Erratum: Fröhlich polaron effective mass and localization length in cubic materials: Degenerate and anisotropic electronic bands [Phys. Rev. B 104, 235123 (2021)]

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An inconsistent choice of phase convention has been discovered in the published version of the article. The i prefactor in three equations has to be removed. Moreover, a subscript is incorrect in another equation. All the other results are unchanged however. The choice of phase convention is discussed, and the connection with choices appearing in the literature is made.

The electron creation operator in Eq. (4) of the original paper has an incorrect subscript, and should be

$$\hat{H}^{\mathrm{Fr}}_{\mathrm{EPC}} = \sum_{\vec{k},\vec{q}} g^{\mathrm{Fr}}(\vec{q})\hat{c}^{+}_{\vec{k}+\vec{q}}\hat{c}_{\vec{k}}\,(\hat{a}_{\vec{q}} + \hat{a}^{+}_{-\vec{q}}). \tag{E1}$$

We thank A. Marini for noticing that this corrected Eq. (4) in conjunction with Eq. (5) of the original paper give a non-Hermitian Hamiltonian. This erroneous formulation of the Fröhlich model comes from an inconsistent choice of phases to deduce Eqs. (4) and (5) of the original paper from the density-functional theory first-principles formulation. In addition, the choices of phase for Eqs. (43) and (44) of the original paper are inconsistent, yielding also a non-Hermitian Hamiltonian. The i has to be removed from Eqs. (5), (6), and (44) of the original paper. All other results are unchanged.

However, this simple fix needs to be discussed, as it is not the only possibility to obtain Hermiticity, and the reason for this mistake in the original paper might be quite obscure. The generalized Fröhlich Hamiltonian is deduced from the density-functional theory applied to the electron-phonon interaction, as exposed in the review on electron-phonon interactions from first principles by Giustino [1]. Equation (43) of the original paper is obtained, provided that Eq. (18) of the original paper is fulfilled, namely,

$$e_{\kappa\alpha,\nu}(-\vec{q}) = e^{*}_{\kappa\alpha,\nu}(\vec{q}). \tag{E2}$$

Giustino mentions that this is a convention, and refers to a publication by Maradudin and Vosko [2] for the discussion of such convention. Indeed, in the discussion by Ref. [2], Eq. (E2) is mentioned to be the choice of Born and Huang [3], Eq. (24.18), while another convenient choice,

$$e_{\kappa\alpha,\nu}(-\vec{q}) = -e^{*}_{\kappa\alpha,\nu}(\vec{q}), \tag{E3}$$

can be found in the book by Leibfried [4].

We will now see that this choice of phase convention has a direct influence on Eqs. (5), (6), and (44) of the original paper.

The generalized Fröhlich coupling in the cubic case, which is the topic of of the original paper, must be deduced from Eq. (5) of Ref. [5], in which the mode polarity vector $\vec{p}_j(\hat{q})$ depends on the above-mentioned choice of phase. The mode polarity in the cubic case is always aligned with the direction $\hat{q}$, and can be written in terms of its length p_j as

$$\vec{p}_j(\hat{q}) = \eta_j(\hat{q})\hat{q}p_j, \tag{E4}$$

where $\eta_j(\hat{q})$ is a phase, so that $|\eta_j(\hat{q})| = 1$. In cubic materials, the length p_j does not depend on the direction $\hat{q}$. However, the phase $\eta(\hat{q})$ might depend on the direction, and should be chosen coherently with the convention for $e_{\kappa\alpha,\nu}(\vec{q})$ that delivers the mode-polarity vector [see Eq. (16) in the Supplementary Information of Ref. [5]]. Using this Eq. (E4), one deduces from Eq. (5) of Ref. [5] that

$$g^{\mathrm{gFr}}(\vec{k}nn', \vec{q}j) = \eta_j(\hat{q})\frac{i}{q}\frac{4\pi}{\Omega_0}\left(\frac{1}{2\omega_{j\mathrm{LO}}V_{\mathrm{BvK}}}\right)^{1/2}\frac{p_{j\mathrm{LO}}}{\epsilon^{\infty}}\sum_{m} s_{n'm}(\hat{k}')[s_{nm}(\hat{k})]^{*}. \tag{E5}$$

Comparing with Eq. (44) of the original paper, one realizes that the prefactor $\eta_j(\hat{q})$ has been added.

