Weierstraß–Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e. V.

5th Workshop

Multiscale Problems in Quantum Mechanics
and Averaging Techniques

Berlin, September 22–23, 2005

W I A S

Analysis, Modeling and Simulation of Multiscale Problems

Schwerpunktprogramm der Deutschen Forschungsgemeinschaft

DFG

Synopsis

The Weierstrass Institute for Applied Analysis and Stochastics (WIAS) hosts the 5th workshop on *Multiscale Problems in Quantum Mechanics and Averaging Techniques* in the framework of the DFG Priority Program 1095 *Analysis, Modeling and Simulation of Multiscale Problems.*

The focus of the workshop is on averaging methods for partial differential equations and multiscale problems arising from the quantum mechanical modeling and simulation of semiconductor nanostructures and their embedding into semiconductor devices.

Topics are: many-particle systems, quantum-classical coupling, time averages, quantum hydrodynamics, adiabatic and scaling limits, semiconductor nanostructures, electronic structure calculation, upscaling to semi-classical models.

Special Guests

Irene Gamba, Peter Markowich, Francis Nier, Riccardo Sacco

Organizers

Anton Arnold, Ansgar Jüngel, and Hans-Christoph Kaiser

World Wide Web

http://www.wias-berlin.de/workshops/mspqcm05

Program

Thursday September 22, 2005

Forenoon Session

9:00 Registration

9:30 Opening Address

9:45 Opening Lecture: P. Markowich

10:30 Coffee Break

11:00 Barbara Niethammer

11:30 Josipa-Pina Milisic

12:00 Lunch Break

Afternoon Session

2:00 Burkhard Schmidt

2:30 Caroline Lasser

3:00 Ulrich Mauthner

3:30 Coffee Break

4:00 Lecture: Francis Nier

4:45 Break

5:15 Matheon Lecture: I. Gamba

Evening Program

6:15 Open Discussion: Perspectives in Multiscale Quantum Mechanics

8:00 Dinner at the historical restaurant "Raabe–Diele"

Friday September 23, 2005

9:00 Heinz-Jürgen Flad

9:30 Hongjun Luo

9:45 Lecture: Riccardo Sacco

10:30 Coffee Break

11:00 Matthias Ehrhardt

11:30 Francesco Maggi

12:00 Sebastian Bauer

12:30 The End

Abstracts

Sebastian Bauer

Radiative friction in classical electrodynamics

We study the dynamics of many charged particles interacting with the Maxwell field. This coupled system is governed by the Vlasov-Maxwell equations. If the initial velocities of the particles are small compared to the speed of light then in lowest order, the Newtonian or classical limit, their motion is governed by the Vlasov-Poisson system. We study higher order corrections including dissipative corrections due to radiation damping.

Matthias Ehrhardt

Discrete Non-Local Boundary Conditions for Split-Step Padé Approximations of the One-Way Helmholtz Equation

This talk deals with the efficient numerical solution of the two-dimensional one-way Helmholtz equation posed on an unbounded domain. In this case one has to introduce artificial boundary conditions to confine the computational domain. The main topic of this work is the construction of so-called discrete transparent boundary conditions for state-of-the-art parabolic equations methods, namely a split-step discretization of the high-order parabolic approximation and the split–step Padé algorithm of Collins which allows for a parallel implementation. Finally, several numerical examples arising in optics and underwater acoustics illustrate the efficiency and accuracy of our approach.

Heinz-Jürgen Flad

Best N-term approximation in electronic structure calculations

We discuss best N-term approximation spaces for reduced density matrices and two-particle correlation functions. These functions can be considered as basic building blocks in electronic structure calculations. The approximation spaces for anisotropic wavelet tensor product bases have been recently characterized by Nitsche. Our results are based on certain regularity assumptions at the electron-electron and electron-nuclear cusps.

Irene Gamba

Quantum charged hydrodynamic transport and the boundary value problem

We consider quantum hydrodynamic models (QHM)-Poisson systems in bounded domains with inflow boundary conditions in the context of charged transport induced by an electric field for a rather general thermatization closure. These problems appear in the modeling of nano-scale electronic devices as well as Bose Einstein condensates and other approximations to charged non-linear Shroedinger transport by WKB expansions. We show non-existence of weak solutions to stationary states for a large set of boundary conditions, and, in particular, a blow up in finite time for transient solutions. However the stationary problem is solvable when a nonlinear viscous-friction term is present.

This presentation is a result of a series of collaborations with A. Jüngel and P. Zhang.

