Phonon Hydrodinamics in solids and superfluids
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Book of Abstract

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Sixty years of phonon hydrodynamics

04 July
10:00

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First, we will present an overview of the historical development of phonon hydrodynamics since in its formulation in 1963 by Sussman and Thellung [1] to some of its recent results. Second, we will briefly discuss eight open and active current lines of phonon hydrodynamics, namely microscopic derivations, experiments, thermodynamic derivations, boundary conditions, nonlinear effects, generalizations to complex systems, applications to phononic devices, and transitions to other transport regimes (normal conduction, ballistic transport, second sound ...). Third, we will present two particular recent proposals in nonlinear phonon hydrodynamics, regarding the possible appearance of a spatial distribution of heat vortices analogous to the von Karman street of hydrodynamic vortices [2], due to nonlinear convective terms, and a nonlinear formulation of phonon hydrodynamics analogous to the power-law model in rheology in usual fluids [3].

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Higher-grade elastic solids with heat conduction and viscosity

04 July
10:30

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A generalized Coleman-Noll procedure is applied to analyze thermoviscoelastic solids of grade N, namely, solids with constitutive equations depending on the Nth spatial gradient of the deformation. Some new forms of stress tensor and specific entropy are obtained. For onedimensional elastic solids in the presence of small deformations, it is proved that the relaxation of the heat flux does not ensure the hyperbolicity of the system of balance laws. For onedimensional viscoelastic solids of grade 3, the equilibrium problem is studied An explicit form of the displacement is calculated. Comparison is made with the equilibrium theory of Korteweg fluids.

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04 July
11:30

Large-scale behaviour of starting vortices in superfluid helium-4

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We study experimentally the starting vortices shed by relatively large objects, accelerating uniformly from rest in superfluid helium-4, at various values of temperature and acceleration. The flow-induced motions of relatively small solid particles, suspended in the liquid and illuminated by a laser sheet, are captured by a digital camera. The trajectories and relative strengths of the shed vortices are estimated from the particle positions and velocities. The experimental results are also compared with a self-similar scaling theory, derived for an inviscid fluid. We find that the starting vortex trajectories do not depend appreciably on the liquid temperature, while their strengths are influenced significantly by the imposed acceleration. Additionally, the visualized vortices move considerably faster than predicted by the theory and, apart from a relatively short initial period, they do not appear to follow the scaling laws obtained analytically. Overall, the outcome can be attributed to viscosity, i.e. the study supports, once more, the idea that large-scale turbulent flows of superfluid helium-4 can be similar to analogous flows of Newtonian fluids, especially when thermal effects can be neglected.

We thank P. Dabnichki for providing the plastic objects used in this study; we acknowledge financial support from the Ministry of Education, Youth and Sports of the Czech Republic under grant no. LL2326.

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04 July
12:00

Wigner equations for phonon transport and quantum heat flux

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The enhanced miniaturization of electron and mechanical devices makes the thermal effects increasingly relevant [1–3] requiring the use of physically accurate models. At kinetic level a good description is that based on the semiclassical Peierls-Boltzmann equation for each phonon branch. However, for typical lengths smaller than the phonon mean-free path also quantum effects must be considered (see [4]). TheWigner equation is a natural approach that better reveal the wave nature of phonons in such circumstances, gives the Peierls-Boltzmann equation as semiclassical limit and still keeps the structure of a kinetic formulation. In this work, the focus is on the acoustic and optical phonons dynamics with a general dispersion relation. Starting from the quantum Liouville equation for the density operator and applying the Weyl quantization, Wigner equations for the longitudinal and transversal optical and acoustic phonons are deduced. The equations are valid for any solid, including 2D crystals like graphene. With the use of Moyal's calculus [5] and its properties the pseudo-differential operators are expanded up to the second order in $\hbar$. The phonon-phonon collision operators are modelled in a BGK form and describe the relaxation of the Wigner functions to a local equilibrium function, depending on a local equilibrium temperature which is definite according to [1]. An energy transport model is obtained by using the moment method with closures based on a quantum version of the Maximum Entropy Principle [6–12]. An explicit form of the thermal conductivity with quantum correction is obtained under a suitable scaling.

