Bastien Mussard, Peter Reinhardt, János G. Ángyán, and Julien Toulouse

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Cubic-scaling algorithm and self-consistent field for the random-phase approximation with second-order screened exchange


Bastien Mussard,1,2,3,a) Peter Reinhardt,2,3 János G. Ángyán,4,5 and Julien Toulouse2,3,b)

1 Sorbonne Universités, UPMC Univ Paris 06, Institut du Calcul et de la Simulation, F-75005 Paris, France
2 Sorbonne Universités, UPMC Univ Paris 06, UMR 7616, Laboratoire de Chimie Théorique, F-75005 Paris, France
3 CNRS, UMR 7616, Laboratoire de Chimie Théorique, F-75005 Paris, France
4 CRM2, Institut Jean Barriol, Université de Lorraine, F-54506 Vandœuvre-lès-Nancy, France
5 CRM2, Institut Jean Barriol, CNRS, F-54506 Vandœuvre-lès-Nancy, France

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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,2 should take the following forms (previously published in Ref. 2):

\[
E_{c}^{\text{dRPA-II}} = \frac{1}{2} \int_{0}^{1} d\alpha \, \text{tr} \left[ \frac{1}{2} Q_{\alpha}^{\text{dRPA}} (A_{\alpha}^{II} + B_{\alpha}^{II}) + \frac{1}{2} (Q_{\alpha}^{\text{dRPA}})^{-1} (A_{\alpha}^{II} - B_{\alpha}^{II}) - \frac{1}{2} A_{\alpha}^{II} \right]
\]

and

\[
E_{c}^{\text{RPAx-II}} = \frac{1}{4} \int_{0}^{1} d\alpha \, \text{tr} \left[ \frac{1}{2} Q_{\alpha}^{\text{RPAx}} (A_{\alpha}^{II} + B_{\alpha}^{II}) + \frac{1}{2} (Q_{\alpha}^{\text{RPAx}})^{-1} (A_{\alpha}^{II} - B_{\alpha}^{II}) - \frac{1}{2} A_{\alpha}^{II} \right],
\]

where the matrix \(Q_{\alpha}\) is defined as follows:

\[
Q_{\alpha} = (A_{\alpha} - B_{\alpha})^{1/2}(M_{\alpha})^{-1/2}(A_{\alpha} - B_{\alpha})^{1/2}
\]

with matrices \(A_{\alpha}^{II}\) and \(B_{\alpha}^{II}\) used to construct \(Q_{\alpha}^{\text{dRPA}}\) and matrices \(A_{\alpha}^{II}\) and \(B_{\alpha}^{II}\) used to construct \(Q_{\alpha}^{\text{RPAx}}\). Note that the matrices \(A_{\alpha}^{II}\), \(A_{\alpha}^{II}\), \(B_{\alpha}^{II}\), \(B_{\alpha}^{II}\), as well as \(M_{\alpha}\) are defined in our article1 but that, on the other hand, the matrix \(A_{\alpha}^{II}\) appearing in Eqs. (1) and (2) of this erratum needs to be defined here,

\[
(A_{\alpha}^{II})_{ia,jb} = \alpha \langle ib||aj \rangle.
\]

It differs from \(A_{\alpha}^{II}\) 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 \(Q_{\alpha}\) are related to the matrices \(P_{c,\alpha}\) that appear in our article3 by \(P_{c,\alpha} = Q_{\alpha} - I\) (where \(I\) is the identity matrix) and that one can make the following approximations to the matrices \((Q_{\alpha})^{-1}\), as explained in Ref. 2:

\[
(Q_{\alpha}^{\text{dRPA}})^{-1} = (I + P_{c,\alpha}^{\text{dRPA}})^{-1} \approx I - P_{c,\alpha}^{\text{dRPA}} = 2 \, I - Q_{\alpha}^{\text{dRPA}}
\]

and

\[
(Q_{\alpha}^{\text{RPAx}})^{-1} = (I + P_{c,\alpha}^{\text{RPAx}})^{-1} \approx I - P_{c,\alpha}^{\text{RPAx}} = 2 \, I - Q_{\alpha}^{\text{RPAx}}.
\]

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

\[
E_{c}^{\text{dRPA-IIa}} = \frac{1}{2} \int_{0}^{1} d\alpha \, \text{tr}[B_{\alpha}^{II} P_{c,\alpha}^{\text{dRPA}}],
\]

\[
E_{c}^{\text{RPAx-IIa}} = \frac{1}{4} \int_{0}^{1} d\alpha \, \text{tr}[B_{\alpha}^{II} P_{c,\alpha}^{\text{RPAx}}].
\]

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

3 Electronic mail: bastien.mussard@upmc.fr
b) Electronic mail: julien.toulouse@upmc.fr