Erratum: Lattice-dynamical model for the filled skutterudite $\text{LaFe}_4\text{Sb}_{12}$: Harmonic and anharmonic couplings [Phys. Rev. B **89**, 224304 (2014)]

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While doing more accurate calculations of force constants in filled skutterudites, we discovered a number of small errors in our earlier publication, which do not affect its substance.

There was an error in our calculations for quartic anharmonic coefficients that affects only one quartic tensor component (3,1,2,1) in Table VI for columns labeled Fe-7.5, Fe-9.9, Sb-5.7, Sb-7.7, Sb-9.4, and Sb-10.7. The values for this component should be as follows: -0.06 , -0.06 , -1.08 , 0.01 , 0.11 , and -0.04 , respectively.

There was a misprint in Table VI: Two different values are mistakenly reported for one force constant (3,1,2,2), and there is a missing entry for (1,1,2,2). The first value for (3,1,2,2) is the value for (1,1,2,2) and the second value for (3,1,2,2) is the correct value.

We inadvertently omitted results for some longer-range forces that, although most likely do not effect measurable properties, are calculable due to the large size of the computational cell. In particular, results for Sb-La distances 11.06, 12.3, and 13.3 Å were ignored as were results for a La-Fe distance of 11.9 Å. It is possible that the Gruneisen parameter defined in the paper may depend on these interactions.

Finally, our very small estimated values for the nearest-neighbor La-La force constant are unreliable as we found through the use of a more accurate density functional parameter set. The true value is more than an order of magnitude larger, consistent with the results of Koza *et al.* [1], who have noted the extreme smallness of our projector augmented wave results in comparison to their calculated value for this force constant. None of the other published results so strongly deviate from our newer calculations, although factor of 2 differences are common for the smaller La-La interactions as well as for other beyond-nearest-neighbor interactions. Notwithstanding these deviations, the anomalously large second neighbor La-La force constant is reliable.

The most significant change that made the newer calculations more accurate was the choice of smearing function in the VASP code. The earlier calculation used the default, i.e., the method of Methfessel-Paxton [2] with order 1, whereas the newer calculations used the more stable Gaussian smearing. The recent calculations also applied the projectors in reciprocal space and increased the plane-wave energy cutoff to 400 eV, although those changes appeared to have only a negligible effect on the force constants, indicating that the original values are sufficient. We also spot-checked the effect of a denser Brillouin-zone mesh ($4 \times 4 \times 4$ for the $2 \times 2 \times 2$ supercell), which appears to change some force constants by a few percent, suggesting that this is a reasonable estimate of the remaining convergence error in the force constants.

[1] M. M. Koza, M. Boehm, E. Sischka, W. Schnelle, H. Mutka, and A. Leithe-Jasper, *Phys. Rev. B* **91**, 014305 (2015).

[2] M. Methfessel and A. T. Paxton, *Phys. Rev. B* **40**, 3616 (1989).