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Erratum to " Accurate GW_0 band gaps and their phonon-induced renormalization in solids"

Tong Shen(申彤)[1,2], Xiao-Wei Zhang(张小伟)[1,3,†], Min-Ye Zhang(张旻烨)[4], Hong Jiang(蒋鸿)[4,‡], and Xin-Zheng Li(李新征)[1,2,§]

[1] *Interdisciplinary Institute of Light-Element Quantum Materials, Research Center for Light-Element Advanced Materials, and Collaborative Innovation Center of Quantum Matter, Peking University, Beijing* 100871, *China*

[2] *State Key Laboratory for Artificial Microstructure and Mesoscopic Physics, Frontier Science Center for Nano-optoelectronics and School of Physics, Peking University, Beijing* 100871, *China*

[3] *International Center for Quantum Materials, Collaborative Innovation Center of Quantum Matter, and School of Physics, Peking University, Beijing* 100871, *China*

[4] *Beijing National Laboratory for Molecular Sciences, College of Chemistry and Molecular Engineering, Peking University, Beijing* 100871, *China*

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The derivation of Eq. (28) in the original paper [*Chin. Phys. B* **30** 117101 (2021)] is corrected.

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After having Eq. (25), since

$$\sum_I \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \frac{\partial v^{\mathrm{KS}}(\boldsymbol{r})}{\partial R_{I\kappa\alpha}}\bigg|_{\boldsymbol{R}=\boldsymbol{R}^0} = \sum_I \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{R}_I)} \frac{\partial v^{\mathrm{KS}}(\boldsymbol{r}-\boldsymbol{R}_I)}{\partial R_{0\kappa\alpha}}\bigg|_{\boldsymbol{R}=\boldsymbol{R}^0} \tag{1}$$

has the lattice periodicity, the matrix in Eq. (25) can be reduced as

$$\begin{aligned}
&\langle n\boldsymbol{k} \mid \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \sum_{I\kappa\alpha} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{R}_I)} \frac{\partial v^{\mathrm{KS}}(\boldsymbol{r}-\boldsymbol{R}_I)}{\partial R_{0\kappa\alpha}}\bigg|_{\boldsymbol{R}=\boldsymbol{R}^0} \mid m\boldsymbol{k}'\rangle \\
&= \frac{1}{N}\int \mathrm{d}^3\boldsymbol{r}\, \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}'-\boldsymbol{q})\cdot\boldsymbol{r}} \sum_{I\kappa\alpha} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{R}_I)} \frac{\partial v^{\mathrm{KS}}(\boldsymbol{r}-\boldsymbol{R}_I)}{\partial R_{0\kappa\alpha}}\bigg|_{\boldsymbol{R}=\boldsymbol{R}^0} u^*_{n\boldsymbol{k}}(\boldsymbol{r}) u_{m\boldsymbol{k}'}(\boldsymbol{r}) \\
&= \frac{1}{N}\sum_J \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}'-\boldsymbol{q})\cdot\boldsymbol{R}_J} \int_\Omega \mathrm{d}^3\boldsymbol{r}\, \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}'-\boldsymbol{q})\cdot(\boldsymbol{r}-\boldsymbol{R}_J)} \sum_{I\kappa\alpha} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{R}_J-\boldsymbol{R}_I)} \frac{\partial v^{\mathrm{KS}}(\boldsymbol{r}-\boldsymbol{R}_J-\boldsymbol{R}_I)}{\partial R_{0\kappa\alpha}}\bigg|_{\boldsymbol{R}=\boldsymbol{R}^0} u^*_{n\boldsymbol{k}}(\boldsymbol{r}) u_{m\boldsymbol{k}'}(\boldsymbol{r}) \\
&= \delta_{\boldsymbol{k}=\boldsymbol{k}'+\boldsymbol{q}} \int_\Omega \mathrm{d}^3\boldsymbol{r} \sum_{I\kappa\alpha} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{R}_I)} \frac{\partial v^{\mathrm{KS}}(\boldsymbol{r}-\boldsymbol{R}_I)}{\partial R_{0\kappa\alpha}}\bigg|_{\boldsymbol{R}=\boldsymbol{R}^0} u_{n\boldsymbol{k}}{}^*(\boldsymbol{r}) u_{m\boldsymbol{k}-\boldsymbol{q}}(\boldsymbol{r}) \\
&= \langle u_{n\boldsymbol{k}} \mid \sum_{I\kappa,\alpha} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{R}_I)} \frac{\partial v^{\mathrm{KS}}(\boldsymbol{r}-\boldsymbol{R}_I)}{\partial R_{0\kappa\alpha}}\bigg|_{\boldsymbol{R}=\boldsymbol{R}^0} \mid u_{m\boldsymbol{k}-\boldsymbol{q}}\rangle_\Omega \delta_{\boldsymbol{k}=\boldsymbol{k}'+\boldsymbol{q}},
\end{aligned} \tag{2}$$

where the subscript Ω represents the integral is within a unit cell. Therefore, Eq. (25) can be rewritten as

$$\hat{H}_1 = N^{-1/2} \sum_{nm\boldsymbol{k}} \sum_{\boldsymbol{q}\nu} g_{nm\nu}(\boldsymbol{k},\boldsymbol{q}) \hat{a}^\dagger_{n\boldsymbol{k}} \hat{a}_{m\boldsymbol{k}-\boldsymbol{q}} \left(\hat{b}_{\boldsymbol{q}\nu} + \hat{b}^\dagger_{-\boldsymbol{q}\nu}\right). \tag{3}$$

Here, we define the electron–phonon coupling matrix element

$$g_{nm\nu}(\boldsymbol{k},\boldsymbol{q}) = \left\langle u_{n\boldsymbol{k}} \middle| \nabla_{\boldsymbol{q}\nu} v^{\mathrm{KS}} \middle| u_{m\boldsymbol{k}-\boldsymbol{q}} \right\rangle_\Omega, \tag{4}$$

where $\nabla_{\boldsymbol{q}\nu} v^{\mathrm{KS}} = \sum_{I\kappa} \left(\frac{1}{2M_\kappa \omega_{\boldsymbol{q}\nu}}\right)^{\frac{1}{2}} \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{R}_I)} \xi_\kappa(\boldsymbol{q}\nu) \cdot \nabla_{\boldsymbol{R}_{0\kappa}} v^{\mathrm{KS}}(\boldsymbol{r}-\boldsymbol{R}_I)$.

References

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†Corresponding author. E-mail: willzxw@pku.edu.cn

‡Corresponding author. E-mail: jianghchem@pku.edu.cn

§Corresponding author. E-mail: xzli@pku.edu.cn

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