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Erratum: "Spin-unrestricted random-phase approximation with range separation: Benchmark on atomization energies and reaction barrier heights" [J. Chem. Phys. 142, 154123 (2015)]

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After publication of our article,[1] we realized that the expressions for the antisymmetrized direct RPA (dRPA-II) and antisymmetrized RPA with exchange (RPAx-II) correlation energies, shown in Eqs. (2) and (4) of the article,[1] should take the following forms (previously published in Ref. 2):

$$E_c^{\text{dRPA-II}} = \frac{1}{2}\int_0^1 \mathrm{d}\alpha \ \mathrm{tr}\left[\frac{1}{2}\mathbf{Q}_\alpha^{\text{dRPA}}\left(\mathbf{A}_1'^{\text{II}} + \mathbf{B}_1^{\text{II}}\right) + \frac{1}{2}\left(\mathbf{Q}_\alpha^{\text{dRPA}}\right)^{-1}\left(\mathbf{A}_1'^{\text{II}} - \mathbf{B}_1^{\text{II}}\right) - \mathbf{A}_1'^{\text{II}}\right] \tag{1}$$

and

$$E_c^{\text{RPAx-II}} = \frac{1}{4}\int_0^1 \mathrm{d}\alpha \ \mathrm{tr}\left[\frac{1}{2}\mathbf{Q}_\alpha^{\text{RPAx}}\left(\mathbf{A}_1'^{\text{II}} + \mathbf{B}_1^{\text{II}}\right) + \frac{1}{2}\left(\mathbf{Q}_\alpha^{\text{RPAx}}\right)^{-1}\left(\mathbf{A}_1'^{\text{II}} - \mathbf{B}_1^{\text{II}}\right) - \mathbf{A}_1'^{\text{II}}\right], \tag{2}$$

where the matrix $\mathbf{Q}_\alpha$ is defined as follows:

$$\mathbf{Q}_\alpha = (\mathbf{A}_\alpha - \mathbf{B}_\alpha)^{1/2}(\mathbf{M}_\alpha)^{-1/2}(\mathbf{A}_\alpha - \mathbf{B}_\alpha)^{1/2} \tag{3}$$

with matrices $\mathbf{A}_\alpha^{\text{I}}$ and $\mathbf{B}_\alpha^{\text{I}}$ used to construct $\mathbf{Q}_\alpha^{\text{dRPA}}$ and matrices $\mathbf{A}_\alpha^{\text{II}}$ and $\mathbf{B}_\alpha^{\text{II}}$ used to construct $\mathbf{Q}_\alpha^{\text{RPAx}}$. Note that the matrices $\mathbf{A}_\alpha^{\text{I}}$, $\mathbf{A}_\alpha^{\text{II}}$, $\mathbf{B}_\alpha^{\text{I}}$, $\mathbf{B}_\alpha^{\text{II}}$, as well as $\mathbf{M}_\alpha$ are defined in our article[1] but that, on the other hand, the matrix $\mathbf{A}_1'^{\text{II}}$ appearing in Eqs. (1) and (2) of this erratum needs to be defined here,

$$\left(A_\alpha'^{\text{II}}\right)_{ia,jb} = \alpha \ \langle ib||aj\rangle. \tag{4}$$

It differs from $\mathbf{A}_\alpha^{\text{II}}$ in that it does not contain the differences of spin-orbital energies.

All results shown in the original article were obtained using Eqs. (1) and (2) of this erratum and are thus correct.

Note that the matrices $\mathbf{Q}_\alpha$ are related to the matrices $\mathbf{P}_{c,\alpha}$ that appear in our article[1] by $\mathbf{P}_{c,\alpha} = \mathbf{Q}_\alpha - \mathbf{I}$ (where $\mathbf{I}$ is the identity matrix) and that one can make the following approximations to the matrices $(\mathbf{Q}_\alpha)^{-1}$, as explained in Ref. 2:

$$\left(\mathbf{Q}_\alpha^{\text{dRPA}}\right)^{-1} = \left(\mathbf{I} + \mathbf{P}_{c,\alpha}^{\text{dRPA}}\right)^{-1} \approx \mathbf{I} - \mathbf{P}_{c,\alpha}^{\text{dRPA}} = 2\,\mathbf{I} - \mathbf{Q}_\alpha^{\text{dRPA}} \tag{5}$$

and

$$\left(\mathbf{Q}_\alpha^{\text{RPAx}}\right)^{-1} = \left(\mathbf{I} + \mathbf{P}_{c,\alpha}^{\text{RPAx}}\right)^{-1} \approx \mathbf{I} - \mathbf{P}_{c,\alpha}^{\text{RPAx}} = 2\,\mathbf{I} - \mathbf{Q}_\alpha^{\text{RPAx}}, \tag{6}$$

which lead to the so-called "IIa" approximations to the dRPA-II and RPAx-II correlation energies,

$$E_c^{\text{dRPA-IIa}} = \frac{1}{2}\int_0^1 \mathrm{d}\alpha \ \mathrm{tr}\left[\mathbf{B}_1^{\text{II}}\,\mathbf{P}_{c,\alpha}^{\text{dRPA}}\right], \tag{7}$$

$$E_c^{\text{RPAx-IIa}} = \frac{1}{4}\int_0^1 \mathrm{d}\alpha \ \mathrm{tr}\left[\mathbf{B}_1^{\text{II}}\,\mathbf{P}_{c,\alpha}^{\text{RPAx}}\right]. \tag{8}$$

These are the expressions that were erroneously shown in the original article.

[1]B. Mussard, P. Reinhardt, J. G. Ángyán, and J. Toulouse, J. Chem. Phys. **142**, 154123 (2015).
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