The Born and Huang convention yields (with the replacement of ν by j to follow the notation of the original paper)

$$\vec{p}_j(-\vec{q}) = [\vec{p}_j(\vec{q})]^{*}, \tag{E6}$$

while the Leibfried convention yields

$$\vec{p}_j(-\vec{q}) = -[\vec{p}_j(\vec{q})]^{*}. \tag{E7}$$

Equivalently, with the Born and Huang convention,

$$\eta_j(-\vec{q}) = -\eta_j^*(\vec{q}), \tag{E8}$$

while with the Leibfried convention,

$$\eta_j(-\vec{q}) = \eta_j^*(\vec{q}). \tag{E9}$$

The choices $\eta_j(\hat{q}) = 1$ or $\eta_j(\hat{q}) = -1$ are coherent with Leibfried convention, while the choices $\eta_j(\hat{q}) = i$ or $\eta_j(\hat{q}) = -i$ are coherent with the Born and Huang convention. Since Eq. (43) of the original paper has been obtained with the Born and Huang convention, this convention should have been used also for the corresponding Eq. (44), and similarly for Eqs. (5) and (6) of the original paper. This was not the case in the original paper, where $\eta_j(\hat{q}) = 1$ had been taken. Choosing $\eta_j(\hat{q}) = -i$, the corrected Eq. (44) of the original paper is

$$g^{\mathrm{gFr}}(\vec{k}nn', \vec{q}j) = \frac{1}{q}\frac{4\pi}{\Omega_0}\left(\frac{1}{2\omega_{j\mathrm{LO}}V_{\mathrm{BvK}}}\right)^{1/2}\frac{p_{j\mathrm{LO}}}{\epsilon^\infty}\sum_m s_{n'm}(\hat{k}')[s_{nm}(\hat{k})]^*. \tag{E10}$$

Similarly, the corrected Eqs. (5) and (6) of the original paper are

$$g^{\mathrm{Fr}}(\vec{q}) = \frac{1}{q}\left[\frac{2\pi\omega_{\mathrm{LO}}}{V_{\mathrm{BvK}}}\left(\frac{1}{\epsilon^\infty} - \frac{1}{\epsilon^0}\right)\right]^{1/2} \tag{E11}$$

and

$$g^{\mathrm{Fr}}(\vec{q}) = \frac{1}{q}\left[\frac{2\sqrt{2}\pi}{V_{\mathrm{BvK}}}\frac{\omega_{\mathrm{LO}}^{3/2}}{\sqrt{m^*}}\alpha\right]^{1/2}. \tag{E12}$$

One sees that the i prefactor is suppressed in these equations. The similar equation [Eq. (13)] in the Supplementary Information of Ref. [5] has to be changed as well by suppressing its i prefactor.

At variance, if the Leibfried convention is followed, the Eqs. (5), (6), and (44) of the original paper are obtained. As mentioned above, the presentation in the Giustino review (Ref. [1]) is consistent with the Born and Huang convention. If one were to use the Leibfried convention, Eq. (37) and several others in Ref. [1] would also have to be adapted. The whole set of equations for the Leibfried convention will not be presented here, only the equations present in the original paper.

As a result of such phase change, the term with the annihilation and creation operators in Eq. (37) of the Giustino review is changed, from $(\hat{a}_{\mathbf{q},\nu} + \hat{a}^+_{-\mathbf{q},\nu})$ to $(\hat{a}_{\mathbf{q},\nu} - \hat{a}^+_{-\mathbf{q},\nu})$.

