Electronic transport simulations in complex bandstructure thermoelectric materials

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1. Abstract

Thermoelectric materials convert heat through temperature gradients into electricity, and vice versa provide cooling capabilities once a potential difference is applied across them. The realization of complex bandstructure materials and their alloys, as well as nanostructured materials, have revived the field of thermoelectric from decades of moderate activity, as they allow possibilities to largely improved performance. Theory and simulation of electro-thermal transport properties of materials has also been rapidly advancing. A variety of simulation software and techniques has been developed, or are in the process of being developed to improve the accuracy of these calculations. The most common simulations for the thermoelectric properties of complex materials employ *ab initio* techniques (DFT) for the dispersion of materials, which are then used within the Boltzmann Transport Equation (BTE) formalism to extract the thermoelectric coefficients. In the majority of studies, the solutions to the BTE assume the constant relaxation time approximation, despite the fact that we know that the scattering mechanisms are not only energy, but momentum, and band dependent. This is due to the vast computational costs in treating energy dependent scattering mechanisms properly. This paper introduces the BTE formalism, and explains the numerical implementation of the energy dependent relaxation time approximation.