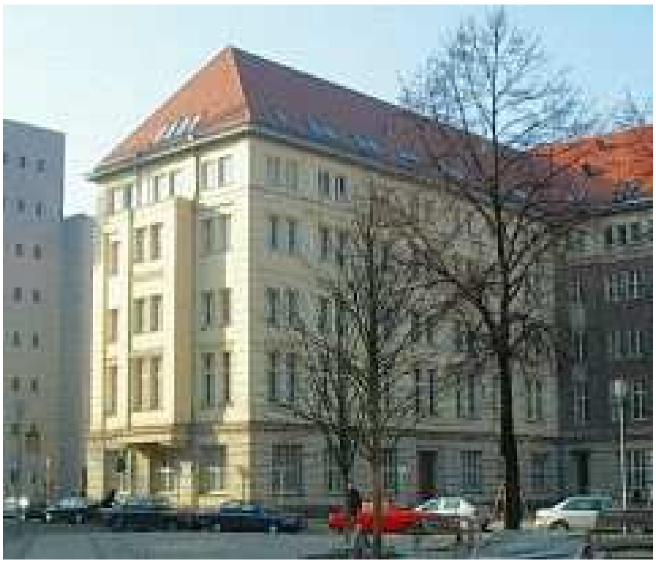
4th Workshop on

Mathematical Models for Transport in Macroscopic and Mesoscopic Systems

Program
Abstracts
Participants



February 8 – 9, 2008

Weierstrass Institute for Applied Analysis and Stochastics

Berlin, Germany

4th Workshop on

Mathematical Models for Transport in Macroscopic and Mesoscopic Systems

The Workshop is supported by

- German Research Foundation (DFG)
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  "Analysis, Modelling and Simulation of Multiscale Problems"

Organizers

Horia Cornean
Hagen Neidhardt
Paul Racec
Joachim Rehberg

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Friday, 08.02.2008, 08:00 - 22:00

08:00 - 08:50	Registration
08:50 - 09:00	Opening
	Chairman: Gheorghe Nenciu
9:00	Scattering and resonances in leaky quantum-wire systems **Pavel Exner**
9:30	Quantum transport in resonant tunneling diodes: comparison between asymptotic models and full simulation of Schrödinger–Poisson systems **Francis Nier**
10:00 - 10:30	Coffee break
	Chairman: Thierry Goudon
10:30	Numerical WKB-scheme for the stationary Schrödinger equation **Anton Arnold**
11:00	A hierarchy of diffusive higher-order moment models for semiconductors **Ansgar Jüngel**
11:30	Quantum-classical coupling in Multi Quantum Well lasers **Uwe Bandelow**
12:00 - 13:30	Lunch
	Chairman: Anton Arnold
13:30	Time-dependent transport in quantum dot systems: from transient regime to steady-state **Valeriu Moldoveanu**
14:00	Magnetotransport through systems embedded in a quantum wire **Vidar Gudmundsson**
14:30	Quantum scaling behavior of nanotransistors **Ulrich Wulf**
15:00 - 15:30	Coffee break
	Chairman: Pavel Exner
15:30	Time-dependent coupling and non-equilibrium steady state limit **Valentin Zagrebnov**
16:00	Time averaging for the strongly confined nonlinear Schrödinger equation, using almost periodicity **François Castella**
16:30	Localization on quantum graphs with random couplings **Konstantin Pankrashkin**
17:00	Generalised discrete Laplacians and quantum graphs **Olaf Post**
18:30 - 22:00	Conference dinner

Saturday, 09.02.2008, 09:00 - 17:15

	Chairman: Francis Nier
09:00	Optimally localized Wannier functions for quasi one-dimensional nonperiodic systems **Gheorghe Nenciu**
09:30	Reduction of dimension for the Schrödinger–Poisson system **Florian Méhats**
10:00 - 10:30	Coffee break
	Chairman: Ansgar Jüngel
10:30	On the current in continuous systems with an adiabatically switched-on electrical bias **Pierre Duclos**
11:00	Asymptotics problems for Laser-matter modeling; quantum and classical models **Thierry Goudon**
11:30	Discrete transparent boundary conditions for the Schrödinger equation on circular domains **Matthias Ehrhardt**
12:00 - 14:00	Lunch
	Chairman: Pierre Duclos
14:00	Fano resonances in transport through open two-dimensional quantum systems **Roxana Racec**
14:30	On the numerics of the 3D Kohn-Sham system **Kurt Hoke**
15:00 - 15:30	Coffee break
	Chairman: Valentin Zagrebnov
15:30	Nanotubes in magnetic fields **Evgeny Korotyaev**
16:00	A thermodynamic approach to transient Kohn-Sham theory **Hans-Christoph Kaiser**
16:30 - 16:45	Closing

Numerical WKB-scheme for the stationary Schrödinger equation

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We present a new second order finite difference scheme for the Schrödinger equation (scalar and vectorial) in the highly oscillatory regime. Transforming out the dominant oscillations, it is not necessary to resolve each oscillation. Moreover, in the classical limit the scheme reproduces the correct weak limit using just a constant number of grid points.

