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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(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(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(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(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(ph) are qualitatively explained using the lowest non-diverging contribution of a perturbation expansion.

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