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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 Eq. (37) altered the trial pair density in a way not fully described by Eqs. (47) and (48). We started, in fact, by a Hartree–Fock pair density amplitude written in the following form:

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

where with the notation used in Eq. (38)

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

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:

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

and not simply as written in Eq. (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 in the search of a model Pauli potential for a given trial pair density amplitude. A further point to be noted concerns the 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,

TABLE II. 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	$\langle r^{-2} \rangle$	$\langle r^{-1} \rangle$	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle r^3 \rangle$
4	0.9835	−14.660(4)	0.878(3)	9.7	4.369	15.41	53.47	225
5	0.9847	−14.669(4)	0.864(3)	9.9	4.405	15.35	53.18	224
6	0.9860	−14.669(4)	0.855(3)	10.0	4.428	15.31	52.98	223
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 the reported difference $T_{ex}-T_w^{(1)}$ and moments are from Refs. 2 and 3.
[b]Moments from Ref. 3.

TABLE III. Total energy (E), Pauli kinetic energy (T_p), and some moments $\langle r^k \rangle$ for C^{2+} 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	$\langle r^{-2} \rangle$	$\langle r^{-1} \rangle$	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle r^3 \rangle$
5	1.000 90	−36.538(9)	3.253(8)	25.2	7.57	7.993	13.99	29.7
6	1.000 63	−36.538(9)	3.226(8)	25.4	7.60	7.987	13.99	29.7
7	1.000 55	−36.539(9)	3.204(8)	25.7	7.62	7.978	13.98	29.7
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, the reported difference $T_{ex}-T_w^{(1)}$ and moments are from Refs. 2 and 3.
[b]Moments from Ref. 2.

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TABLE IV. 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.

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	1.000 05	−68.40(1)	6.91(1)	48.5	10.74	5.499	6.61	9.89
8	1.000 03	−68.40(1)	6.91(1)	48.7	10.75	5.498	6.61	9.89
9	1.000 03	−68.41(1)	6.90(1)	49.0	10.78	5.493	6.60	9.87
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, the reported difference $T_{ex}-T_w^{(1)}$ and moments are from Refs. 2 and 3.
[b] Moments from Ref. 2.

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 II–IV. The agreement of these new values with the most accurate from literature, in the spirit of our study, is good.

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[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).