Wigner formulation of thermal transport in solids

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Two different heat-transport mechanisms are discussed in solids: in crystals, heat carriers propagate and scatter particle-like as described by Peierls' formulation of the Boltzmann transport equation for phonon wavepackets. In glasses, instead, carriers behave wave-like, diffusing via a Zener-like tunneling between quasi-degenerate vibrational eigenstates, as described by the Allen-Feldman equation. Recently, it has been shown that these two conduction mechanisms emerge from a Wigner transport equation, which unifies and extends the Peierls-Boltzmann and Allen-Feldman formulations, allowing to describe also complex crystals where particle-like and wave-like conduction mechanisms coexist. Here, we discuss the theoretical foundations of such transport equation as is derived from the Wigner phase-space formulation of quantum mechanics, elucidating how the interplay between disorder, anharmonicity, and the quantum Bose-Einstein statistics of atomic vibrations determines thermal conductivity.
We rationalize the conditions determining the crossover from particle-like to wave-like heat conduction, showing that phonons below the Ioffe-Regel limit (i.e. with a mean free path shorter than the interatomic spacing) contribute to heat transport due to their wave-like capability to interfere and tunnel. Finally, we show that the present approach overcomes the failures of the Peierls-Boltzmann formulation for crystals with ultralow or glass-like thermal conductivity, with case studies of materials for thermal barrier coatings and thermoelectric energy conversion.

Wigner signed-particles: computational challenges and simulation opportunities

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Wigner signed-particle methods are attractive options for solving transient quantum electron transport problems via kinetic Monte Carlo approaches. The ability to treat electrons as waves of numerical particles allows for naturally investigating prototypical quantum phenomena, such as interference effects. This is essential for many fields of quantum electronics, ranging from electron quantum optics to nanoelectronic devices and systems. Although multi-dimensional simulations have been made possible via parallelized signed-particle methods, the key challenge is still the exponential increase in particles, in particular for long evolution times, inclusion of general electromagnetic fields, and for three-dimensional spatial domains. This talk will summarize the involved computational challenges and highlight some solution approaches as well as simulation opportunities.