TT 24: Poster Session: Transport

Time: Thursday 13:30–16:00 Location: P

TT 24.1 Thu 13:30 P

Efficient steady-state solver for the hierarchical equations of motion approach: formulation and application to charge transport through nanosystems — •Christoph Kaspar and Michael Thoss — University of Freiburg

We present an iterative algorithm [1] to efficiently solve the hierarchical equations of motion (HEOM) [2,3] for the steady-state of open quantum systems. The approach reduces the computational resources required by traditional steady-state solvers, in particular for larger systems or the low temperature regime. It uses the method of matrix equations in combination with a efficient preconditioning technique and a hierarchy truncation scheme. We illustrate the numerical performance of the method by applications to models of charge transport in single-molecule junctions.

[1] Kaspar *et al.*, J. Phys. Chem. A **125**, 23, 5190-5200 (2021)
[2] Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008)
[3] Tanimura, J. Chem. Phys. **153**, 020901 (2020)

TT 24.2 Thu 13:30 P

Spin-orbit interaction induces charge beatings in a lightwave-STM – single molecule junction — •Moritz Frankerl and Andrea Donarini — Institute for Theoretical Physics, University of Regensburg, 93049 Regensburg, Germany

Experiments based on lightwave-STM have shown how to obtain both space and time resolution of single molecule vibrations on their intrinsic length and time scales [1]. We investigate theoretically the electronic dynamics of a copper-phthalocynanine in a lightwave-STM by simulating the full pump-probe cycle [2]. Beatings in the transferred charge reveal the intertwined spin and orbital dynamics, modulated by a tip induced exchange field [3]. We study the dynamics directly in the time domain within a generalized master equation approach. A deeper understanding of our numerical results is obtained via coupled Bloch like equations for the molecular spin and pseudospin [4].

[1] T. L. Cocker et al., Nature 539, 263-267 (2016)
[2] M. Frankerl et al, Phys. Rev. B 103, 085420 (2021)
[3] M. Braun et al., Phys. Rev. B 70, 195345 (2004)
[4] M. Maurer et al., Phys. Rev. Research 2, 033440 (2020)

TT 24.3 Thu 13:30 P

Pseudospin resonances reveal synthetic spin-orbit interaction — •Christoph Rohrmeier and Andrea Donarini — Institute of Theoretical Physics University of Regensburg, Regensburg, Germany

The interplay between interference and interaction produces several effects in degenerate quantum systems, including spin torques [1], dark states formation [2] and multilevel coherences [3]. In this context, a spin resonance without spin splitting has been first predicted for a single quantum dot spin valve [4]. We investigate a spinful double quantum dot coupled to leads in a pseudospin valve configuration. We predict in the stability diagram a rich variety of current resonances which are modulated by the system parameters [5]. In the presence of ferromagnetic leads and pseudospin anisotropy, those resonances split, turn into dips, and acquire a Fano shape, thus revealing a synthetic spin-orbit interaction induced on the double quantum dot. A set of rate equations derived for a minimal model captures those features. The model accurately matches the numerical results obtained for the full system in the framework of a generalized master equation and calculated within the next to leading order approximation.

[1] M. Braun et al., Phys. Rev. B 70, 195345 (2004)
[2] A. Donarini et al., Nature Comm. 10, 381 (2019)
[3] M. Maurer et al., Phys. Rev. Research 2, 033440 (2020)
[4] M. Hell et al., Phys. Rev. B 91, 195404 (2015)
[5] C. Rohrmeier et al., Phys. Rev. B 103, 205420 (2021)

TT 24.4 Thu 13:30 P

Feynman-Vernon influence functional approach to quantum transport in interacting nanojunctions: An analytical hierarchical study — •Luca Magazzu and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We present a nonperturbative and formally exact approach for the charge transport in interacting nanojunctions based on the Feynman-Vernon influence functional. By borrowing the nomenclature of the famous spin-boson model, we parametrize the two-state dynamics of each single-particle fermionic degree of freedom, in the occupation number representation, in terms of blips and sojourns. We apply our formalism to the exactly solvable resonant level model (RLM) and to the single-impurity Anderson model (SIAM), the latter being a prototype system for studying strong correlations. For both systems, we demonstrate a hierarchical diagrammatic structure. While the hierarchy closes at the second-tier for the RLM, this is not the case for the interacting SIAM. Upon inspection of the current kernel, known results from various perturbative and nonperturbative approximation schemes to quantum transport in the SIAM are recovered. Finally, a novel noncrossing approximation for the hierarchical kernel is developed, which enables us to systematically decrease temperature at each next level of the approximation.

