Erratum: First-principles calculation of nonlinear optical responses by Wannier interpolation **[Phys. Rev. B *96*, 115147 (2017)]**

Chong Wang , Xiaoyu Liu, Lei Kang, Bing-Lin Gu, Yong Xu, and Wenhui Duan

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Four minor errors and typographical errors in the original paper are corrected as follows.

(I) Equation (5) should be corrected as

$$r_{nm;a}^b = \frac{i\hbar^2}{E_{nm}} \left[\frac{v_{nm}^b \Delta_{nm}^a + v_{nm}^a \Delta_{nm}^b}{E_{nm}} + \sum_{p \neq n,m} \left(\frac{v_{np}^b v_{pm}^a}{E_{pm}} - \frac{v_{np}^a v_{pm}^b}{E_{np}} \right) \right] + \frac{1}{iE_{nm}} \langle n | \partial_a \partial_b \hat{H}(\mathbf{k}) | m \rangle (n \neq m).$$

This equation was not used in the calculations.

(II) Throughout the original paper, e is the charge of electron, such that $e = -|e|$. Unfortunately, the authors made a sign error in the code for the shift current. Therefore, the lines in Figs. 1(c) and 1(d) and Figs. 3(b)–3(d) should be flipped with respect to the horizontal axis. The results of Ref. [9] should also be flipped due to a different choice of the coordinate system. Therefore, our result and Ref. [9]’s result are still consistent with reasonable accuracy. For the reader’s convenience, we plot the corrected figures in Figs. 1 and 2 here.

(III) The interband term of second harmonic generation in Appendix A should be

$$\chi_e(\omega) = \frac{e^3}{2\hbar^2} \sum_{nml} \int \frac{d^3k}{(2\pi)^3} \frac{r_{nm}^a (r_{ml}^b r_{ln}^c + r_{ml}^c r_{ln}^b)}{\omega_{ln} - \omega_{ml}} \left[\frac{2f_{nm}}{\omega_{mn} - 2\omega} + \frac{f_{ln}}{\omega_{ln} - \omega} + \frac{f_{ml}}{\omega_{ml} - \omega} \right].$$

This typographical error did not enter the code and the relevant calculations were correct.

FIG. 1. The corrected Fig. 1 of the original paper.

FIG. 2. The corrected Fig. 3 of the original paper.

(IV) For $n = m$, Eq. (8) should be clarified with

$$(U^\dagger \partial_a \partial_a U)_{nm} = - \sum_{l \neq m} \frac{\langle m | H_a^{(W)} | l \rangle \langle l | H_a^{(W)} | m \rangle}{(E_l - E_m)^2}.$$

This equation in the original paper was correct. However, the subscript n on the left-hand side of the equation was reused as a summation index on the right-hand side, which may cause confusion for the readers. Similarly, for $a \neq b$ and $n = m$, Eq. (8) should be presented as

$$(U^\dagger \partial_b \partial_a U)_{nm} = - \frac{1}{2} \left(\sum_{l \neq m} \frac{\langle m | H_b^{(W)} | l \rangle \langle l | H_a^{(W)} | m \rangle}{(E_l - E_m)^2} + \sum_{l \neq m} \frac{\langle m | H_a^{(W)} | l \rangle \langle l | H_b^{(W)} | m \rangle}{(E_l - E_m)^2} \right).$$

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