

## Erratum: “Temperature dependence of the electronic structure of semiconductors and insulators” [J. Chem. Phys. 143, 102813 (2015)]

S. Poncé, Y. Gillet, J. Laflamme Janssen, A. Marini, M. Verstraete, and X. Gonze

Citation: *The Journal of Chemical Physics* **146**, 099901 (2017);

View online: <https://doi.org/10.1063/1.4977571>

View Table of Contents: <http://aip.scitation.org/toc/jcp/146/9>

Published by the [American Institute of Physics](#)

---

### Articles you may be interested in

[Temperature dependence of the electronic structure of semiconductors and insulators](#)

*The Journal of Chemical Physics* **143**, 102813 (2015); 10.1063/1.4927081

[Preface: Special Topic on Frontiers in Molecular Scale Electronics](#)

*The Journal of Chemical Physics* **146**, 092101 (2017); 10.1063/1.4977469

[Perspective: Theory and simulation of hybrid halide perovskites](#)

*The Journal of Chemical Physics* **146**, 220901 (2017); 10.1063/1.4984964

[Parameter-free driven Liouville-von Neumann approach for time-dependent electronic transport simulations in open quantum systems](#)

*The Journal of Chemical Physics* **146**, 092331 (2017); 10.1063/1.4976731

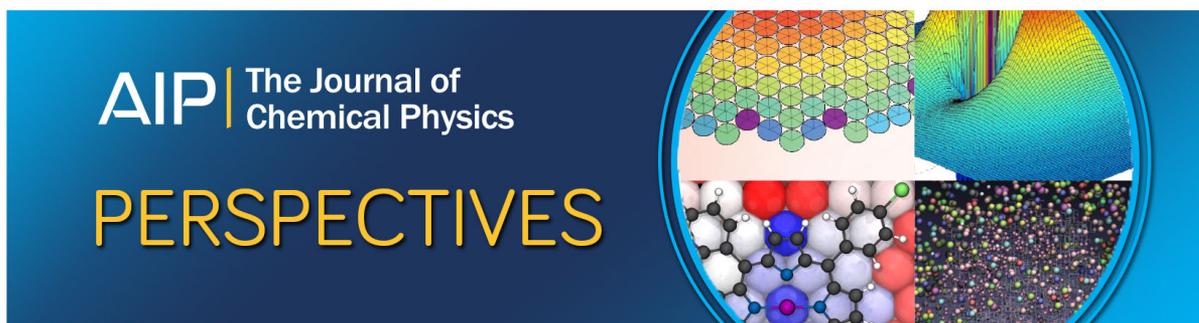
[Screened hybrid density functionals applied to solids](#)

*The Journal of Chemical Physics* **124**, 154709 (2006); 10.1063/1.2187006

[Density matrix renormalization group \(DMRG\) method as a common tool for large active-space CASSCF/CASPT2 calculations](#)

*The Journal of Chemical Physics* **146**, 094102 (2017); 10.1063/1.4976644

---



## Erratum: “Temperature dependence of the electronic structure of semiconductors and insulators” [J. Chem. Phys. 143, 102813 (2015)]

S. Poncé,<sup>1,a)</sup> Y. Gillet,<sup>1</sup> J. Laflamme Janssen,<sup>1</sup> A. Marini,<sup>2</sup> M. Verstraete,<sup>3</sup> and X. Gonze<sup>1</sup>

<sup>1</sup>European Theoretical Spectroscopy Facility and Institute of Condensed Matter and Nanosciences,

Université catholique de Louvain, Chemin des étoiles 8, bte L07.03.01, B-1348 Louvain-la-Neuve, Belgium

<sup>2</sup>Consiglio Nazionale delle Ricerche (CNR), Via Salaria Km 29.3, CP 10, 00016 Monterotondo Stazione, Italy

<sup>3</sup>European Theoretical Spectroscopy Facility and Physique des Matériaux et Nanostructures,

Université de Liège, Allée du 6 Août 17, B-4000 Liège, Belgium

(Received 6 February 2017; accepted 15 February 2017; published online 2 March 2017)

[<http://dx.doi.org/10.1063/1.4977571>]

The following amendments to the paper<sup>1</sup> have to be made.

