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Spherical Harmonic Expansion Method for Coupled Electron-Phonon Boltzmann Transport MARCO SANTIA, JOHN ALBRECHT, Michigan State University — Thermoelectric transport modeling often relies on independent Boltzmann transport equations (BTEs) for electrons and phonons which work best near equilibrium (linearized) and steady-state. Device design relies heavily on this baseline approximation. Monte Carlo methods can allow for complex physical interactions (e.g., anharmonicity) but their stochastic nature has practical limits. Distribution functions with wide disparities in population (e.g., ratios $> 10^8$ between majority and minority carriers.[1]) are a computational challenge. We present a coupled BTE solver based on a k-space spherical harmonic expansion (SHE) of the distribution functions and eigenstates of electrons and phonons. The method is deterministic and allows for detailed treatments of scattering processes, yet ameliorates the issues with population disparity within phase space. We set the formalism and examine the accuracy of the SHE for phonon band structures, calculate scattering rates determined within that representation, and compare our preliminary results for distribution statistics in control examples such as thermal conductivity and drift velocity.

[1]The SHE method has treated majority/minority carriers in bipolar transistors, S.-M. Hong, et al, IEEE Trans. Electr. Dev. **57**, 2390 (2010).

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