[1] arXiv:2104.14497 (2021)

TT 24.5 Thu 13:30 P

An Atomistic Study of the Thermoelectric Signatures of CNT Peapods — •Alvaro Gaspar Rodriguez Mendez[1,2], Leonardo Medrano Sandonas[3], Arezoo Dianat[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Tu Dresden, 01062 Dresden, Germany. — [2]Max Planck Institute for Complex Systems, 01187 Dresden, Germany. — [3]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg.

Carbon-based nanomaterials have a great potential for the development of high performance thermoelectric (TE) materials because of their low-cost and for being environmentally friendly. Carbon nanotubes have, however, high electrical and thermal conductivities so that further nanoscale engineering is required to exploit them as TE materials. We investigate electron and phonon transport in CNT peapods to elucidate their potential advantage over pristine CNTs. We show their transport properties are sensitively modified by C60 encapsulation, when the CNT-C60 intermolecular interaction is strong enough to produce a periodic buckling of the CNT walls. Moreover, the phonon transmission is strongly suppressed at low and high frequencies, leading to a reduction of the phonon contribution to the overall thermal conductance, similar effect observed in recently proposed phononic metamaterials. We obtain in general a larger TE figure of merit over a broad temperature range for the CNT peapod when compared with the pristine CNT. Our findings show an alternative route for the enhancement of the TE performance of CNT-based devices.

TT 24.6 Thu 13:30 P

Evolution of Molecular Binding in Mechanically Controlled Break-Junctions — •Lokamani Lokamani[1,3], Florian Günther[2], Filip Kilibarda[3], Jeffrey Kelling[1], Guido Juckeland[1], Artur Erbe[3], and Sibylle Gemming[4] — [1]Department of Information Services and Computing, HZDR, Dresden, Germany — [2]Instituto de Física de São Carlos, Universidade de São Paulo, Brazil — [3]Department of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [4]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

Electrical properties of single molecules can be investigated with extreme precision using atomically sharp metallic electrodes in mechanically controllable break junctions (MCBJs). The current-voltage (IV) characteristics in such junctions are considerably affected by the binding positions of the anchoring groups on the tip-facets and the configuration of the molecule. Hence, characterizing the electronic transport properties during a single tip-tip opening provides interesting insights into the tip-molecule interaction.

Here, we present a novel high-throughput approach to reproduce the time evolution of the electronic transport characteristics. We performed transport calculations using the self-consistent charge scheme of the density-functional-based tight binding approach and the Green's function formalism. In particular, we evaluated the energy level and the coupling of the dominating transport channel using the single level model. In contrast to standard approaches, we consider many thermodynamically relevant configurations.

TT 24.7 Thu 13:30 P

Revealing channel polarization of atomic contacts of ferromagnets and strong paramagnets by shot-noise measure-

ments — Martin Prestel, •Marcel Strohmeier, Wolfgang Belzig, and Elke Scheer — University of Konstanz, 78457 Konstanz, Germany

We report measurements of the shot noise of atomic contacts using the mechanically controllable break junction (MCBJ) technique at low temperatures. In accordance with theoretical predictions [1, 2] single-atom contacts of the ferromagnets Co and Gd with conductance smaller than the conductance quantum show reduced noise compared to the expectation for the spin-degenerate single-channel transport. Additionally we focus on the strong paramagnets Pt [3], Pd [4], and Ir [5], where a nonmonotonic magnetotransport has been reported for atomic contacts, interpreted as emerging magnetic ordering in small dimension, which is expected due to the Stoner instability [6, 7]. Our recent measurements on Pd, Pt, and Ir reveal noise levels which are above, but close to the threshold to the spin-degenerate single-channel situation. An anticorrelation between the minimum noise and the bulk Stoner parameter of these elements is observed. We discuss by how far this might indicate that spin polarization is reflected in the noise signal.

[1] Olivera et al., PRB 95, 075409 (2017)
[2] Häfner et al., PRB 77, 104409 (2008)
[3] Strigl et al., Nature Comm. 6, 6172 (2015)
[4] Strigl et al., PRB 94, 144431 (2016)
[5] Prestel et al., PRB 100, 214439 (2019)
[6] Delin et al., PRL 92, 057201 (2004)
[7] Delin et al., PRB 68, 144434 (2003)

TT 24.8 Thu 13:30 P

Theory of coherent phonon mode excitation in metal nanoparticles — •Robert Salzwedel[1], Dominik Hoeing[2], Yannic Staechelin[2], Florian Schulz[2], Holger Lange[2], Andreas Knorr[1], and Malte Selig[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für Physikalische Chemie, Universität Hamburg, 20146 Hamburg, Germany

Metal nanoparticles perform radial breathing mode oscillation upon excitation by a light pulse. Typically, these oscillations are assumed to be driven by the thermalization of hot electrons that impulsively heat the lattice [1,2].

