The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

Recent Progress in Thermal Transport Theory and Experiments | (SMR 3711)

30 May 2022 - 03 Jun 2022
ICTP, Trieste, Italy

P01 - BEARDO Albert

Hydrodynamic heat transport signatures in Silicon and Germanium

P02 - DRIGO Enrico

Thermal transport coefficient computation via energy density auto-correlation function

P03 - IZZO Maria Grazia

Thermal transport coefficient computation via energy-density correlation functions

P04 - MCBENNETT Brendan

Directional thermal transport channeling near nanoscale heaters: in-plane scattering enhances cross-plane conduction

P05 - NGUYEN Thi Kim Thanh

Open Kondo circuit as a detector for electron-electron interactions in a Luttinger Liquid

P06 - QIN Guangzhao

Performance Regulation of Heat Transfer in Semiconductors

P07 - ZERAATI Majid

Strongly anharmonic phonons in pyrope

P01

Hydrodynamic heat transport signatures in Silicon and Germanium

Recent experiments revealed non-Fourier thermal conduction in semiconductors like Silicon [1-3] or Germanium [4]. This can be interpreted in a unifying way using hydrodynamic-like heat transport modeling [5-7]. In this poster, we discuss two relevant experiments. First, we consider the process of energy release from nanoscale heat sources towards a Silicon substrate [2,3]. We demonstrate that the heater temperature transient evolution follows a double exponential decay as predicted by the hydrodynamic model. This system response cannot be explained if using Fourier's law with effective parameters to model the substrate conduction, which predicts a single exponential thermal decay followed by a power law. Furthermore, we derive analytical expressions for the decay times and provide a simple analogy based in an electrical circuit to illustrate the heater thermal evolution. Second, we study thermal memory effects in rapidly varying temperature fields [4]. We demonstrate the emergence of second sound in bulk natural Ge between 7 K and room temperature by studying the phase lag of the thermal response under a harmonic high-frequency external thermal excitation and addressing the relaxation time and the propagation velocity of the heat waves. References: [1] A. Ziabari et.al., Nat. Comm. 9, 255 (2018). [2] A. Beardo, J. Knobloch, et al. ACS Nano 15, 8, 13019–13030 (2021) [3] S. Alajlouni, A. Beardo et al. Nano Research 14 945–952 (2020) [4] A. Beardo et. al., Science Advances 7, eabg4677 (2021) [5] L. Sendra et al. Phys Rev. B 103, L140301 (2021) [6] A. Beardo et al. Phys Rev. B 105, 165303 (2022) [7] A. Beardo et al. Phys Rev. B 101, 075303 (2020)

P02

Thermal transport coefficient computation via energy density auto-correlation function

A rigorous algebraic identity [B.J. Berne, J. P. Boop, S. A. Rice, J. Chem. Phys. 45, 1086; H. Mori, Progr. Theoret. Phys. 34, 423] states that $K = \lim_{\omega\to 0}\lim_{k\to 0}\phi^{GK}(\boldsymbol{k},\omega) = \lim_{k\to 0}\lim_{\omega\to 0}\frac{\chi(\boldsymbol{k})}{k^2 S(\boldsymbol{k},\omega)}$, where K is the transport coefficient, $\phi^{GK}(\boldsymbol{k},\omega)$ is the related Green-Kubo formula, $S(\boldsymbol{k},\omega)$ is the dynamic structure factor at frequency ω and wavevector $\boldsymbol{k}$ obtained from the density auto-correlation function of the pertinent conserved quantity, uncoupled to the other constants of motion, with diffusive dynamics, $\chi(\boldsymbol{k})$ is the associated wavevector-dependent static susceptibility. Since the identity is mathematically exact in the macroscopic limit, any property holded by the Green-Kubo relation, relevantly including the so-called *gauge invariance* [A. Marcolongo, P. Umari, S. Baroni, Nat. Phys. 12, 80], is retained by the expression via the density auto-correlation function. We combine this two major concepts in order to evaluate accurately the thermal transport coefficient from the energy density auto-correlation function. In order to achieve a statistically consistent estimation of the macroscopic limit, we made an extensive use of the cepstral analysis [L. Ercole, A. Marcolongo, S. Baroni, Sci. Rep. 7, 15835] and of an ad hoc developed Bayesian linear regression procedure. We apply the theory to the model case of a molecular fluid, H_2O, showing that the protocol is operationally efficient, requiring relatively short molecular dynamics trajectories and small simulations box. This condition is possibly still holding for different disordered systems, where the non-Fourier regime is reached only at very small wavevectors. A similar approach has been recently exploited in [B. Cheng, D. Frenkel, Phys. Rev. Lett. 125, 130602].

