

Erratum: “How accurate is the strongly orthogonal geminal theory in predicting excitation energies? Comparison of the extended random phase approximation and the linear response theory approaches” [J. Chem. Phys.140, 014101 (2014)]

Katarzyna Pernal, Koushik Chatterjee, and Piotr H. Kowalski

Citation: *The Journal of Chemical Physics* **140**, 189901 (2014); doi: 10.1063/1.4876720

View online: <http://dx.doi.org/10.1063/1.4876720>

View Table of Contents: <http://scitation.aip.org/content/aip/journal/jcp/140/18?ver=pdfcov>

Published by the [AIP Publishing](#)

Articles you may be interested in

Publisher's Note: “Derivative couplings between TDDFT excited states obtained by direct differentiation in the Tamm-Dancoff approximation” [J. Chem. Phys.141, 024114 (2014)]

J. Chem. Phys. **141**, 069903 (2014); 10.1063/1.4891539

Linear response theory for the density matrix renormalization group: Efficient algorithms for strongly correlated excited states

J. Chem. Phys. **140**, 024108 (2014); 10.1063/1.4860375

How accurate is the strongly orthogonal geminal theory in predicting excitation energies? Comparison of the extended random phase approximation and the linear response theory approaches

J. Chem. Phys. **140**, 014101 (2014); 10.1063/1.4855275

Erratum: “The role of the reference state in long-range random phase approximation correlation” [J. Chem. Phys.131, 154106 (2009)]

J. Chem. Phys. **138**, 019901 (2013); 10.1063/1.4773899

Erratum: “Hybrid functionals including random phase approximation correlation and second-order screened exchange” [J. Chem. Phys.132, 094103 (2010)]

J. Chem. Phys. **133**, 179902 (2010); 10.1063/1.3501928



NEW Special Topic Sections

NOW ONLINE
Lithium Niobate Properties and Applications:
Reviews of Emerging Trends

AIP | Applied Physics
Reviews

Erratum: “How accurate is the strongly orthogonal geminal theory in predicting excitation energies? Comparison of the extended random phase approximation and the linear response theory approaches” [J. Chem. Phys. **140**, 014101 (2014)]

Katarzyna Pernal,^{1,a)} Koushik Chatterjee,² and Piotr H. Kowalski²

¹*Institute of Physics, Technical University of Lodz, ul. Wolczanska 219, 90-924 Lodz, Poland*

²*Faculty of Chemistry, Technical University of Lodz, ul. Zeromskiego 116, 90-924 Lodz, Poland*

(Received 1 May 2014; accepted 4 May 2014; published online 14 May 2014)

[<http://dx.doi.org/10.1063/1.4876720>]

In the original publication¹ the expression for elements of the **A** and **B** matrices, Eq. (A1) in the Appendix, is mistaken. The correct form reads

$$\begin{aligned}
 \forall_{\substack{p \neq q \\ r \neq s}} B_{pq,rs} = A_{pq,rs} = & (n_p - n_q)(\delta_{ps}h_{qr} - \delta_{qr}h_{ps}) \\
 & + (c_p c_s \delta_{I_p I_s} + c_q c_r \delta_{I_q I_r})(\langle pq|rs\rangle + \langle pq|sr\rangle) \\
 & + [n_p n_s (1 - \delta_{I_p I_s}) + n_q n_r (1 - \delta_{I_q I_r}) - n_p n_r (1 - \delta_{I_p I_r}) - n_q n_s (1 - \delta_{I_q I_s})] \langle pr||qs\rangle \\
 & - \delta_{qr} c_p \sum_t \delta_{I_p I_t} c_t \langle ps|tt\rangle - \delta_{ps} c_q \sum_t \delta_{I_q I_t} c_t \langle qr|tt\rangle - \delta_{pr} c_r \sum_t \delta_{I_r I_t} c_t \langle qs|tt\rangle - \delta_{qs} c_s \sum_t \delta_{I_s I_t} c_t \langle pr|tt\rangle \\
 & + \delta_{ps} \sum_t n_t [n_p (1 - \delta_{I_p I_t}) - n_q (1 - \delta_{I_q I_t})] \langle qt||rt\rangle - \delta_{qr} \sum_t n_t [n_p (1 - \delta_{I_p I_t}) - n_q (1 - \delta_{I_q I_t})] \langle pt||st\rangle,
 \end{aligned}$$

where

$$\langle pq||rs\rangle = 2 \langle pq|rs\rangle - \langle pq|sr\rangle.$$

¹K. Pernal, K. Chatterjee, and P. H. Kowalski, *J. Chem. Phys.* **140**, 014101 (2014).

^{a)}Electronic mail: pernak@gmail.com