Quantum-classical coupling in Multi Quantum Well lasers

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The presence of quantum wells in laser diodes introduces a new length scale, being in the order of the Fermi-wavelength of the carriers. This induces a mixed spectral density, where the carriers localizing within the quantum wells belong to the discrete spectrum and the free-roaming carriers belong to the continuous spectrum. Consequently, this divides the carriers into species which exhibit different properties. In particular, the latter species is viewed as a "classical" species, carrying classical transport on a large scale (some μm). By quantum well design the properties of the localized "quantum" species can be tuned and optimized for applications. Due to their localized nature the above "quantum" species cannot carry a current within a single-particle approach and therefore acts as a null-space for the transport. In consequence, their occupation remains fixed forever - which is contradicting to physics.

Interaction as phonon-carrier and carrier-carrier scattering will change this simplified picture and causes kinetical processes for all the species. Among others, carriers can then migrate from one species to another. Above a certain time-scale such processes can be modeled in some approximation in terms of a dynamics which effectively counts the amount of carriers being captured by the quantum wells as well as the amount of carriers escaping from the quantum wells.

Time averaging for the strongly confined nonlinear Schrödinger equation, using almost periodicity

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We study the limiting behavior of a nonlinear Schrödinger equation describing a three dimensional gas that is strongly confined along the vertical, z direction. The confinement induces fast oscillations in time, that need to be averaged out. Since the Hamiltonian in the z direction is merely assumed confining, without any further specification, the associated spectrum is discrete but arbitrary, and the fast oscillations induced by the nonlinear equation entail countably many frequencies that are arbitrarily distributed as well. For that reason, averaging can not rely on small denominator estimates or like. To overcome these difficulties, we prove that the fast oscillations are almost periodic in time, with values in a Sobolev-like space that we completely identify. We then exploit the existence of long time averages for almost periodic function to perform the necessary averaging procedure in our nonlinear problem.

This is a joint work with N. Ben Abdallah (Toulouse) and F. Mehats (Rennes).

On the current in continuous systems with an adiabatically switched-on electrical bias

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Consider a system which looks like a cross connected pipe system, i.e. a small sample coupled to a finite number of leads. We investigate the current running through this system, in the linear response regime, when we adiabatically turn on an electrical bias between leads. The main technical tool is the use of a finite volume regularization, which allows us to define the current coming out of a lead as the time derivative of its charge. We finally prove the conductivity tensor is given by a Landauer-Büttiker type formula. This is a work obtained in collaboration with H. Cornean, G. Nenciu and R. Purice, arXiv:0708.0303.

Discrete transparent boundary conditions for the Schrödinger equation on circular domains

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We propose transparent boundary conditions for the time-dependent Schrödinger equation on a circular computational domain. First we derive the two-dimensional discrete TBCs in conjunction with a conservative Crank-Nicolson-type finite difference scheme. The presented discrete boundary-valued problem is unconditionally stable and completely reflection-free at the boundary. Then, since the discrete TBCs for the Schrödinger equation with a spatially dependent potential include a convolution w.r.t. time with a weakly decaying kernel, we construct approximate discrete TBCs with a kernel having the form of a finite sum of exponentials, which can be efficiently evaluated by recursion. Finally, we describe several numerical examples illustrating the accuracy, stability and efficiency of the proposed method.

We also comment briefly on the situation in different geometries, like straight line, wave guide and general convex geometry.

Scattering and resonances in leaky quantum-wire systems

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We discuss a model of quantum-wire systems which takes tunneling into account, being formally described by Hamiltonians of the type $-\Delta - \alpha\delta(x - \Gamma)$ in $L^2(\mathbb{R}^2)$ where $\Gamma \subset \mathbb{R}^2$ is a metric graph with asymptotically straight "leads". Such systems can exhibit interesting spectral and scattering properties provided we exclude the trivial case when $\Gamma = \Gamma_0$ is just a straight line. We will analyze negative-energy scattering in the situation when Γ is a local deformation of Γ_0. We will also recall an approximation result for these operators which gives numerical hints for existence of resonances due to the global geometry, and mention some open problems.

