Mathematical Challenges of Quantum Transport in Nano-Optoelectronic Systems

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Weierstrass Institute for Applied Analysis and Stochastics, Berlin

Organizers

Horia Cornean
Hagen Neidhardt
Paul Racec

February 4 – 5, 2010
Weierstrass Institute for Applied Analysis and Stochastics
Berlin, Germany

Scope

The goal of the workshop is to give the opportunity to interchange ideas about modeling of charge transport and their interaction with external fields in nano-optoelectronic devices. This workshop is a part of a series initiated among others by Pierre Duclos in Bucharest in 2005.

The models developed are important for describing the influence of light on the electrical current, for example in solar cells and photodetectors, but also the influence of electrical current on the light emission, for example in light emitting diodes. The research area is of interest for theoretical understanding, experimental study as well as for efficient and optimal applicability of these systems.

We bring together experimental physicists, who can give an overview of the actual studied phenomena in quantum dots and nanowires, engineers working on the practical problems about the production and optimization of devices, for example of thin film solar cells, and mathematicians and theoretical physicists, developing suitable models and their analysis for efficient numerical implementation.

The workshop gives also an oportunity for young researchers to enter this very interesting and rapidly developing research area.

Topics

- quantum dots and nanowires as optoelectronic devices: theory and experiments
- light coupling to charge carriers in open quantum systems
- modeling of semiconductor and optoelectronic quantum devices
- quantum effects in thin film solar cells
- Landauer–Büttiker formula
- non-equilibrium steady states for optoelectronic devices
- numerical challenges

Invited Speakers

- Anton Arnold (Vienna, Austria)
- Raffaella Calarco (Berlin, Germany)
- Tony C. Dorlas (Dublin, Irland)
- Pavel Exner (Prague, Czech Republic)
- Klaus-Jürgen Friedland (Berlin, Germany)
- Vidar Gudmundsson (Reykjavik, Iceland)
- Ansgar Jüngel (Vienna, Austria)
- Andrei Manolescu (Reykjavik, Iceland)
- Francis Nier (Rennes, France)
- Igor Popov (St. Petersburg, Russia)
- Roxana Racec (Cottbus, Germany)
- Radu Purice (Bucharest, Romania)
- Ulrich Wulf (Cottbus, Germany)

Friday, 04.02.2011, 08:00 - 21:00

08:00 - 09:00	REGISTRATION
09:00 - 09:15	OPENING
09:15 - 10:25	Chairman: Arnold, Anton
09:15	Spectra of periodic quantum graphs and the effect of local perturbations **Pavel Exner**
09:50	Eigenfunctions decay for magnetic pseudodifferential operators **Radu Purice**
10:25 - 11:00	COFFEE BREAK
11:00 - 12:45	Chairman: Gudmundsson, Vidar
11:00	Asymptotically correct finite difference schemes for highly oscillatory ODEs **Anton Arnold**
11:35	Size dependences in III-nitride nanowires **Raffaella Calarco**
12:10	Thermal properties of quantum transistors **Ulrich Wulf**
12:45 - 14:30	PHOTO + LUNCH
14:30 - 15:40	Chairman: Calarco, Raffaella
14:30	Semi-classical modeling of quantum dot lasers with microscopic treatment of Coulomb scattering **Thomas Koprucki**
15:05	Theory of Coulomb scattering in semiconductor quantum dot lasers **Alexander Wilms**
15:40 - 16:10	COFFEE BREAK
16:10 - 17:55	Chairman: Jüngel, Ansgar
16:10	Model of zero-range potentials with internal structure for Maxwell operator **Igor Yu. Popov**
16:45	R-matrix and finite volume method for cylindrical nanowire heterostructures **Paul Racec**
17:20	Heat transport in hybrid nanosystems using the atomic Green's functions **Mathias Käso**
17:55 - 19:00	DISCUSSIONS
19:00 - 21:00	DINNER

Program

Saturday, 05.02.2011, 09:00 - 17:30

09:00 - 10:10	Chairman: Popov, Igor Yu.
09:00	An explicit model for the adiabatic evolution of quantum observables driven by 1D shape resonances **Francis Nier**
09:35	Diffusion in quantum fluid models for semiconductors **Ansgar Jüngel**
10:10 - 10:40	COFFEE BREAK
10:40 - 12:25	Chairman: Purice, Radu
10:40	High-mobility electron transport on cylindrical surfaces **Klaus-Jürgen Friedland**
11:15	Time-dependent transport through a nanostructure coupled to an electromagnetic field in a cavity **Vidar Gudmundsson**
11:50	Coulomb and spin-orbit interactions in nanorings **Andrei Manolescu**
12:25 - 14:30	LUNCH
14:30 - 16:15	Chairman: Exner, Pavel
14:30	Fano effect in open quantum systems **Roxana Racec**
15:05	On the Keldysh formalism applied to mesoscopic quantum systems **Horia Cornean**
15:40	An abstract approach to the Landauer-Büttiker formula with application to an LED toy model **Lukas Wilhelm**
16:15 - 16:30	CLOSING