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04 July
12:30

Dynamics of Quantum Vortices in Exciton-Polariton Superfluids

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Low energy excitations of quantum gases and fluids are of fundamental interest and have widespread applications, with significant results being obtained in superfluid helium and Bose-Einstein condensates of ultracold atoms. Light propagation in nonlinear media can be seen as a gas of interacting photons, exhibiting, under suitable conditions, intriguing many-body behaviors such as Bose-Einstein condensation and superfluidity. Based on this concept, several groups have focused on investigating quantum fluids of light over the last two decades, particularly in the paradigmatic example of exciton polaritons in semiconductor microcavities [1,2]. One of the main advantages of optical systems is the ability to directly measure both the phase and density of quantum fluids.

Here, we present our latest results on vortex hydrodynamics in exciton-polariton quantum fluids. We focus on the Bogoliubov dispersion of polariton superfluids, highlighting the consequences of the out-of-equilibrium nature of these many-body systems, where the steady state results from a balance between pumping and dissipation [3,4]. We also demonstrate precise control over vortex dynamics, particularly showcasing the onset of vortex clustering and the build-up of the inverse energy cascade in 2D exciton-polariton superfluids [5,6,7].

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Non-Fourier Heat Transport in Nanostructures

04 July
15:00

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One of the most intriguing results from the first computer simulations of dynamical systems was the discovery of non-Fourier heat transport in low-dimensional models, such as the Fermi-Pasta-Ulam-Tsingou model. While this phenomenon is now widely accepted, the occurrence of anomalous heat transport in real nanoscale systems is still a matter of both theoretical and experimental investigations [1]. In this talk, I will discuss recent progress on anomalous lattice thermal transport in nanostructures from atomistic simulations. Our approach combines molecular dynamics simulations and anharmonic lattice dynamics calculations, to obtain a comprehensive understanding of phonon transport in lowdimensional and confined systems including both classical and quantum mechanical statistics. This talk addresses the lengthdependent thermal conductivity of carbon nanotubes [2], and the effect of thickness and layer spacing on the cross-plane thermal conductivity of layered materials and heterostructures [3, 4].

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04 July
15:30

Constructed evolution: Extended Thermodynamics and Internal Variables for heat conduction

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In nonequilibrium thermodynamics there are several methods to construct constitutive evolution equations. For example, in Extended Thermodynamics, the dissipative fluxes are independent fields and their evolution equations are constructed constitutively using the Second Law of Thermodynamics. There are two test methods that can be used to check the viability of the theories: compatibility with the moment series expansion of the Boltzmann equation, and stability of the thermodynamic equilibrium. However, there are some generalisations of Fourier heat conduction that are theoretically plausible and compatible with the Second Law, but do not fit into extended thermodynamics. These are, for example, the Burgers type or Quintanilla equations. It is shown that these equations can be treated by introducing internal variables but not as dissipative fluxes and by generalising the entropy flow. The stability properties are convincing in the sense that the linear stability of homogeneous thermodynamic equilibrium is satisfied without any further conditions beyond thermodynamics.

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04 July
16:30

A kinetic approach to study the thermal effects in monolayer graphene simulated by a deterministic method

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Under the action of an electric field, charge carriers generate an electric current in a semiconductor material. In turn, the energy gained from the electrons is released to the lattice with a heating effect. For applications in the industry, it is crucial to accurately model both the electric current and the crystal heating. Graphene is one of the materials that has recently garnered significant attention for future applications in nanoelectronic devices due to its excellent mechanical properties and its outstanding ability to conduct heat and electricity [1]. In particular, graphene has a very high thermal conductivity due to its unique lattice structure, making it a promising candidate for thermal management applications in nanoelectronic circuits. An accurate way to model electrical and thermal properties is represented by the semiclassical Boltzmann equations for electrons and phonons [2-3]. If the lattice is at a thermal bath then several methods have been developed to solve numerically the transport equations for electrons. Coupling them with the phonon transport equations and numerically solving the system is a hard task. With some physical approximations, the simulation of electron-phonon coupling and heating dynamics in suspended monolayer graphene has been tackled by Direct Simulation Monte Carlo analysis (DSMC)[4-5]. In DSMC the phonon energy density production term is usually determined by counting the number of emission and absorption scatterings multiplied by the correct physical weight [6-7]. In this work, we propose a kinetic version of the energy density production term derived directly from the collisional operator. In this case, numerical solutions can be obtained with a deterministic approach. A comparison of the simulation results demonstrates the equivalence of the two approaches.

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04 July
17:00

Analysis of nonlinear genera-lizations of the Maxwell-Cattaneo equation in heat pulse propagation

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The nonlinear terms resulting from temperature dependence of thermal conductivity and relaxation time are not negligible when studying applications to nanosystems. Two nonlinear generalizations of the Maxwell-Cattaneo-Vernotte equation for thermal transport with relaxation effects are introduced. A comparison of the consequences of these different nonlinear Cattaneo type equations on thermal pulse propagation is obtained and discussed. The differences in the corresponding velocities and in the corresponding heights of the perturbation peaks turn out to be significant and could be experimentally detected.