Asymptotics problems for Laser-matter modeling; quantum and classical models

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This joint work with F. Castella and P. Degond is devoted to the asymptotic analysis of both quantum and classical models which are intended to describe the evolution of electrons subject to the potential of an atomic crystal perturbed by the highly oscillating potential of external electro-magnetic waves. The problem combines homogenization aspects of transport like equation with relaxation phenomena. We derive either Einstein rate equations or diffusion equations with respect to the energy variable, depending on whether the initial model is quantum or classical. We point out the analogies and differences in the treatment of the two models, considering successively the cases of (quasi-)periodic perturbations or random ones. We point out the different role of the relaxation effects according to the nature of the perturbation.

Magnetotransport through systems embedded in a quantum wire

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We show how transport in a 2D-quantum wire in a perpendicular magnetic field can be described using the Lippmann-Schwinger scattering formalism. The concept of coupled channel transport will be introduced, and the interplay between geometry and the magnetic field will be investigated for embedded subsystems as quantum dots, antidots, and rings. We introduce the extension of this formalism to the time-domain.

On the numerics of the 3D Kohn-Sham system

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The Schrödinger-Poisson system with exchange-correlation potential (Kohn-Sham system) in three dimensions is solved using the fixed point iteration scheme proposed by Kerkhoven. This scheme goes in line with the analytical description used by H.-Chr. Kaiser and J. Rehberg as a fixed point mapping. It separates in two parts, which intend to stabilize and accelerate the pure fixed point iteration. First, underrelaxation with some carefully adapted relaxation-factor is used for stabilization. Secondly, acceleration is reached by switching to Newton's method and applying a derivative-free version of the GMRES method.

A hierarchy of diffusive higher-order moment models for semiconductors

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A hierarchy of diffusive partial differential equations is derived by a moment method and a Chapman-Enskog expansion from the semiconductor Boltzmann equation assuming dominant collisions. The moment equations are closed by employing the entropy maximization principle of Levermore. The new hierarchy contains the well-known drift-diffusion model, the energy-transport equations, and the six-moments model of Grasser et al. It is shown that the diffusive models are of parabolic type. Two different formulations of the models are derived: a drift-diffusion formulation, allowing for a numerical decoupling, and a symmetric formulation in generalized dual-entropy variables, inspired by nonequilibrium thermodynamics. An entropy inequality (or H-theorem) follows from the latter formulation.

A thermodynamic approach to transient Kohn-Sham theory

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The drift-diffusion Kohn-Sham theory provides a thermodynamically motivated model for charge transport in heterogeneous semiconductor materials with non-local operators for the charge carrier densities. The mobilities are chosen in accordance with the theory of large deviations in stochastic processes. The theory is in the general framework of Transient Density Functional Theory.

Nanotubes in magnetic fields

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We consider the Schrödinger operator with a periodic potential on a quasi 1D continuous periodic model of zigzag (or armchair) nanotubes in R^3 in a uniform magnetic field (with amplitude $B \in R$), which is parallel to the axis of the nanotube. The spectrum of this operator consists of an absolutely continuous part (spectral bands separated by gaps) plus an infinite number of eigenvalues with infinite multiplicity. We describe all compactly supported eigenfunctions with the same eigenvalue. We define a Lyapunov function, which is analytic on some Riemann surface. On each sheet, the Lyapunov function has the same properties as in the scalar case, but it has branch points, which we call resonances. We prove that all resonances are real for zigzag nanotubes but they can be complex for armchair nanotubes. We determine the asymptotics of the periodic and anti-periodic spectrum and of the resonances at high energy. We show that endpoints of the gaps are periodic or anti-periodic eigenvalues or resonances (real branch points of the Lyapunov function). We describe the spectrum as a function of B. For example, 1) if $B \to B_{k,s} = 163(\pi 2 - \pi k N + \pi s) \tan \pi 2N, k = 1, 2, .., N, s \in Z$, then some spectral band shrinks into a flat band, i.e., an eigenvalue of infinite multiplicity, 2) we determine the asymptotics of spectral gaps and effective masses as $B \to 0$, 3) we obtain identities and a priori estimates in terms of effective masses and gap lengths.

Time-dependent transport in quantum dot systems: from transient regime to steady-state

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Consider a few-level noninteracting quantum dot described by a lattice Hamiltonian. At $t = 0$ the system is coupled suddenly to biased leads. We compute the transient currents within the non-equilibrium Green-Keldysh formalism and discuss the charge dynamics inside many-level quantum dots. The Dyson equation for the two-times Green function is transformed into an algebraic equation which can be numerically implemented and solved by standard algorithms. We also investigate the passage to steady-state transport and identify traces of the many-level structure in this intermediate regime. When periodic signals are applied to the contacts the system operates as a turnstile pump. In this case we present a unified description of adiabatic and nonadiabatic pumping.

