MM 7: Transport I: Electronic and thermal transport

Time: Monday 11:30–12:45 Location: H53

MM 7.1 Mon 11:30 H53

Non-linear conductance in mesoscopic weakly disordered wires - Interaction and magnetic field asymmetry — Christophe Texier[1,2] and •Johannes Mitscherling[1,3] — [1]LPTMS, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France — [2]Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France — [3]Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

Whereas it is well known that the linear conductance of a two-terminal device is symmetric with respect to magnetic field reversal, the electronic interaction causes an asymmetry of the non-linear conductance $\mathcal{G} \sim \partial^2 I/\partial V^2|_{V=0}$, which can thus be used as a probe of interaction as it was proposed in quantum dots in the ergodic regime [1,2].
We study the non-linear transport in weakly disordered metallic wires in the diffusive regime [3]. The analysis is based on the scattering approach including the effect of electronic interaction (screening) proposed by Büttiker. The dependence of the non-linear conductance in the phase coherence length is determined. The role of thermal fluctuations is also considered.

[1] D. Sánchez and M. Büttiker, Phys. Rev. Lett. 93, 106802 (2004)
[2] B. Spivak and A. Zyuzin, Phys. Rev. Lett. 93, 226801 (2004)
[3] C. Texier and J. Mitscherling, arXiv:1510.02214 (2015)

MM 7.2 Mon 11:45 H53

Evidence for hydrodynamic electron flow in PdCoO2 — Philip Moll[1,2], Pallavi Kushwaha[3], •Nabhanila Nandi[3], Burkhard Schmidt[3], and Andrew Mackenzie[3,4] — [1]Laboratory for Solid State Physics, ETH Zurich, Switzerland — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [4]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

The electrical resistance is conventionally determined by the momentum-relaxing scattering of electrons by the host solid and its excitations. Hydrodynamic fluid flow through channels, in contrast, is determined by geometrical factors, boundary scattering and the viscosity of the fluid, which is governed by momentum-conserving internal collisions. A longstanding question in the physics of solids has been whether the viscosity of the electron fluid plays an observable role in determiningthe resistance. At first sight this seems unlikely, because in almost all known materials the rate of momentum-relaxing collisions dominates that of the momentum-conserving ones that give the viscous term. Here, we show this is not always the case. We report experimental evidence that the resistance of restricted channels of the ultra-pure two-dimensional metal PdCoO2 has a large viscous contribution. Comparison with theory allows an estimate of the electronic viscosity to be similar to water at room temperature or liquid nitrogen at 75 K.

MM 7.3 Mon 12:00 H53

Hyperfine Interactions in Pd foils during D/H electrochemical loading — •Eric Bernardo da Silva[1], Juliana Schell[2,3], João G. M. Correia[2,4], Graham K. Hubler[5], Vittorio Violante[6], Moustapha Thioye[7], Jinghao He[5], and Michel Zoghby[8] — [1]Instituto de Pesquisas Energéticas e Nucleares, São Paulo University, Brazil — [2]ISOLDE-CERN — [3]Universität des Saarlades, Germany — [4]C2TN, Centro de Ciências e Tecnologias Nucleares, Instituto Superior Técnico, University of Lisbon, Portugal — [5]Sidney Kimmel Institute for Nuclear Renaissance, Dept. of Physics and Astronomy, University of Missouri, USA — [6]ENEA, Italian Agency for Energy New Technologies and Sustainable Development, Rome, Italy — [7]State University of New York, Stony Brook, USA — [8]Consultant, Thoiry, France

Since 1989, the Fleischmann and Pons Effect (FPE), the appearance of anomalous excess heat (AHE) during electrolytic loading of hydrogen in metal, has been observed, well above measurement uncertainty, in numerous calorimetric experiments. In the present work, Perturbed Angular Correlations (PAC) was used to probe Pd samples, implanted at 80keV with low concentration of radioactive 181Hf (181Ta). During loading of D2O or H2O, three different EFG distributions were observed; static, dynamic, and a specific. These EFG distributions, which are only felt by about 10, 15 percent of the Hf/Ta probe atoms and only appear during D loading above 81 percent ([D]/[Pd]), could be explained by a temporary atomic rearrangement of D atoms in some zones of the Pd lattice.

MM 7.4 Mon 12:15 H53

Thermal Conductivities in Solids from First Principles: Accurate Computations and Rapid Estimates — •Christian Carbogno and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

In spite of significant research efforts, a first-principles determination of the thermal conductivity κ at high temperatures has remained elusive. Boltzmann transport techniques that account for anharmonicity perturbatively become inaccurate under such conditions. *Ab initio* molecular dynamics (MD) techniques using the *Green-Kubo* (GK) formalism capture the full anharmonicity, but can become prohibitively costly to converge in time and size. We developed a formalism that accelerates such GK simulations by several orders of magnitude and that thus enables its application within the limited time and length scales accessible in *ab initio* MD. For this purpose, we determine the *effective* harmonic potential occurring during the MD, the associated temperature-dependent phonon properties and lifetimes. Interpolation in reciprocal and frequency space then allows to extrapolate to the macroscopic scale. For both force-field and *ab initio* MD, we validate this approach by computing κ for Si and ZrO_2, two materials known for their particularly harmonic and anharmonic character. Eventually, we demonstrate how these techniques facilitate reasonable estimates of κ from existing MD calculations at virtually no additional computational cost.

MM 7.5 Mon 12:30 H53

Strain engineering of thermal transport in 2D grain boundaries — •Leonardo Medrano Sandonas[1,2], Rafael Gutierrez[1], Alessandro Pecchia[3], Gotthard Seifert[4], and Gianaurelio Cuniberti[1,5,6] — [1]Institute for Materials Science, TU Dresden, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Consiglio Nazionale delle Ricerche, ISMN, Rome, Italy — [4]Physical Chemistry Deparment, TU Dresden, Dresden, Germany — [5]Center for Advancing Electronics Dresden, TU Dresden, Dresden, Germany — [6]Dresden Center for Computational Materials Science, TU Dresden, Dresden, Germany

Grain boundaries (GBs) in two-dimensional materials have attracted great attention in recent years due to its unique physical properties. However, many questions are still unanswered about the influence of external factors on their thermal properties. Thus, we want to provide some insights in understanding the influence of strain on the thermal transport in 2D materials with grain boundaries. To do this, we employ Green's functions technique combined with DFTB theory. Our main focuses are grain boundaries in novel two-dimensional materials like hBN, Phosphorene, and MoS2, which are potential candidates for developing novel approaches to nanoscale electronics and phononics. Among the GBs studied in the present work (5|7 and 4|8), 4|8 GB has the stronger influence on the thermal transport. Moreover, we have found an anomalous behavior of the thermal conductance after increasing the uniaxial strain. This trend is associated to the strain dependence of the bond length and the force constants of the material.