MP 9: Quantenmechanik I

Time: Wednesday 11:45–12:45

Location: HFT-FT 101

MP 9.1 Wed 11:45 HFT-FT 101 Transfer matrices and excitations with matrix product states — •VALENTIN ZAUNER¹, DAMIAN DRAXLER¹, LAURENS VANDERSTRAETEN², MATTHIAS DEGROOTE², JUTHO HAEGEMAN², MAREK M RAMS³, VID STOJEVIC⁴, NORBERT SCHUCH⁵, and FRANK VERSTRAETE¹ — ¹University of Vienna, Vienna, Austria — ²University of Ghent, Ghent, Belgium — ³Krakow University of Technology, Krakow, Poland — ⁴University College London, London, UK — ⁵RWTH Aachen, Aachen, Germany

We investigate the relation between static correlations in the ground state of local many-body Hamiltonians and the low energy dispersion relations using the formalism of tensor network states. We show that the Matrix Product State Transfer Matrix (MPS-TM) - a central object in the computation of static correlation functions - provides important information about the location and magnitude of the minima of the low energy dispersion and present numerical data for onedimensional lattice and continuum models as well as two-dimensional lattice models. We elaborate on the peculiar structure of the MPS-TM's eigenspectrum and give several arguments for the close relation between the structure of the low energy spectrum of the system and the form of static correlation functions. Finally, we discuss how the MPS-TM connects to the exact Quantum Transfer Matrix. We also present a renormalization group argument which allows to reinterpret variational MPS techniques (such as the Density Matrix Renormalization Group) as an application of Wilson's Numerical Renormalization Group along the virtual (imaginary time) dimension of the system.

MP 9.2 Wed 12:05 HFT-FT 101

Quantum interference in dangling bond loops — •ANDRII KLESHCHONOK, RAFAEL GUTIÉRREZ, and GIANAURELIO CUNIBERTI — Institute for Materials Science, Dresden University of Technology, Hallwachstr. 3, 01069 Dresden, Germany

Dangling bonds can be produced with atomic precision by selectively removing hydrogen atoms from a Si passivated surface with a scanning tunneling microscope (STM). Dangling bond wires (DBW) and dangling bond loops open fascinating possibilities for becoming the building bocks of novel planar, atomic-scale electronic circuits and logic elements. We perform a realistic study of transport properties of the DBW connected to the carbon nanoribbon leads and quantum interference effects in DBW loops by combining density-functional based approaches with equilibrium and non-equilibrium Green function methods. We develop methodology to study different topologies (half row, full row, zigzag), length of the loops, lead coupling strength and position.

MP 9.3 Wed 12:25 HFT-FT 101 Pseudospin-driven spin relaxation mechanism in graphene. — •DINH VAN TUAN — ICN2 - Institut Catala de Nanociencia i Nanotecnologia, Campus UAB, 08193 Bellaterra (Barcelona), Spain

The extremely small intrinsic spin-orbit coupling (SOC) of graphene and the lack of hyperfine interaction with the most abundant carbon isotope have led to intense research into possible applications of this material in spintronic devices due to the possibility of transporting spin information over very long distances. However, the spin relaxation times are found to be orders of magnitude shorter than initially predicted, while the major physical process for spin equilibration and its dependence on charge density and disorder remain elusive. Experiments have been analyzed in terms of the conventional Elliot-Yafet and Dyakonov-Perel processes, yielding contradictory results. Here, we unravel a spin relaxation mechanism for nonmagnetic samples that follows from an entanglement of spin and pseudospin degrees of freedom driven by random SOC, which makes it unique to graphene and is markedly different to conventional processes. We show that the mixing between spin and pseudospin-related Berry's phases results in unexpectedly fast spin dephasing, even when approaching the ballistic limit, and leads to increasing spin relaxation times away from the Dirac point, as observed experimentally. This hitherto unknown phenomenon points towards revisiting the origin of the low spin relaxation times found in graphene. It also opens new perspectives for spin manipulation using the pseudospin degree of freedom, a tantalizing quest for the emergence of radically new information storage and processing technologies.