Reply to Shvaika et al.: Presence of a boson peak in anharmonic phonon models with Akhiezer-type damping

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There were two unintentional mistakes in our original paper, which have been now corrected. All the physical conclusions and results of the original paper, including the prediction of boson peak due to anharmonicity, remain valid in the corrected version.

As pointed out in [1], our Eq.(7) in Ref.[2] contains an obvious mathematical inconsistency due to the absence of the 3D volume factor $q^2 dq$. Moreover, in [2], we assumed the low-energy phonon dispersion relation $\Omega(q) = vq$ which does not take into account the ubiquitous bending of the acoustic branch towards larger wavevector near the Brillouin-zone (BZ) boundary. In this Reply, we correct these issues and show that the main physical conclusions of [2] remain unchanged.

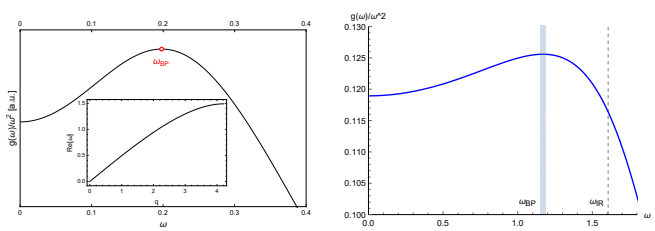

Figure 1. **Left:** the presence of a BP arising from Eqs.(1)-(2). Here $v = 0.5, a_4 = 0.007, D = 0.012, q_D = 5.95$. Finally, $\omega_{BZ} \approx 1.5 \gg \omega_{BP}$. The inset shows the acoustic dispersion relation used to compute the VDOS as given by Eq.(2). **Right:** The correlation between the BP and IR frequencies. For completeness, also the longitudinal branch (L) has been added. In these plots , $v_T = 0.5, a_4^T = 0.003, D_T = 0.045, v_L = 1.051, a_4^L = 0.01, D_L = 0.05, k_D = 5.95$. Using these parameters, we have $\omega_{IR}/\omega_{BP} = 1.3$.

Neglecting the longitudinal modes, the correct expression for the vibrational density of states (VDOS) is given by:

$$g(\omega) \;=\; -\,\frac{2\,\omega}{\pi\, q_D^3}\int_0^{q_D} \mathrm{Im}\,\mathrm{G}(\omega,q)\,q^2\,dq \qquad (1)$$

where:

$$\mathrm{G}(\omega,q) \;=\; \frac{1}{\omega^2 \;-\; v^2\,q^2 \;+\; a_4\,q^4 \;+\; i\,\omega\,D\,q^2} \qquad (2)$$

is the propagator given by hydrodynamic expansion in powers of q (which cannot be extrapolated beyond the point at which the dispersion relation flattens).

Eq.(1) combined with Eq.(2) predicts a boson peak (BP) anomaly in the Debye normalized VDOS $g(\omega)/\omega^2$, which is well separated from the edge of the BZ, ω_{BZ}, as shown in Fig.1. The emergence of the BP is due to the anharmonic Akhiezer-type phonon damping $\Gamma = Dq^2$ in the propagator of Eq.(2), without which no BP can be predicted. Also the prediction that the BP frequency ω_{BP} is close to the frequency of the Ioffe-Regel crossover ω_{IR} remains confirmed in the corrected version of the model, see the right panel of Fig. 1.

We demonstrated the *presence of a BP in anharmonic phonon models with Akhiezer-type damping*, which invalidates the arguments presented in the Comment by Svhaika et al. [1] and supports the validity of our original model [2].

[1] A. Shvaika, M. Shpot, W. Schirmacher, T. Bryk, and G. Ruocco, "Absence of a boson peak in anharmonic phonon models with akhiezer-type damping," (2021).

[2] M. Baggioli and A. Zaccone, Phys. Rev. Lett. **122**, 145501 (2019).