Erratum: Quantitative validation of the Boltzmann transport equation phonon thermal conductivity model under the single-mode relaxation time approximation [Phys. Rev. B 69, 094303 (2004)]

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When calculating the phonon relaxation times, τ, we incorrectly multiplied the time constant obtained from the decay of the phonon-mode energy autocorrelation function by two. The reported thermal conductivities are therefore too large by a factor of two. As a result, by comparing to thermal conductivities predicted using the Green-Kubo method, we incorrectly concluded that the thermal transport in Lennard-Jones argon is well-described under the isotropic assumption.

Turney *et al.*[1] recently predicted the thermal conductivity of Lennard-Jones argon using our formulation. Using the correct values of the relaxation times, they found that the isotropic assumption underpredicts the thermal conductivity compared to values obtained using Green-Kubo or direct method molecular dynamics approaches. The thermal conductivities they predict using phonons from the entire Brillouin zone are in good agreement with the Green-Kubo and direct method values up to a temperature of 50 K. Their results validate the Boltzmann transport equation phonon thermal conductivity model under the single-mode relaxation time approximation.

Please consider the following when reading our original paper:

The values and spreads of the relaxation times in Table II should be divided by two.

The $1/\tau$ data plotted in Figs. 5(a), 5(b), and 5(c) should be multiplied by two. The curves corresponding to Eq. (16) in Fig. 5(a) are unchanged. Because the slopes of these curves are very large at the maximum frequencies, the thermal conductivity predictions are unaffected.

All thermal conductivities in Tables III (except k_{GK}) and IV should be divided by two. The comparison between the different approximations in Table IV is still valid.

The k_{BTE}, k_L, and k_T values in Figs. 7(a) and 9 should be divided by two.

We recommend that readers consult our original paper for details on obtaining phonon properties from molecular dynamics simulations, and Turney *et al.*[1] for the numerical results for Lennard-Jones argon.

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[1] J. E. Turney, E. S. Landry, A. J. H. McGaughey, and C. H. Amon, Phys. Rev. B **79**, 064301 (2009).

