SEMICLASSICAL AND QUANTUM TRANSPORT OF PHONONS

Vittorio Romano[1,*], Vito Dario Camiola[1], Giovanni Nastasi[2], Giorgia Vitanza[2]

[1]Department of Mathematics and Computer Science, University of Catania, viale A. Doria 6, 95125 Catania, Italy
[2]University "Kore", Enna, Italy
[*]vittorio.romano@unict.it

ABSTRACT

Thermal effects in micro and nano electronic and mechanical devices has acquired an increasingly relevant importance [7; 8; 9] and their description requires accurate physical models beyond the standard Fourier law. At kinetic level a good model can be formulated by introducing the phonons, which are bosonic quasi particles, whose dynamic in the semiclassical case (mean-free path greater or equal the characteristic length of the phenomenum) is described by the Peierls-Boltzmann equation for each phonon branch. In the case of typical lengths smaller than the phonon mean-free path quantum effects must be taken into account as well (see [10]). A natural extension of the Peierls-Boltzmann equation is the Wigner one that better reveals the wave nature of phonons and still keeps the structure of a kinetic formulation. However, in the literature an almost standard approximation is to consider the Wigner equation with quadratic dispersion relation. We focus on the inclusion of general dispersion relation into the Wigner equation and then we consider as particular cases the group velocity of acoustic and optical phonons.

The approach is based on Weyl quantization and Moyal's calculus [11]. In order to get asymptotic expression for the heat flux the pseudo-differential operators are expanded up to the second order in $\hbar$ while the phonon-phonon collision operators are modelled in a relaxation form depending on a local equilibrium temperature which is definite according to [7].

An energy transport model is obtained by using the moment method with closures based on a quantum version of the Maximum Entropy Principle [12; 13; 14; 15; 16; 17; 18]. An explicit form of the thermal conductivity with quantum correction is obtained under a suitable scaling. Numerical results are presented in the semiclassical limit for thermal effects in graphene.

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