Erratum: Phonon-mediated high-temperature superconductivity in the ternary borohydride KB₂H₈ under pressure near 12 GPa [Phys. Rev. B **104, L100504 (2021)]**Miao Gao , Xun-Wang Yan, Zhong-Yi Lu, and Tao Xiang

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The projected phonon density of states (DOS) of KB₂H₈ presented in Fig. 3(b) was calculated with the quasiharmonic approximation (QHA) package in QUANTUM ESPRESSO. Very recently, we find that there is a bug in the QHA codes, whereas the phonon displacements rather than phonon eigenvectors are employed to construct the projected phonon DOS by default. The normalized phonon displacements are the eigenvectors divided by the square root of the mass. The correct definition of projected phonon DOS reads

$$\text{DOS}^\alpha(\omega) = \frac{1}{N_{\mathbf{q}}} \sum |\mathbf{e}_{\mathbf{q}\nu}^\alpha|^2 \delta(\omega - \omega_{\mathbf{q}\nu}). \quad (1)$$

Here, $\mathbf{q}$ is the wave vector. $N_{\mathbf{q}}$ is the total number of $\mathbf{q}$ points. ν is the index of phonon branch. $\omega_{\mathbf{q}\nu}$ represents the vibrational frequency for phonon $\mathbf{q}\nu$. $\mathbf{e}_{\mathbf{q}\nu}^\alpha$ is the phonon eigenvector of atom α for phonon mode $\mathbf{q}\nu$. Finally, the DOS is normalized to $3N$ with N being the number of atoms in the unit cell.

The revised projected phonon DOS for KB₂H₈ under 12 GPa is presented in Fig. 1. As expected, the vibration of K atoms dominates acoustic phonon modes. The contribution of the boron to the DOS mainly locates in intervals from 20 to 50 meV. The updated projected phonon DOS has no influence on the results of electron-phonon coupling and superconductivity for KB₂H₈.

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FIG. 1. Projected phonon density of states of KB₂H₈ under 12 GPa.