P03

Thermal transport coefficient computation via energy density auto-correlation function

A rigorous algebraic identity [B.J. Berne, J. P. Boop, S. A. Rice, J. Chem. Phys. 45, 1086 (1966); H. Mori, Progr. Theoret. Phys. 34, 423 (1965)] states that $K = \lim_{\omega\to 0}\lim_{k\to 0}\phi^{GK}(\boldsymbol{k},\omega) = \lim_{k\to 0}\lim_{\omega\to 0}\frac{\chi(\boldsymbol{k})}{k^2 S(\boldsymbol{k},\omega)}$, where K is the transport coefficient, $\phi^{GK}(\boldsymbol{k},\omega)$ is the related Green-Kubo formula, $S(\boldsymbol{k},\omega)$ is the dynamic structure factor at frequency ω and wavevector $\boldsymbol{k}$ obtained from the density auto-correlation function of the pertinent conserved quantity, uncoupled to the other constants of motion, with diffusive dynamics, $\chi(\boldsymbol{k})$ is the associated wavevector-dependent static susceptibility. Since the identity is mathematically exact in the macroscopic limit, any property holded by the Green-Kubo relation, relevantly including the so-called *gauge invariance* [A. Marcolongo, P. Umari, S. Baroni, Nat. Phys. 12, 80 (2016)], is retained by the expression via the density auto-correlation function. We combine this two major concepts in order to evaluate accurately the thermal transport coefficient from the energy density auto-correlation function. In order to achieve a statistically consistent estimation of the macroscopic limit, we made an extensive use of the cepstral analysis [L. Ercole, A. Marcolongo, S. Baroni, Sci. Rep. 7, 15835 (2017)] and of an ad hoc developed Bayesian linear regression procedure. We apply the theory to the model case of a molecular fluid, H_2O, showing that the protocol is operationally efficient, requiring relatively short molecular dynamics trajectories and small simulations box. This condition is possibly still holding for different disordered systems, where the non-Fourier regime is reached only at very small wavevectors. A similar approach has been recently exploited in [B. Cheng, D. Frenkel, Phys. Rev. Lett. 125, 130602 (2020)].

P04

Directional thermal transport channeling near nanoscale heaters: in-plane scattering enhances cross-plane conduction

Using nonequilibrium molecular dynamics simulations of periodic heated nanostructures on a silicon thin film, we uncover two novel phonon transport behaviors. First, we use spectral energy density calculations to show that the nanostructure geometry affects phonon lifetimes in the substrate. Reducing the nanostructure periodicity, we observe decreased in-plane phonon lifetimes, indicating a deviation from bulk phonon scattering behavior in the vicinity of the nanostructures. Second, reduced in-plane phonon lifetimes coincide with enhanced cross-plane thermal conduction, as phonons are channeled downwards by in-plane scattering events. This anisotropic “channeling” effect may explain recent experimental observations documenting a return towards Fourier-like transport efficiency in the vicinity of close-packed nanoheaters.

P05

Open Kondo circuit as a detector for electron-electron interactions in a Luttinger Liquid

We investigate the effects of the electron-electron interactions on quantum transport in a one-dimensional system. We demonstrate it by considering the model in which a quantum dot is sandwiched between two finite quantum wires or quantum point contacts. We show that the open quantum dot can be used as an electron-electron interaction detector: the temperature scaling of the electric conductance is affected by the interaction in the electron gas through the Luttinger parameter g. Two limits: L << a and L >> a are considered with L and a are the size of the Luttinger liquid wires and the quantum dot, correspondingly. We also discuss the influence of e-e interactions on the non Fermi liquid behavior of the conductance at the two channel Kondo fixed point. Besides, our results bring back the electron interaction independent dc conductance e2/h in the finite length quantum wires.

P06

Performance Regulation of Heat Transfer in Semiconductors

High-performance thermal management is of great significance to the operational stability of integrated chip and electronic devices, where the heat transfer performance of the core semiconductors plays a key role. In this poster, I would like to introduce our recent work on the performance regulation of heat transfer focusing on few typical semiconductors, such as gallium nitride, boron nitride, boron arsenide, silicene, etc. Based on a concise strategy of accelerating evaluation of converged lattice thermal conductivity, the regulation effects of lots of manners, such as temperature controlling, strain engineering, applying external field, alloying, etc, have been systematically investigated. The fundamental mechanism is revealed based on the deep analysis of the electronic structures. The performance regulation of heat transfer and the underlying mechanism would be helpful on future studies of thermal and electrical coupling in emerging energy materials.

P07

Strongly anharmonic phonons in pyrope

Crystalline materials in which there are low frequencies of rattling phonons make up an important class of materials with low thermal conductivity. In this study, we observed the strong temperature dependence of Mg rattling phonon modes in pyrope Mg3Al2(SiO4)3 by performing the lattice dynamics and effective harmonic method. This hardening of rattling optical phonons reduces the phonon interaction and increases the lifetime of phonons as heat carrying. Also, using the molecular dynamics method with machine learning interatomic potentials, the results obtained from the lattice dynamics method and the Boltzmann transport equation solution were verified.