Erratum to: Introducing the γ function in quantum theory, Int. J. Quantum. Chem. 120 e26221 (2020)

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On page 9. of paper[1], in Section 5., the (unnumbered) equation for the integral $(11|11)$ contains some misprints. Its correct form is:

$$(11|11) \;=\; \frac{1}{16\pi^2 r_0^4} \iint \gamma^2(r_1 - r_0)\, \frac{1}{r_{12}}\, \gamma^2(r_2 - r_0) dV_1 dV_2.$$

A more severe error is that in the next line it is wrongly stated that this expression *"is clearly divergent"*. The qualitative explanation provided there, *"the repulsion of two charged particles distributed uniformly on the surface of the same sphere is infinite."* is also false. The integral has now been evaluated correctly via expanding $\frac{1}{r_{12}}$ in terms of spherical harmonics Y_{lm} to yield:

$$\begin{aligned}
(11|11) \;&=\; \frac{1}{r_0^4} \iint \delta(r_1 - r_0)\, \frac{1}{r_{12}}\, \delta(r_2 - r_0)\, Y_{00}^4\, dV_1 dV_2 \\
&=\; \frac{4\pi}{r_0^4} \sum_{l,m} \frac{Y_{00}^2}{2l+1}\, (-1)^m \int_0^\infty\!\!\int r_1^2\, r_2^2\, dr_1 dr_2\, \delta(r_1 - r_0)\, \delta(r_2 - r_0)\, \frac{r_<^l}{r_>^{l+1}} \\
&\quad \times \underbrace{\int_0^\pi\!\!\int \sin\vartheta_1 \sin\vartheta_2\, d\vartheta_1 d\vartheta_2 \int_0^{2\pi}\!\!\int d\varphi_1 d\varphi_2\, Y_{00} Y_{lm}^*(\vartheta_1, \varphi_1)\; Y_{00} Y_{lm}(\vartheta_2, \varphi_2)}_{\delta_{l0}\,\delta_{m0}} \\
&=\; \frac{1}{r_0}
\end{aligned}$$

in standard notations. Using this result for the integral (11|11) in the potential energy for the He atom discussed in Sect. 5. of Ref.[1] corresponds to an uncorrelated (Hartree-Fock type) treatment, and results the total energy

$$E_{\mathrm{He}} \;=\; -2.25 \text{ a.u.},$$

instead of the value obtained in Ref.[1] in the somewhat overcorrelated "north-south" model yielding -3.06 a.u. The latter is much closer to the experimental energy of -2.90 a.u. One concludes that, apart from the erroneous statement on the integral cited above, the conclusions of Ref.[1] about the treatment of He remain valid.

References

1. P. R. Surján, Int. J. Quantum Chem. **120**, e26221 (2020).