1} \rangle$	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle r^3 \rangle$
5	1.00090	-36.538(9)	3.253(8)	25.2	7.57	7.993	13.99	29.71
6	1.00063	-36.538(9)	3.226(8)	25.4	7.60	7.987	13.99	29.71
7	1.00055	-36.539(9)	3.204(8)	25.7	7.62	7.978	13.98	29.67
HF ^(a)		-36.408	3.475	27.06	7.716	7.945	13.863	29.06
corr ^(b)		-36.534	—	25.50	7.548	8.118	14.502	31.14

^(a) In the T_p column is reported the difference $T_{ex} - T_w^{(1)}$ and moments are from refs. [2, 3].

^(b) Moments from [2].

Table 2: Total energy (E), Pauli kinetic energy (T_p) and some moments $\langle r^k \rangle$ for C²⁺ atomic ion for different choices of the correlation function parameter a and the scaling constant λ calculated in this work and comparison with HF and correlated literature data. Data are in atomic units.

a	λ	E	T_p	$\langle r^{-2} \rangle$	$\langle r^{-1} \rangle$	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle r^3 \rangle$
7	1.00005	-68.40(1)	6.91(1)	48.5	10.74	5.499	6.614	9.891
8	1.00003	-68.40(1)	6.91(1)	48.7	10.75	5.498	6.612	9.890
9	1.00003	-68.41(1)	6.90(1)	49.0	10.78	5.493	6.603	9.872
HF ^(a)		-68.257	7.374	51.8	10.887	5.455	6.469	9.167
corr ^(b)		-68.411	—	49.17	10.694	5.570	6.769	9.843

^(a) In the T_p column is reported the difference $T_{ex} - T_w^{(1)}$ and moments are from refs. [2, 3].

^(b) Moments from [2].

Table 3: Total energy (E), Pauli kinetic energy (T_p) and some moments $\langle r^k \rangle$ for O^{4+} atomic ion for different choices of the correlation function parameter a and the scaling constant λ calculated in this work and comparison with HF and correlated literature data. Data are in atomic units.