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Analysis of the whirling heat current density in the Guyer-Krumhansl equation

04 July
17:30

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Among the numerous heat conduction models, the Guyer-Krumhansl equation [1] has a special role. Besides its various application possibilities in nanotechnology, cryotechnology, and even in case of modeling heterogeneous materials [2–4], it poses additional mathematical challenges compared to the Fourier or Cattaneo equations. Furthermore, the Guyer-Krumhansl equation is the first heat conduction model, which includes the curl of the heat flux density in the evolution equation [5]. Here, we place our focus on the consequences of the existence of such whirling heat current density by solving the two-dimensional Guyer-Krumhansl equation with a space and time-dependent heat pulse boundary conditions.

The discretization poses further challenges in regard to the boundary conditions for which we propose a particular extrapolation method. Furthermore, with the help of the Helmholtz decomposition, we show the analogy with the linearized acoustics of Newtonian fluids, which reveals how the heat flux density plays the role of the velocity field. Our solutions also reveal an unexpected temperature evolution caused by the whirling heat flux density, namely, the temperature can locally be decreased for a short time in a case when the curl of the heat flux density dominates the heat conduction process.

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05 July
09:00

Microstructure-induced finite speed heat propagation in polarizable ceramics

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Fourier's law that links heat flux $\mathbf{q}$ and temperature gradient through the conductivity k, here assumed to be constant, namely $\mathbf{q} = -k\nabla\theta$, reduces in rigid conductors the balance of energy to the classical parabolic equation $c_v\dot{\theta} = k\Delta\theta$, where c_v is the specific heat at constant volume. The scheme foresees heat propagation with infinite speed, which contradicts the everyday experience of heating bodies. Attempts to overcome this physical inconsistency rest on different but not necessarily mutually excluding viewpoints:

1. As a constitutive equation implied by the Clausius–Duhem inequality, Fourier's law is insufficient. Non–equilibrium states require a refined description.

2. The relation between heat flux and temperature is, instead, a balance law, not a constitutive structure, and should be derived as such.

3. The way we describe the conductor (even when it is considered to be rigid) is insufficient. In other words, the physical evidence that temperature variations propagate at finite speed is consequent to the presence of material microstructure in real bodies.

The present talk focuses on the third item. To account for "independent" microstructural events at a low spatial scale, which influence the global behavior, we consider phase fields ν describing the microstructural morphology. Pertinent bulk and contact actions are defined by the power that they perform in the time rate of ν and satisfy appropriate balance equations. When we presume a generic internal constraint linking ν to the temperature θ, neglect macroscopic strain and make a few special assumptions, although accepting Fourier's law, the local form of the energy balance reduces to

$$\zeta \cdot \nabla\dot{\theta} - k\Delta\theta + (c_v + \delta)\dot{\theta} + \xi \cdot \nabla\theta + (\hat{\gamma} - r) = 0, \tag{1}$$

where the coefficients are in general state functions [1]. We focus first on equation (1). Primary and tertiary pyroelectric effects in Strontium–titanate ceramics – the class $Ba_{1-x}Sr_xTiO_3$ – fall within the assumptions leading to equation (1). For them ν represents at x and t a temperature–induced polarization. First we show simulations in two-dimensional setting of temperature time variations and the pertinent time rate as governed by equation (1). Numerical results are a clear indication towards experiments. Thus, we consider deformations and introduce a theory of pyroelectricity in large strain regime. It is based on invariance requirements and accounts even for the possible presence of external electric fields determining potential switching phenomena in the case of points groups 1 and 10. The pertinent results refine and generalize the 2017 analysis [1] leading to equation (1).

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Hydrodynamic experimental observations in bulk semiconductors

05 July
09:30

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A large number of experimental observations incompatible with the classical Fourier description of thermal transport at the nanometer and in the picosecond scales has been reported in the last decade [1,2]. Despite the theoretical efforts done in the topic, a model able to describe the gathered data at all length and time scales is still not available.