Asymptotically correct finite difference schemes for highly oscillatory ODEs

Arnold, Anton
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We are concerned with the numerical integration of ODEs of the form $\epsilon 2\psi_{xx} + a(x)\psi = 0$ for given $a(x) \geq \alpha > 0$ in the highly oscillatory regime $0 < \epsilon \ll 1$ (appearing as a stationary Schrödinger equation, e.g.). In two steps we derive an accurate finite difference scheme that does not need to resolve each oscillation:

1 With a WKB-ansatz the dominant oscillations are "transformed out", yielding a much smoother ODE.
2 For the resulting oscillatory integrals we devise an asymptotic expansion both in ϵ and h.

In contrast to existing strategies, the presented method has (even for a large spatial step size h) the same weak limit (in the classical limit $\epsilon \to 0$) as the continuous solution. Moreover, it has an error bound of the order $O(\epsilon 3h2)$. We shall give applications to $\boldsymbol{k} \cdot \boldsymbol{p}$-Schrödinger systems and to the simulation of semiconductor-nanostructures.

Ref: A. ARNOLD, N. BEN ABDALLAH and C. NEGULESCU: WKB-based schemes for the Schrödinger equation in the semi-classical limit, preprint 2010.

Abstracts

Size dependences in III-nitride nanowires

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In recent years III-nitride based nanowires (NWs) have attracted a lot of interest because of their potential applications for nanoelectronic devices. The growth of Nitride nanowires by MBE occurs on various substrates under N-rich conditions without using a liquid-phase catalyst. We addressed the optimization [1, 2] of the crystalline and optical quality of GaN and InN. The growth of GaN NWs on bare Si(111) is characterized by a long nucleation period [3-5], which results in a broad distribution of the nanowire sizes. The investigation of the electrical properties of GaN NWs showed that the band-to-band photoelectric effect varies by orders of magnitude as a function of the nanowire diameter [6]. Photovoltage Spectroscopy and Spectral Photoconductivity (SPC) measurements have been carried out to analyze the near band-edge absorption in GaN nanowires [7]. A strong diameter dependence of the band absorption tail was found by SPC measurements. The band-edge tailoring and its wire-diameter dependence can be explained by the Franz-Keldysh effect induced by the electric field at the wire surface. In InN NWs a highly conductive surface accumulation was observed [8]. We performed also Raman characterization on nanowire ensemble in comparison with single nanowire measurements [9, 10]. The ensemble spectra of GaN NWs did not reveal a deviation from the selection rules for the wurtzite structure, in contrast in the single wire spectra, only A1(TO) was observed, which intensity is almost suppressed if the laser polarization was perpendicular to the nanowire axis. These results indicate that the penetration of the laser light and the Raman scattering in isolated GaN nanowires thinner than 100 nm is governed by size effects.

This is a joint work with T. Stoica, E. Sutter, P. Sutter, E.O. Schäfer-Nolte, T. Schäpers, Michel Marso, Hans Lüth, A. Cavallini, L. Polenta, T. Schumann, T. Gotschke, F. Limbach, D. Grützmacher.

[1] R. Meijers et al. J. Cryst. Growth 289, 381 (2006).
[2] T. Stoica et al. Nano Letters, 6(7), 1541-1547 (2006)
[3] R. Calarco et al. Nano Letters, 7 (8), 2248 -2251, (2007).
[4] R. K. Debnath et al. Appl. Phys. Lett., 90, 123117 (2007).
[5] T. Stoica et al. Small 4, 751 (2008).
 [6] R. Calarco et al. Nano Letters 5, 981 (2005).
[7] A. Cavallini et al. Nano Letters, 7, 2166 (2007).
[8] T. Richter et al. Nano Lett. 8, 2834 (2008).
[9] E.O. Schäfer-Nolte et al. Appl. Phys. Lett. 96, 091907 (2010).
[10] T. Stoica et al. Nanotechnology 21, 315702 (2010).

On the Keldysh formalism applied to mesoscopic quantum systems

Cornean, Horia
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This talk is intended as a “vulgarisation” of the Keldysh formalism towards mathematicians. We show in particular that the Keldysh contour-ordering is not necessary when calculating transient or steady-state currents through noninteracting mesoscopic systems. The Langreth rules can also be derived using elementary operations, only.

