**Numerical simulation of quantum transport of the electrons and holes in graphene devices**

Omar MORANDI
Department of Physics, University of Graz, Austria

Graphene is an allotropic form of carbon where atoms are densely packed in a mono-layer in form of honeycomb-lattice. As a result of the conically shaped electronic band, the dynamics of electrons and holes in graphene is governed by the Dirac equation and they propagate as massless Fermions. In this contribution, quantum corrections to the electron-hole motion in graphene are investigated by applying the quantum phase-space approach. The Wigner-Weyl formalism is used to reduces the overall complexity of the system and a quasi-diagonalization procedure on the pseudo-spin degree of freedom is proposed. The resulting formulation of the equation of motion reveals to be particularly close to the classical description of the particle motion. The stationary state of graphene-based devices in the presence of strong electric fields and quantum barriers is numerically investigated. The connection of our formalism with the Barry-phases approach is also presented.

**Open Boundary Conditions for Ballistic Transport Equations**

Walter PÖTZ
Department of Physics, University of Graz, Austria

We discuss a physically motivated approach to realize open boundary conditions based on scattering theory. It assumes flat potential regions outside of the simulated region and is based on slow variation of S-matrix elements. It is equally suited to treat pure state (wave packet) and mixed state (density matrix) dynamics. In fact is has first been applied to the quasi-one-dimensional nonlinear Schrödinger equation and mixed states[1]. Here we discuss application to multi-component wave equations, specifically the Bogoliubov-deGennes and 1+1 Dirac equation, each of which represent two-component wave equations. The case of time-independent external potentials offers a special case which, within this method, allows for a very simple and stable solution. We discuss pitfalls arising from discretization schemes which lead to non-trivial modifications of the energy spectrum, such as fermion doubling for the Dirac equation or the non-Hermiticity (complex eigenvalues), and eigenfunctions.

[1] M. A. Talebian and W. Pötz, Superlattices and Microstructures, Volume 20, Number 3, October 1996 , pp. 267-272(6); M. A. Talebian und W. Pötz, ,,Open boundary conditions for a time-dependent analysis of the resonant tunnelling structure“,Appl. Phys. Lett., Bd. 69, Nr. 8, S. 1148-1150, 1996.

Work supported by FWF Project Nr. I395-N16

**Deterministic Numerical Solution of the Boltzmann Transport Equation**

Karl RUPP
Institute for Microelectronics, University of Technology, Vienna, Austria

Monte-Carlo methods are typically employed to solve the Boltzmann Transport Equation for semiconductors numerically. However, they suffer from high computational costs and resolve low-probability regions of the carrier distribution function inaccurately. These limitations can be overcome with deterministic methods at the cost of high memory consumptions. A memory reduction scheme for the most prominent deterministic solution approach, the Spherical Harmonics Expansion method, is presented. It allows to save up to two orders of magnitude in

memory by storing the resulting system matrix in a factorized form. Implications on the choice of the iterative solver and efficient implementations are discussed.

### Measure solutions of a 2D Keller-Segel system as limit of a stochastic many particle model

Christian SCHMEISER
Faculty of Mathematics, University of Vienna, Austria

The two-dimensional parabolic-elliptic Keller-Segel system is a model for the aggregation of particles under the influence of diffusion and of an attractive binary interaction. Depending on the value of a dimensionless parameter proportional to the total mass, either diffusion wins and the particles are dispersed, or attraction wins and concentration of particles occurs in finite time. In the latter case, solutions of the Keller-Segel system can be extended as time dependent measures globally in time.
A stochastic many particle model will be presented, which can be used as the basis of numerical simulations of measure solutions. It can also be shown that in the limit of infinitely many particles, the (Boltzmann) hierarchy for the sequence of marginals possesses a solution preserving molecular chaos, where the one-particle marginal is a measure solution of the Keller-Segel system.

This is joint work with Jan Haskovec.

### Computation of spin transport and magnetization dynamics in ferromagnetic/normal metal heterostructures using a drift-diffusion model

Markus WENIN
Department of Physics, University of Graz, Austria

We present a self-consistent simulation of the magnetization dynamics and the spin dynamics in ferromagnetic/normal metal/ferromagnetic (FNF) heterostructures. We use the stationary solution of a drift-diffusion equation (SDDE) to compute the spin dynamics and the Landau-Lifshitz-Gilbert equation to compute the magnetization dynamics. Both equations couple via the spin-transfer torque and the magnetic field in the SDDE.

### Fluid Dynamic Limit to the Riemann Solutions of Euler Equations

Tong YANG
Department of Mathematics, City University of Hong Kong, P.R.China

Fluid dynamic limit to the compressible Euler equations from the compressible Navier-Stokes and Boltzmann equation has been an active topic. Even though intensive studies have been made when the solution to the Euler equations has noninteracting single waves, the problem on the genuine Riemann problem is still open. In this talk, we present some recent results on this problem when the Riemann solution contains a superposition of either shock-rarefaction wave or rarefaction wave contact discontinuity. In addition, uniform convergence rates in terms of the physical parameters will also be given.

This is joint work with Feimin Huang and Yi Wang.