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 paper,[1] we realized that the expressions for the dRPA-II and RPAx-II correlation energies, shown in equations (2) and (4) of the paper,[1] should take the following forms (previously published in Ref. [2]):

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

and:

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

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

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

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

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

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

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

Note that the matrices $\mathbf{Q}_\alpha$ are related to the matrices $\mathbf{P}_{\mathrm{c},\alpha}$ that appear in our paper[1] by $\mathbf{P}_{\mathrm{c},\alpha} = \mathbf{Q}_\alpha - \mathbf{I}$ (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]:

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

and

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

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

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

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

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

[1]B. Mussard, P. Reinhardt, J.G. Ángyán, J. Toulouse, J. Chem. Phys. **142**, 154123 (2015).
[2]J. G. Ángyán, R.-F. Liu, J. Toulouse and G. Jansen, J. Chem. Theory Comput. **7**, 3116 (2011).

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