

# Erratum: “Exchange-Correlation Energy Densities and Response Potentials: Connection between Two Definitions and Analytical Model for the Strong-Coupling Limit of a Stretched Bond” [J. Phys. Chem. A 2020, 124, 2473-2482]

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With this Erratum, we intend to rectify a mistake in the original publication.<sup>1</sup>

Namely, in the line between eq (39) and eq (40) we write  $\langle \frac{\partial \Phi_\lambda}{\partial \lambda} | \hat{h}_\lambda | \Phi_\lambda \rangle_{2\dots N} + \langle \Phi_\lambda | \hat{h}_\lambda | \frac{\partial \Phi_\lambda}{\partial \lambda} \rangle_{2\dots N} = 2 \langle \Phi_\lambda | \hat{h}_\lambda | \frac{\partial \Phi_\lambda}{\partial \lambda} \rangle_{2\dots N}$ . However, despite  $\hat{h}_\lambda$  being an Hermitian operator, this equation is not true in general, because  $\hat{h}_\lambda$  contains the laplacian with respect to the variable  $\mathbf{r}$ , which is not integrated (we remind that we use the Dirac brackets  $\langle \dots | \dots \rangle_{2\dots N}$  for  $\int d\sigma d\mathbf{x}_2 \dots \mathbf{x}_N$ ). Then, the full term, which we now label  $\delta_{\partial_\lambda \Phi_\lambda}$ ,

$$\delta_{\partial_\lambda \Phi_\lambda} = \langle \frac{\partial \Phi_\lambda}{\partial \lambda} | \hat{h}_\lambda | \Phi_\lambda \rangle_{2\dots N} + \langle \Phi_\lambda | \hat{h}_\lambda | \frac{\partial \Phi_\lambda}{\partial \lambda} \rangle_{2\dots N}, \quad (1)$$

should appear in place of  $2 \langle \Phi_\lambda | \hat{h}_\lambda | \frac{\partial \Phi_\lambda}{\partial \lambda} \rangle_{2\dots N}$  wherever this latter had been used. Note that this term is always integrated in  $\lambda$  between 0 and 1 in the remaining of the original paper. In particular, the two fundamental equations connecting the two gauges should read

$$\epsilon_{\text{kin+hole}} - \epsilon_{\text{xc}} = \int_0^1 \delta_{\partial_\lambda \Phi_\lambda} d\lambda \quad (2)$$

$$\bar{v}_{\text{resp}} = v_{\text{resp}} - v_{\text{c,kin}} + 2 \int_0^1 \delta_{\partial_\lambda \Phi_\lambda} d\lambda \quad (3)$$

as well as the graphical abstract (see corrected fig 1) among others.

Nonetheless, recognising these two terms as being different does not alter any of the conclusions of the paper,

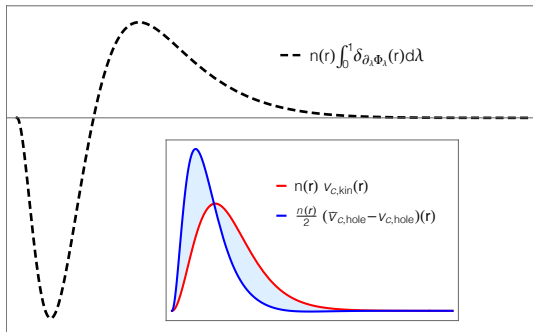


FIG. 1. Local difference,  $n(\mathbf{r}) \int_0^1 \delta_{\partial_\lambda \Phi_\lambda} d\lambda(\mathbf{r})$ , between the two energy densities definitions for the Hydrogen anion.

once  $2 \langle \Phi_\lambda | \hat{h}_\lambda | \frac{\partial \Phi_\lambda}{\partial \lambda} \rangle_{2\dots N}$  is replaced with  $\delta_{\partial_\lambda \Phi_\lambda}$ . For example, the following equation

$$\delta_{\partial_\lambda \Phi_\lambda} = \frac{\partial}{\partial \lambda} v_{\lambda,\text{kin}} + \frac{\lambda}{2} \frac{\partial}{\partial \lambda} v_{\lambda,\text{cond}}, \quad (4)$$

which amends eq (52) of the paper, still supports the analysis in the last two columns of the section. In particular, for the case of a stretched bond, we have

$$\int_0^1 \delta_{\partial_\lambda \Phi_\lambda} d\lambda \sim v_{\text{c,kin}}, \quad (5)$$

instead of eq (57), which still supports

$$v_{\text{xc,hole}}(x) \sim \bar{v}_{\text{xc,hole}}(x) \quad (6)$$

$$\bar{v}_{\text{resp}}(x) \sim v_{\text{c,kin}}(x) + v_{\text{resp}}(x), \quad (7)$$

appearing as eqs (58) and (59) of the original publication.

<sup>1</sup>S. Giarrusso and P. Gori-Giorgi, The Journal of Physical Chemistry A **124**, 2473 (2020).