Abstracts

Spectra of periodic quantum graphs and the effect of local perturbations

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I am going to review several recent results about spectra of quantum graphs. Speaking first about periodic graphs, I will show how their spectral bands and gaps can behave asymptotically at high energies in case of a general self-adjoint vertex coupling. Furthermore, it will be demonstrated that even for $\mathbb{Z}$-periodic graphs spectral edges may not correspond to the periodic or antiperiodic situation unless the graph is a chain, the components of which are connected by single edges. Using the examples of chain and comb graphs I will also show how local perturbations give rise to eigenvalues and resonances in such systems.

High-mobility electron transport on cylindrical surfaces

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The self-rolling of thin, pseudomorphically strained semiconductor bilayer systems based on epitaxial heterojunctions grown by molecular-beam epitaxy allows to realize motion of electrons on curved surfaces. We realized a high-mobility, two-dimensional electron gas in which the low-temperature mean free path of the electrons is as large as the curvature radius of the tube, which allow us to study the interesting effects, in particular ballistic transport phenomena and the quantum Hall effect on a curved surface. The curvature of the surface results in a spatial change of the component of the magnetic field which is perpendicular to the surface, therefore, the filling factor changes gradually. For the quantum Hall effect we observe additional contributions in the longitudinal resistance. The phenomenon results from a specific current distribution in the quantized phase and can not be explained by the conventional Landauer–Büttiker approach which presupposes besides conductance along one-dimensional Landau channels a fully localized transport in the bulk. Moreover, we develop a model including the transport along incompressible stripes and the compressible (metallic) bulk. We also observe a new type of resistance oscillations in the ballistic transport of two-dimensional electrons on cylindrical surfaces with a tangentially directed magnetic field. The longitudinal resistance oscillates with a periodicity proportional to the square root of the magnetic field $\boldsymbol{B}$, which indicates on a commensurability between the channel width and a length scale related to the gradient of the perpendicular to the surface component of the magnetic field. We show, that the lengths of a stripe with free electrons, forming the so called 'snake'-like trajectories is basic for the $\sqrt{\boldsymbol{B}}$ oscillations. We speculate about a process, including spin procession of electrons in the one-dimensional 'skin'-channel forming around the $\boldsymbol{B} = 0$ position, which causes this new type of resistance oscillations.

Abstracts

Time-dependent transport through a nanostructure coupled to an electromagnetic field in a cavity

Gudmundsson, Vidar
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In the talk I shall describe preliminary results for a model calculation of transport of Coulomb interacting electrons through a nanostructure coupled to a photon field of a microwave cavity.

Diffusion in quantum fluid models for semiconductors

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Quantum fluid models have been recently derived by Degond, Mehats, and Ringhofer from the Wigner-BGK equation by a moment method with a quantum Maxwellian closure. In the $O(\epsilon^4)$ approximation, where ϵ is the scaled Planck constant, this leads to local quantum diffusion or quantum hydrodynamic equations. In this talk, we present recent results on the modeling, analysis, and numerical approximation of these models. First, we consider quantum diffusion models containing highly nonlinear fourth-order or sixth-order differential operators. The existence results are obtained from a priori estimates using entropy dissipation methods. Second, a quantum Navier-Stokes model, derived by Brull and Mehats, will be analyzed. This system contains nonlinear third-order derivatives and a density-depending viscosity. The key idea of the mathematical analysis is the reformulation of the system in terms of a new “osmotic velocity” variable, leading to a viscous quantum hydrodynamic model. Surprisingly, this variable has been also successfully employed by Bresch and Desjardins in (non-quantum) viscous Korteweg models.

Abstracts

Heat transport in hybrid nanosystems using the atomic Green's functions

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At the beginning of the talk we will be presenting the general formalism of the "Atomistic Green's Functions (AGF)". This formalism allows us to study phononic heat transport problems in nanoscale devices. Then we will use this method to describe one dimensional, open systems with the typical contact-device-contact structure. Especially for the homogeneous atomic chain we will derive an analytical expression of the thermal conductance. Subsequently we discuss this result for low and for high temperatures.

Semi-classical modeling of quantum dot lasers with microscopic treatment of Coulomb scattering

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Drift-diffusion models provide a semi-classical description of the carrier transport in semiconductor devices. Self-consistently coupled to equations for the optical field they are established models for the simulation of semiconductor lasers. We consider quantum dot lasers with optically active regions consisting of quantum dots grown on a wetting layer. We present a drift-diffusion based modeling approach for the simulation of quantum dot lasers which uses a multi-species description of the carriers along the quantum dot active region and includes microscopically determined scattering rates describing the capture of the carriers into the quantum dots by Coulomb scattering.