Here we present a hydrodynamic theory based on the Heisenberg equation of motion formalism for the optical excitation of the electron gas in metal nanoparticles and the related electron-phonon interaction.

Our analysis reveals that spatial gradients of the electron density which are induced by the optical pump already drive coherent phonon oscillations whereas thermalization is found to be of reduced importance.

[1] Hodak, J. H. et al. (1999), *JOCP*, **111**(18)
[2] Ng, M. Y. et al. (2011), *JOCP*, **134**(9), 094116

TT 24.9 Thu 13:30 P

Direct current from AC driving of Dirac Fermions — •Adrian Seith, Jakob Schlosser, Jan Wilhelm, and Ferdinand Evers — Institut für Theoretische Physik, Universy of Regensburg, Germany

Recent developments in systems driven by an ultra-short laser pulse demonstrate the high-order harmonic generation in topological systems with a Dirac-type (surface) bandstructure [1]. We investigate the current-density that results from the laser pulse close to the surface. Simulations based on the Semiconductor Bloch equations as implemented in the CUED code [2] indicate the emergence of a DC-like current with a lifetime by far exceeding the pulse duration. An analytical solution within a model system of Dirac Fermions is possible explaining the effect rigorously together with the observed dependence on the carrier envelope phase (CEP). Consequences for experiments with realistic band structures are discussed, as well as applications to light-wave-electronics.

[1] Schmid et. al., Nature 593, 385 (2021)
[2] Wilhelm et. al., Phys. Rev. B 103, 125419 (2021)

TT 24.10 Thu 13:30 P

Laser-waveform control of high-harmonic emission - a theoretical analysis — •Jan Wilhelm, Maximilian Graml, Maximilian Nitsch, Patrick Grössing, and Ferdinand Evers — Institute of Theoretical Physics, University of Regensburg

When irradiating solids with a short, i.e. subcycle, laser pulse, the corresponding electric field initiates ultrafast electron dynamics in the material. Fingerprints of it are encoded in the emission spectrum that features high-harmonic generation. High-harmonic emission from a topological insulator has been observed recently in experiment [1] opening a platform to explore topology and quasi-relativistic quantum physics using strong laser fields. Strikingly, the high-harmonic orders can be shifted to non-integer multiples of the driving frequency by varying the carrier-envelope phase (CEP) of the driving field. We theoretically analyze the mechanisms leading to CEP shifts using semiconductor Bloch equations [2-4] finding that an interplay of chirp and CEP of the laser pulse lead to arbitrary CEP shifts.

[1] C. P. Schmid, et al., Nature 593, 385-390 (2021)
[2] W. Schäfer, M. Wegener, Semiconductor Optics and Transport Phenomena, Springer, Berlin (2002)
[3] M. Kira, S. W. Koch, Semiconductor Quantum Optics, Cambridge University Press (2011)
[4] J. Wilhelm, P. Grössing, A. Seith, J. Crewse, M. Nitsch, L. Weigl, C. Schmid, F. Evers, Phys. Rev. B 103, 125419 (2021)

TT 24.11 Thu 13:30 P

High-harmonic geneneration in topological insulator surface states — •Vanessa Junk[1], Cosimo Gorini[1,2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Germany — [2]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

High-order harmonics are typically generated when matter is interacting with strong-field light. In most materials efficient scattering and dephasing destroy coherences in the emitted spectra. In topological insulator (TI) surface states however, scattering is strongly suppressed. This opens up the possibility to observe signatures of coherent transport.

We present how Berry curvature effects imprint into the dynamics of strong-field light driven electrons in TI surface states. In the semiclassical framework, a non-zero Berry curvature leads to the emergence of a velocity component perpendicular to the external driving. Here, we compare the semiclassical predictions with a full quantum mechanical simulation. The high harmonics spectra we calculate from the dynamics show an alternating polarization as has recently also been observed in experiment [1].

[1] C. Schmid, L. Weigl, P. Grössing, V. Junk, C. Gorini, S. Schlauderer, S. Ito, M. Meierhofer, N. Hofmann, D. Afanasiev, J. Crewse, K. Kokh, O. Tereshchenko, J. Güdde, F. Evers, J. Wilhelm, K. Richter, U. Höfer and R. Huber, Nature **593**, 385-390 (2021)