Reduction of dimension for the Schrödinger–Poisson system

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I will present some joint works with N. Ben Abdallah, F. Castella, F. Fendt and O. Pinaud. We analyze the time-dependent 3D Schrödinger-Poisson system with a singular perturbation modeling the effect of a strong confining potential. I will discuss on two cases : confinement on a plane (for bidimensional electron gases) or on a line (for nanowires), which are qualitatively very different.

Optimally localized Wannier functions for quasi one-dimensional nonperiodic systems

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It is proved that for general, not necessarily periodic one-dimensional systems, the band position operator corresponding to an isolated part of the energy spectrum has discrete spectrum and its eigenfunctions have the same spatial localization as the corresponding spectral projection. As a consequence, an eigenbasis of the band position operator provides a basis of optimally localized Wannier functions.

Quantum transport in resonant tunneling diodes: comparison between asymptotic models and full simulation of Schrödinger–Poisson systems

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After a review of the application of the asymptotic model developed by V. Bonnaillie, F. Nier and Y. Patel for the non linear steady state of far from equilibrium resonant tunneling diodes, a numerical comparison with simulations of the complete Schrödinger-Poisson system will be presented.

Localization on quantum graphs with random couplings

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We study a class of periodic quantum graphs with randomly distributed Kirchhoff coupling constants at all vertices. Using the technique of self-adjoint extensions we obtain conditions for spectral and dynamical localization in terms of finite volume criteria (Aizenman–Molchanov method) for some energy-dependent discrete Hamiltonians.

Generalised discrete Laplacians and quantum graphs

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In this talk, we define a generalisation of the discrete Laplace operator on a combinatorial graph. These generalised Laplacians appear in a natural way from the spectral analysis of quantum graph Laplacians with general vertex boundary conditions. In the case of the standard ("Kirchhoff") boundary conditions, the discrete operator is the usual combinatorial Laplacian. We also comment on trace formulas.

Fano resonances in transport through open two-dimensional quantum systems

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We develop a theory for the measured Fano resonances in the conductance of a quantum dot strongly coupled to the leads. A nonseparable potential is considered which assures for the channel mixing. Our central result is that there is a single, well-defined resonant transmission channel even in presence of channel coupling. This resonant channel is associated with a single pole of the S-matrix. In addition, there is a background part of the S-matrix arising from poles other than the resonant one. It can be shown that this constant part of the S-matrix can be split in one part which interferes coherently with the resonant channel (coherent background) and a noncoherent part (noncoherent background). The interplay between the coherent background and the resonant channel determines the single asymmetry parameter seen in the experiment. The noncoherent background part of the S-matrix results in a noncoherent constant contribution to the conductance which is also seen in the experiment.

This is a joint work with U. Wulf and P. N. Racec.

Quantum scaling behavior of nanotransistors

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In our previous papers on ballistic field effect transistors [J. Appl. Phys. 96, 596 (2004), and ibid. 98, 84308 (2005)] it was demonstrated that under certain conditions ('SMAT' approximation) it is possible to reduce the fully three-dimensional transport problem to an effectively one-dimensional one. It was found that already a simple, piecewise linear ansatz for the effective potential leads to a qualitative description of the output characteristics of ultra-small transistors with channel lengths of several tens of nanometers. Here we want to demonstrate that for an effectively one-dimensional potential a scale invariant description of the transistor-transport-problem is possible. For the particular piecewise linear ansatz it is found that apart from a properly normalized temperature the output characteristics depend only on a single unitless barrier parameter $\beta^{th} = 2m\mu d^2\hbar^{-2}$ which depends on the effective mass m of the electrons, the channel length d, and the chemical potential μ in the source contact. At channel lengths between ten to thirty nanometers and ultra-high n-doping in the source contact β^{th} takes values between a few hundreds ('weak barrier') up to a few thousands ('strong barrier'). At weak barriers relatively high source-drain leakage currents may result so that instead of a clear 'OFF'-state regime a 'quasi-OFF-state' tunneling transistor regime arises. The features of the output- and of the transfer characteristics in this regime are structurally very similar to the 'short-channel effects' resulting in a drift-diffusion model for the transistor. At large β^{th} these undesirable quasi-short-channel effects are significantly reduced.

Time-dependent coupling and non-equilibrium steady state limit

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We consider an example of two semi-infinite one-dimensional leads coupled to a quantum well by two time-dependent point "switchers". The initial condition in the remote past corresponds to the three decoupled systems each at its own thermal equilibrium, whereas in the remote future the "switchers" make the systems fully coupled. We define and study the non-equilibrium steady state generated by this dynamics.

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