Thus, Eq. (43) of the original paper changes, either to

$$\hat{H}^{\mathrm{gFr}} = \sum_{\vec{k},n}\frac{\sigma\vec{k}^2}{2m_n^*(\hat{k})}\hat{c}^+_{\vec{k},n}\hat{c}_{\vec{k},n} + \sum_{\vec{q},j}\omega_{j\mathrm{LO}}\hat{a}^+_{\vec{q},j}\hat{a}_{\vec{q},j} + \sum_{\vec{k}nn',\vec{q}j}g^{\mathrm{gFr}}(\vec{k}nn', \vec{q}j)\hat{c}^+_{\vec{k}+\vec{q},n'}\hat{c}_{\vec{k},n}(\hat{a}_{\vec{q},j} - \hat{a}^+_{-\vec{q},j}), \tag{E13}$$

corresponding to $\eta_j(\hat{q}) = 1$, or to

$$\hat{H}^{\mathrm{gFr}} = \sum_{\vec{k},n}\frac{\sigma\vec{k}^2}{2m_n^*(\hat{k})}\hat{c}^+_{\vec{k},n}\hat{c}_{\vec{k},n} + \sum_{\vec{q},j}\omega_{j\mathrm{LO}}\hat{a}^+_{\vec{q},j}\hat{a}_{\vec{q},j} + \sum_{\vec{k}nn',\vec{q}j}g^{\mathrm{gFr}}(\vec{k}nn', \vec{q}j)\hat{c}^+_{\vec{k}+\vec{q},n'}\hat{c}_{\vec{k},n}(-\hat{a}_{\vec{q},j} + \hat{a}^+_{-\vec{q},j}), \tag{E14}$$

corresponding to $\eta_j(\hat{q}) = -1$, albeit with a transfer of this negative sign from the coupling g^{gFr} to the phonon operators in the last parentheses of the Hamiltonian. Equation (4) of the original paper should be modified similarly.

In the original paper, the phase contained in Eqs. (5), (6), or (44) has no influence on the other results, since the Fröhlich coupling is always multiplied by its complex conjugate.

In the literature, both conventions are present. We give several examples. The classic Feynman work on polarons [6] relies on the Leibfried convention, with $\eta_j(\hat{q}) = -1$, and the transfer of the negative sign from the coupling to the Hamiltonian (Devreese lecture notes [7], also). In the book by Madelung [8], Eq. (3.124) is the Born and Huang convention. In the book by Mahan [9], the Born and Huang convention is used as well. This is clear in equations (1.74), (1.280), (1.281), (7.1), and (7.3), namely, all the equations that relate directly to the Fröhlich model. Equation (1.86) is in appearance following the Leibfried convention, but we note that the combination of phonon operators in Eq. (1.86) is coherent with Born and Huang. Incorporating the i prefactor of Eq. (1.85) into $\xi_{\mathbf{k},\lambda}$ and identifying the resulting polarization vector with our $e_{\kappa\alpha,\nu}(\vec{q})$ satisfies Eq. (E2), which is again the Born and Huang convention, as expected.

Finally, we note that the directional dependence of $\eta_j(\hat{q})$ is not used in the above-mentioned choices. Another natural possibility would be to fix the mode-polarity vector such that it is unchanged when the magnitude of $\vec{q}$ decreases, passes through zero, and emerges on the other side. Indeed, the nonanalytical part of the dynamical matrix, Eq. (60) of Ref. [10], is unchanged when this happens. This would, however, require

$$\vec{p}_j(-\vec{q}) = \vec{p}_j(\vec{q}), \tag{E15}$$

meaning

$$\eta_j(-\vec{q}) = -\eta_j(\vec{q}), \tag{E16}$$

which is neither Born and Huang convention nor Leibfried convention. The directional dependence of $\eta_j(\hat{q})$ might be used to obtain this result, although $\eta_j(\vec{q})$ cannot be made a continuous function of $\vec{q}$ in such case, as one is working in a space of real normed vectors $\hat{q}$ in three dimensions, while the freedom of phase is inside the space of the moduli of complex numbers. In mathematical terms, one can prove in homotopy theory that there is no map from the three-dimensional sphere $\mathbb{S}^2$ to the two-dimensional complex number circle $\mathbb{S}^1$ that fulfills Eq. (E16).

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