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Computational Study of Vibrational Thermal Conductivity - Effects beyond the Peierls-Boltzmann (PB) equation TAO SUN, INFM-CNR DEMOCRITOS and SISSA, P.B. ALLEN, Stony Brook University — The heat flux $j(\text{ph})$ of phonons is the sum over modes of $e(Q)v(Q)N(Q)$ (energy, velocity, and occupation). The PB equation relates $N(Q)$ to the temperature gradient, and gives a theory, exact to second order in anharmonicity, for the high T form $k=C/T$ of the thermal conductivity. We use classical molecular dynamics to evaluate the exact classical $k(T)$ from the heat-current correlation $[j(t)j(0)]$ for a 2-D Lennard-Jones triangular lattice. This keeps three corrections to PB theory: (1) a fully anharmonic potential $V(\text{LJ})$; (2) exact treatment of phonon-phonon interactions, not limited to low order; (3) an “exact” heat current operator j , with anharmonic terms beyond the quasiparticle version $j(\text{ph})$. Our work, which follows Ladd, Moran, and Hoover (Phys. Rev. B34, 5088 (1986)), finds large corrections to the PB form $k=C/T$, even though phonon quasiparticles are fairly well-defined. Restriction to 2-D enhances statistical and finite-size accuracy with little loss of realism. Our findings are (a) truncation of the Taylor expansion of $V(\text{LJ})$ gives the correct $k(T)$, but terms up to 8th order are needed at higher T; (b) anharmonic terms in j are very important even at quite low T; (c) the computed contributions to $k(T)$ from terms of j beyond $j(\text{ph})$ are qualitatively explained using the lowest non-diverging contribution of a perturbation expansion.

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