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Lattice thermal transport through atomically defined systems in a quantum mechanical description.

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There are different theoretical approaches to describe lattice thermal transport through nano-sized solid structures. From those approaches, atomistic calculations represent the smallest level of description, and provide a straight route towards fully understanding the phonon transport process across nanomaterials and interfaces. Within the atomistic descriptions themselves, there are several categories: 1-"classical," such as molecular dynamics, 2-"semi-classical," such as the Boltzmann-Peierls equation, and 3-"quantum-mechanical," such as Green's functions techniques. In this talk we will focus on quantum mechanical effects on nanoscale thermal transport, with specific examples in nanowires, nanotubes, and molecular junctions. Thus, we will discuss specific theoretical techniques from categories 2 and 3 above. We will start from the simplest of these approaches [1], which gives a good account of experimental measurements in semiconductor nanowires. Then we will discuss the more complex problem of thermal conduction in single walled carbon nanotubes, graphene, and graphite. We will see how the character of the 3-phonon scattering process in these systems results in long phonon mean free paths and thermal conductivities [2]. Subsequent experimental results have confirmed findings from the theoretical study [3]. Then, we will discuss a newer technique, based on non-equilibrium Green's functions, that allows to study the quantum mechanical many-body problem of interacting phonons flowing through generic, atomically described, anharmonic structures [4]. This technique is applied to investigate a simple model molecular junction. We will show some strictly quantum mechanical effects that take place in the anharmonic scattering process. Finally, we will present new results on first-principles calculations of phonon conduction across nitrogen impurities in carbon nanotubes [5].

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