- The matrix elements were incorrectly written in Eq. (4) and that have to be changed into

$$\frac{\partial \varepsilon_{n\mathbf{k}}}{\partial n_{m\mathbf{q}}} = \frac{1}{2\omega_{m\mathbf{q}}} \sum_{\substack{\kappa\alpha \\ \kappa'\gamma}} U_{m,\kappa'\gamma}^*(\mathbf{q}) U_{m,\kappa\alpha}(\mathbf{q}) \left\{ \left\langle u_{n\mathbf{k}}^{(0)} \left| \frac{\partial^2 \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(-\mathbf{q}) \partial R_{\kappa'\gamma}(\mathbf{q})} \right| u_{n\mathbf{k}}^{(0)} \right\rangle + \frac{1}{2} \left( \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa\alpha}(\mathbf{q})} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} \right| u_{n\mathbf{k}}^{(0)} \right\rangle \right. \right. \\ \left. \left. + \left\langle u_{n\mathbf{k}}^{(0)} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(-\mathbf{q})} \left| \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} \right\rangle \right) + (\kappa\alpha, \mathbf{q}) \leftrightarrow (\kappa'\gamma, -\mathbf{q}) \right\}.$$

- Also, Eq. (5) has to be replaced with

$$\frac{\partial X}{\partial R_{\kappa\alpha}(\mathbf{q})} = \sum_l e^{i\mathbf{q}\cdot\mathbf{R}_l} \frac{\partial X}{\partial R_{l\kappa\alpha}}.$$

- The Fan contribution in Eq. (7) has to be changed, giving

$$\mathcal{F}_{\kappa'\gamma}^{\kappa\alpha}(\mathbf{q}) \triangleq \frac{1}{2} \left( \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa\alpha}(\mathbf{q})} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} \right| u_{n\mathbf{k}}^{(0)} \right\rangle + \left\langle u_{n\mathbf{k}}^{(0)} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(-\mathbf{q})} \left| \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} \right\rangle \right) + (\kappa\alpha, \mathbf{q}) \leftrightarrow (\kappa'\gamma, -\mathbf{q}). \right.$$

- The Fan term in Eq. (15) should be changed, giving

$$\Delta \varepsilon_{n\mathbf{k}}^{(\text{adiabatic,RIA})}(T) = \Re \frac{1}{N_q} \sum_{\mathbf{q}} \sum_m^{3N} \left( n_{m\mathbf{q}}(T) + \frac{1}{2} \right) \frac{1}{4\omega_{m\mathbf{q}}} \sum_{\substack{\kappa\alpha \\ \kappa'\gamma}} \left\{ \left( \left[ 2 \sum_{n'=1}^M \frac{\left\langle u_{n\mathbf{k}}^{(0)} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(-\mathbf{q})} \right| u_{n'\mathbf{k}+\mathbf{q}}^{(0)} \right\rangle \left\langle u_{n'\mathbf{k}+\mathbf{q}}^{(0)} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} \right| u_{n\mathbf{k}}^{(0)} \right\rangle}{\varepsilon_{n\mathbf{k}}^{(0)} - \varepsilon_{n'\mathbf{k}+\mathbf{q}}^{(0)} + i\delta} \right. \right. \\ \left. \left. + \left\langle \hat{P}_{c\mathbf{k}+\mathbf{q}} \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa\alpha}(\mathbf{q})} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} \right| u_{n\mathbf{k}}^{(0)} \right\rangle + \left\langle u_{n\mathbf{k}}^{(0)} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(-\mathbf{q})} \left| \hat{P}_{c\mathbf{k}+\mathbf{q}} \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} \right\rangle \right] \right. \\ \left. + (\kappa\alpha, \mathbf{q}) \leftrightarrow (\kappa'\gamma, -\mathbf{q}) \right) U_{m,\kappa'\gamma}^*(\mathbf{q}) U_{m,\kappa\alpha}(\mathbf{q}) - \frac{1}{2} \left( \left( \left[ \sum_{n'=1}^M \frac{\left\langle u_{n\mathbf{k}}^{(0)} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(\mathbf{T})} \right| u_{n'\mathbf{k}}^{(0)} \right\rangle \left\langle u_{n'\mathbf{k}}^{(0)} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{T})} \right| u_{n\mathbf{k}}^{(0)} \right\rangle}{\varepsilon_{n\mathbf{k}}^{(0)} - \varepsilon_{n'\mathbf{k}}^{(0)} + i\delta} \right. \right. \\ \left. \left. + \left\langle \hat{P}_{c\mathbf{k}} \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa\alpha}(\mathbf{T})} \left| \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{T})} \right| u_{n\mathbf{k}}^{(0)} \right\rangle \right) + (\kappa\alpha) \leftrightarrow (\kappa'\gamma) \right) + (c.c.) \left( U_{m,\kappa\gamma}^*(\mathbf{q}) U_{m,\kappa\alpha}(\mathbf{q}) + U_{m,\kappa'\gamma}^*(\mathbf{q}) U_{m,\kappa'\alpha}(\mathbf{q}) \right) \left. \right\}.$$