Two different descriptions have been proposed. Phonon hydrodynamics has been used as a framework to model thermal transport in materials where momentum conservation in phonon-phonon collisions is important. For other situations, a kinetic description based on the propagation of independent phonons, in what is called quasiballistic description, has been developed. The fundamental difference between them is in the number of length or time scales required to describe the observations. While in the hydrodynamic approach, a single scale is enough, in the quasiballistic description, the full set of phonon scales is necessary. For graphene and other 2D materials, the hydrodynamic approach has been the traditional main stream, while the quasiballistic approach has been more used for classical bulk semiconductors.

In the last years, some experiments and theoretical descriptions seems to be challenging this traditional splitting. On the one side, some predictions of the hydrodynamic regime for 2D materials like the second sound velocity have put on doubt the standard approach. On the other side, collective phonon behavior like the use of a single time scale to describe thermal decay in a silicon substrate [3] or the observation of second sound in germanium [4] seem to indicate that the hydrodynamic description could be used in these semiconductors. This could be an indication that a more unified framework could be proposed.

The talk will cover some of the most recent evidences in the theoretical and experimental research on thermal transport and we will analyze them in the framework of the Kinetic/Collective model (KCM) [5], developed to give a more generalized framework to describe thermal experiments.

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05 July
10:00

Internal tensorial variables and heat transport equation with inertial, thermal viscosity and vorticity terms

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Taking into account some results obtained within the framework of non-equilibrium thermodynamics with internal variables (NET-IV) in a previous paper [1], where generalized Guyer-Krumhansl evolution equations for the heat flux were derived by the help of non-local vectorial internal variables, in this paper we obtain a heat conduction equation where beside the conductive behaviours of phonons also viscous motions and vortical motions of phonons [2],[3],[4] are described. For the description of thermal vortices of phonons by the GENERIC approach we refer the reader to the Reference [5], where the appearance of a set of vortices analogous to the von Karman vortices in viscous fluids around a cylinder is explored on theoretical grounds. This possibility -as well as some other analogous possibilities- emphasizes the interest of exploring the interactions between the average heat flow and the heat vortices.

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Phonon-boundary scatterings and boundary conditions: Application to the heat transfer in thin nano-wires

05 July
10:30

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At nano-scale several conceptual questions still remain unanswered; some of them are sometimes fervently debated. It is however currently well-known that in nano-systems the phonons always undergo to different scattering mechanisms during the heat propagation. The particular regime of heat transfer, instead, strictly depends on the ratio between the phonon mean-free path and the characteristic size of the system, i.e., the so-called Knudsen number. Among the aforementioned open questions, the role played by the phonon-boundary scatterings, for different values of the Knudsen number, in particular is an interesting research playground. In this talk, therefore, it will be proposed an enhanced model of boundary conditions in order to suitably address the problem of the correct tackling of the phonon-boundary scatterings when heat is flowing in a thin nano-wire.

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05 July
11:30

How embedding nanoparticles affects semiconductor thermal conductivity

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We study how the thermal conductivity of semiconductors is affected by embedding in them nanoparticles, which act as extrinsic phonon scattering centers. The study is based on a new formula for thermal conductivity, which has recently been found on the basis of Extended Thermodynamics. All the other main interactions of phonons among themselves, with isotopes and boundaries are taken into account. Numerical results are shown for the case of germanium nanoparticles embedded in a Si0.7Ge0.3 alloy crystal.

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05 July
12:00

Wave propagation at nano-scale in coupled transport phenomena: Application to thermoelectricity

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The analysis of coupled transport phenomena is one of the most outstanding aspects of non-equilibrium thermodynamics. In this paper the attention is put on thermoelectricity, i.e., the coupling of heat and electricity. We propose a theoretical model which goes beyond the usual relations employed at macro-scale to describe thermoelectric effects. It introduces the non-local effects which should be taken into account in view of the possible applications of thermoelectric effects at nanoscale. The proposed model is here employed to investigate how nonlocal effects may influence the propagation of waves.

Phonon hydrodynamics of short channels in superfluids and solids

05 July
12:30

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In this talk we present some results on the effective thermal conductivity of thin and short channels filled with superfluid helium between two helium reservoirs at slightly different temperatures in the context of phonon hydrodynamics [1]. Further we propose an expression for the heat transfer in solids in narrow and short channels, based on the analogy with heat transport in suerfluid helium. The channels communicate two thermal reservoirs of the same material than the channel, so that there are no interfaces at the longitudinal boundaries of the channel, but only an abrupt change in the width of the system.

References

[1] L. Saluto, D. Jou *Entrance, slip, and turbulent effects in heat transport in superfluid helium across a thin layer*, ZAMP, 71(2), (2020) DOI:10.1007/s00033-020-1277-x

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