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Exploiting non-local analysis of lattice thermal conductivity[1]

PHILIP B. ALLEN, Stony Brook University — Small Q phonons have very slow relaxation rates $1/\tau_Q$. This causes the heat current $j(x)$ to depend on the temperature gradient $dT(x')/dx'$ at long distances $|x - x'|$. In a homogeneous crystal, the Fourier-space representation $j(q) = -\kappa(q)dT/dx(q)$ is helpful; I use this to analyze simulations[2,3] of GaN thermal conductivity. The Peierls-Boltzmann equation in relaxation time approximation gives a formula for $\kappa(q)$. Using a Debye model, explicit results $\kappa_p(q)$ are found for models where $1/\tau_Q \propto Q^p$. Numerics often gives exponents p to be 2, 3, or 4. When $p = 2$, $\kappa_2(q) \sim \kappa_0 - C\sqrt{q}$. This shows that simulations on samples of size L should be extrapolated by plotting $\kappa(L)$ *versus* $1/\sqrt{L}$. For exponent $p \geq 3$, $\kappa(q)$ diverges as $q \to 0$, which means that $\kappa(L)$ diverges as $L \to \infty$. An improved analysis is described, which uses Callaway's version of the relaxation time approximation, treating N and U processes separately.

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[2] X. W. Zhou *et al.*, Phys. Rev. B **79**, 115201 (2009).
[3] Z. Liang *et al.*, J. Appl. Phys. **118**, 125104 (2015).

Philip B. Allen
Stony Brook University

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