- For the same reason, we have to update the Fan term in Eq. (16), but also, the denominator of the (static) Debye-Waller term in this equation was incorrectly written. The corrected Eq. (16) is written as

<sup>a)</sup>Electronic mail: samuel.pon@gmail.com

$$\begin{aligned}
\Delta\varepsilon_{nk}^{(\text{dynamic,RIA})}(T, \omega) = & \Re \frac{1}{N_q} \sum_{\mathbf{q}} \sum_m^{3N} \frac{1}{4\omega_{m\mathbf{q}}} \sum_{\substack{\kappa\alpha \\ \kappa'\gamma}} \left\{ \left( \left[ \sum_{n'=1}^M \langle u_{n\mathbf{k}}^{(0)} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(-\mathbf{q})} | u_{n'\mathbf{k}+\mathbf{q}}^{(0)} \rangle \right. \right. \\
& \times \langle u_{n'\mathbf{k}+\mathbf{q}}^{(0)} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} | u_{n\mathbf{k}}^{(0)} \rangle \left( \frac{n_{m\mathbf{q}}(T) + f_{n'\mathbf{k}+\mathbf{q}}}{\omega - \varepsilon_{n'\mathbf{k}+\mathbf{q}}^{(0)} + \omega_{m\mathbf{q}} + i\eta + i\delta} + \frac{n_{m\mathbf{q}}(T) + 1 - f_{n'\mathbf{k}+\mathbf{q}}}{\omega - \varepsilon_{n'\mathbf{k}+\mathbf{q}}^{(0)} - \omega_{m\mathbf{q}} + i\eta + i\delta} \right) \\
& + \left( \langle P_{c\mathbf{k}+\mathbf{q}} \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa\alpha}(\mathbf{q})} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} | u_{n\mathbf{k}}^{(0)} \rangle + \langle u_{n\mathbf{k}}^{(0)} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(-\mathbf{q})} | \hat{P}_{c\mathbf{k}+\mathbf{q}} \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} \rangle \right) \left( n_{m\mathbf{q}}(T) + \frac{1}{2} \right) \Big] \\
& + (\kappa\alpha, \mathbf{q}) \leftrightarrow (\kappa'\gamma, -\mathbf{q}) \Big) U_{m,\kappa'\gamma}^*(\mathbf{q}) U_{m,\kappa\alpha}(\mathbf{q}) - \frac{1}{2} \left( \left[ \sum_{n'=1}^M \frac{\langle u_{n\mathbf{k}}^{(0)} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(\mathbf{T})} | u_{n'\mathbf{k}}^{(0)} \rangle \langle u_{n'\mathbf{k}}^{(0)} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{T})} | u_{n\mathbf{k}}^{(0)} \rangle \right. \right. \\
& + \left. \left. \langle P_{c\mathbf{k}} \frac{\partial u_{n\mathbf{k}}}{\partial R_{\kappa\alpha}(\mathbf{T})} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{T})} | u_{n\mathbf{k}}^{(0)} \rangle \right] + (\kappa\alpha) \leftrightarrow (\kappa'\gamma) + (c.c.) \right) \left( n_{m\mathbf{q}}(T) + \frac{1}{2} \right) \left( U_{m,\kappa\gamma}^*(\mathbf{q}) U_{m,\kappa\alpha}(\mathbf{q}) \right. \\
& \left. + U_{m,\kappa'\gamma}^*(\mathbf{q}) U_{m,\kappa'\alpha}(\mathbf{q}) \right) \Big\},
\end{aligned}$$