The presented results are joint work with U. Bandelow, K. Gärtner, A. Wilms, and A. Knorr (TU Berlin).

Abstracts

Coulomb and spin-orbit interactions in nanorings

Manolescu, Andrei
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Combined effects of the Coulomb electron-electron interaction and the spin orbit coupling in one- and two-dimensional nanorings will be shown. The Coulomb interaction is treated in a complete many-body manner with the so-called “exact diagonalization” method. The spin-orbit coupling is described by the Rashba and/or Dresselhaus models. The local spin and charge densities will be observed both in the ground state and in the excited states. The influence of an external magnetic field and/or of an external potential will also be discussed.

An explicit model for the adiabatic evolution of quantum observables driven by 1D shape resonances

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We will present explicit analytic calculations for a model of a resonant tunneling structure. Possibly, comparisons with numerical calculations will be discussed.

Abstracts

Model of zero-range potentials with internal structure for Maxwell operator

Popov, Igor Yu.
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Model of zero-range potential for the Maxwell operator in domains with small boundary openings is suggested. It is based on the theory of self-adjoint extensions of symmetric operators. Another version of the model is related with the description of opto-electronic systems. It is a generalization of zero-range potentials with internal structure for the Schrödinger operator. Operator extensions theory technique allows one to switch on point-like interaction between classical electro-magnetic field (Maxwell operator) and electron (Schrödinger operator).

Eigenfunctions decay for magnetic pseudodifferential operators

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We prove rapid decay (even exponential decay under some stronger assumptions) of the eigenfunctions associated to discrete eigenvalues, for a class of self-adjoint operators in $L^2(R^d)$ defined by magnetic pseudodifferential operators. This class contains the relativistic Schrödinger operator with magnetic field.

Abstracts

R-matrix and finite volume method for cylindrical nanowire heterostructures

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The R-matrix formalism allows us to reduce the scattering problem i) to a single eigenvalue problem for a closed domain with Dirichlet and Neumann boundary conditions and ii) the computation of the scattering matrix by matrix multiplication for every energy of interest. We take into account the position dependent effective mass for the heterostructure in the framework of the finite volume method. We will present the variational formulation for a cylindrical heterostructure with linear triangular elements.

This is a joint work with H.-Chr. Kaiser and K. Gärtner (WIAS Berlin).

Fano effect in open quantum systems

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We analyze a quantum dot strongly coupled to the conducting leads via quantum point contacts - Fano regime of transport - and report a variety of resonant states which demonstrate the dominance of the interacting resonances in the scattering process in a low confining potential. As effects of the interaction between resonances, the line shapes of the conductance peaks are described by Fano functions with complex asymmetry parameters and the phases of the transmission amplitudes do not increase monotonically by π through each conductance peak anymore. The phase lapses, typical for the universal behaviour, are obtained as a particular case for weak interacting resonances, while the strong interaction regime is associated with the mesoscopic phase evolution.

Abstracts

An abstract approach to the Landauer–Büttiker formula with application to an LED toy model

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We give a new derivation of the Landauer-Büttiker formula that is inspired by the work of Nenciu, but that does not make use of generalized eigenfunctions or the Lippmann-Schwinger equation. We stay in a purely operator theoretical framework, and our results are even valid for perturbations that are only locally trace class. We then present a toy model for a quantum dot LED to which this derivation can be applied to obtain a Landauer-Büttiker type formula for the electron current in the presence of electron-photon interaction.

Abstracts

Theory of Coulomb scattering in semiconductor quantum dot lasers

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One key requirement for the simulation of laser dynamics is a good description of the optical active region. In high density regime the dynamics of the light carrier interaction in quantum dot lasers are strongly influenced by Coulomb scattering processes. We give an introduction to the theory of Coulomb scattering in quantum dot lasers in the limit of Born-Markov approximation.

The presented results are joint work with A. Knorr, TU Berlin.

Abstracts

Thermal properties of quantum transistors

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We consider a thermal model for an integrated circuit with an active (i. e. heat producing) layer of quantum devices located above a heat sink. As the simplest scenario the heat transport problem between active layer and heat sink is taken as homogeneos in the layer directions and quasi-stationary in time. The temperature of the active device layer can be found from the solution of a fix-point problem when the temperature of the heat sink is given. We analyze the possible numbers of fix-points and their stability for a general device type. Numerical solutions for a device layer of quantum transistors are given for selected parameters.

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For Your Notes

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