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


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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):

\[
E_{\text{c,RPA-II}} = \frac{1}{2} \int_0^1 d\tau \, \text{tr} \left[ \frac{1}{2} Q^{\text{dRPA}}_\alpha (A^I_\alpha + B^I_\alpha) + \frac{1}{2} (Q^{\text{dRPA}}_\alpha)^{-1} (A^I_\alpha - B^I_\alpha) - A^{\text{dRPA}}_1 \right]
\]

(1)

and

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

(2)

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

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

(3)

with matrices \( A^I_\alpha \) and \( B^I_\alpha \) used to construct \( Q^{\text{dRPA}}_\alpha \) and matrices \( A^{\text{RPAx}}_\alpha \) and \( B^{\text{RPAx}}_\alpha \) used to construct \( Q^{\text{RPAx}}_\alpha \). Note that the matrices \( A^I_\alpha \), \( A^{\text{RPAx}}_\alpha \), \( B^I_\alpha \), and \( B^{\text{RPAx}}_\alpha \), as well as \( M_\alpha \), are defined in our article1 but that, on the other hand, the matrix \( A^{\text{dRPA}}_1 \) appearing in Eqs. (1) and (2) of this erratum needs to be defined here,

\[
(A^{\text{dRPA}}_1)_{ia,jb} = \alpha \langle ib|\alpha j \rangle.
\]

(4)

It differs from \( A^{\text{RPAx}}_1 \) 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 article1 by \( P_{c,\alpha} = Q_\alpha - I \) (where \( I \) is the identity matrix) and that one can make the following approximations to the matrices \( Q^{-1}_\alpha \), as explained in Ref. 2:

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

(5)

and

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

(6)

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

\[
E_{\text{c,dRPA-IIa}} = \frac{1}{2} \int_0^1 d\tau \, \text{tr} [B^{\text{dRPA}}_1 P_{c,\alpha}^{\text{dRPA}}],
\]

(7)

\[
E_{\text{c,RPAx-IIa}} = \frac{1}{4} \int_0^1 d\tau \, \text{tr} [B^{\text{RPAx}}_1 P_{c,\alpha}^{\text{RPAx}}].
\]

(8)

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


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