where one can appreciate the static adiabatic nature of the Debye-Waller term.

- Similarly, Eq. (18) should be changed into

$$\begin{aligned}
\frac{1}{2\tau_{nk}^{(\text{non-adiabatic,RIA})}} = & \frac{\pi}{N_q} \sum_{\mathbf{q}} \sum_m^{3N} \frac{1}{4\omega_{m\mathbf{q}}} \sum_{\substack{\kappa\alpha \\ \kappa'\gamma}} U_{m,\kappa'\gamma}^*(\mathbf{q}) U_{m,\kappa\alpha}(\mathbf{q}) \sum_{n'=1}^M \left( \left[ \langle u_{n\mathbf{k}}^{(0)} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(-\mathbf{q})} | u_{n'\mathbf{k}+\mathbf{q}}^{(0)} \rangle \langle u_{n'\mathbf{k}+\mathbf{q}}^{(0)} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} | u_{n\mathbf{k}}^{(0)} \rangle \right. \right. \\
& \times \left. \left. \left( (n_{m\mathbf{q}}(T) + f_{n'\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n\mathbf{k}}^{(0)} - \varepsilon_{n'\mathbf{k}+\mathbf{q}}^{(0)} + \omega_{m\mathbf{q}}) + (n_{m\mathbf{q}}(T) + 1 - f_{n'\mathbf{k}+\mathbf{q}}) \delta(\varepsilon_{n\mathbf{k}}^{(0)} - \varepsilon_{n'\mathbf{k}+\mathbf{q}}^{(0)} - \omega_{m\mathbf{q}}) \right) \right] \right. \\
& \left. + (\kappa\alpha, \mathbf{q}) \leftrightarrow (\kappa'\gamma, -\mathbf{q}) \right).
\end{aligned}$$

- And finally, Eq. (19) should be changed into

$$\begin{aligned}
\frac{1}{2\tau_{nk}^{(\text{adiabatic,RIA})}} = & \frac{\pi}{N_q} \sum_{\mathbf{q}} \sum_m^{3N} \frac{1}{2\omega_{m\mathbf{q}}} \left( n_{m\mathbf{q}}(T) + \frac{1}{2} \right) \sum_{\substack{\kappa\alpha \\ \kappa'\gamma}} \sum_{n'=1}^M U_{m,\kappa'\gamma}^*(\mathbf{q}) U_{m,\kappa\alpha}(\mathbf{q}) \\
& \times \left( \langle u_{n\mathbf{k}}^{(0)} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa\alpha}(-\mathbf{q})} | u_{n'\mathbf{k}+\mathbf{q}}^{(0)} \rangle \langle u_{n'\mathbf{k}+\mathbf{q}}^{(0)} | \frac{\partial \hat{H}_{\mathbf{k},\mathbf{k}}}{\partial R_{\kappa'\gamma}(\mathbf{q})} | u_{n\mathbf{k}}^{(0)} \rangle \delta(\varepsilon_{n\mathbf{k}}^{(0)} - \varepsilon_{n'\mathbf{k}+\mathbf{q}}^{(0)}) + (\kappa\alpha, \mathbf{q}) \leftrightarrow (\kappa'\gamma, -\mathbf{q}) \right).
\end{aligned}$$

These corrections do not affect the numerical results, the ABINIT software package implementation, or the conclusions of the article.

<sup>1</sup>S. Poncé, Y. Gillet, J. Laflamme Janssen, A. Marini, M. Verstraete, and X. Gonze, *J. Chem. Phys.* **143**, 102813 (2015).