Caroline Lasser

Resonances of a conical level crossing

(Joint work with Setsuro Fujiie and Laurence Nedelec.)

In the study of molecular spectra, Schrdinger operators with matrix-valued potentials arise. We present a semiclassical description of the resonant set for the case, that the potential matrix has conically intersecting eigenvalues.

Hongjun Luo

Linearized Approximations to Relativistic Minimax Principle

For the invistigation of the relativistic effects in the electronic systems, it is crucial to have efficient schemes for obtaining energy optimized approximate solutions to the one particle Dirac equations. The Dirac operator is unbounded from bellow, which causes the so called "variational collapse." This problem can be conquered by Minimax method, but on the other hand the Minimax method is non-linear in eigenvalue and potential which causes great difficulties and effort. Therefore we developed linearisations (LARM methods) which approximate the Minimax energies very closely, converge also to the exact ralativistic values when the basis for the large spinor components becomes complete, and are linear in the eigenvalue.

Francesco Maggi

Confining thin elastic sheets and paper folding

(Joint work with Sergio Conti)

Crumpling a sheet of paper leads to the formation of complex folding patterns over several length scales. This can be understood on the basis of the interplay of a nonconvex elastic energy, which favors locally isometric deformations, and a small singular perturbation, which penalizes high curvature.

Based on three-dimensional nonlinear elasticity and by using a combination of explicit constructions and general results from differential geometry, we prove that, in agreement with previous heuristic results in the physics literature, the total energy per unit thickness of such folding patterns scales at most as the thickness of the sheet to the power $5/3$. For the case of a "single fold" we also obtain a corresponding lower bound.

Peter Markowich

On Bose-Einstein Condensation

Ulrich Mauthner

Space-adiabatic perturbation theory for Dirac electrons in a periodic potential

In the last few years, space-adiabatic theory was used extensively to obtain rigorous results for a number of well-known physical problems such as the Born-Oppenheimer problem or the motion of an Bloch electron. This talk shows some results on the case of a relativistic electron in a periodic potential and compares them with the non-relativistic case (i.e. the Bloch electrons).

Josipa Pina Milisic

Numerical approximations of quantum hydrodynamic models

Due to the growing field of nanotechnology applications, mathematical modeling and simulation of charge transport in semiconductors is today a challenging research area. In order to achieve the efficient fabrication of the electronic devices, it is important to derive quantum models which are physically accurate as well as computationally feasible. The quantum hydrodynamic models seem to fulfill these requests.

In this talk, extended quantum hydrodynamic model will be derived from a Wigner equation including collision terms of Fokker-Planck or BGK-type. These models differ from the usual one by additional (viscous, vorticity etc.) terms taking into account the collisional effects. Finally, we present some numerical results for a one-dimensional resonant tunneling diode.

Francis Nier

Computing the steady states of resonant tunneling structures via an asymptotic model

(Joint work with Y. Patel and V. Bonnaillie)

After reviewing the difficulties and some methods used in order to make simulations of nonlinear quantum electronic resonant structures, we will present an algorithm and numerical results based on an asymptotic theoretical analysis.

Barbara Niethammer

An averaging method to capture effective properties in interacting particle systems

Multiscale modeling often requires to investigate higher order terms in order to reveal genuine statistical effects. We illustrate a method to identify higher order corrections with the simple example of the Laplace operator with Dirichlet conditions in a domain with randomly distributed holes.

Riccardo Sacco

Multi-Physics Simulation of Nanoscale Semiconductor Devices

(Joint work with Carlo de Falco)

This lecture deals with the numerical simulation of advanced nanoscale semiconductor devices based on Quantum–Corrected Drift–Diffusion (QCDD) models. QCDD models properly account for electrostatic quantum effects due to strong electron confinement and barrier penetration. Computational efficiency is achieved at the price of neglecting quantum phenomena in transport.

Burkhard Schmidt

Quantum-Classical Liouville Dynamics

In mixed quantum-classical molecular dynamics few but important degrees of freedom of a molecular system are modeled quantum-mechanically while the remaining degrees of freedom are treated within the classical approximation. Such models can be systematically derived as a first order approximation to the partial Wigner transform of the quantum Liouville-von Neumann equation for two–component systems.

Efficient numerical propagation is based on Rothe methods established in the theory of partial differential equations where time discretization is achieved by virtue of the implicit trapezoidal rule. The resulting stationary equations are solved by Monte Carlo based particle methods employing sets of Gaussian packets in phase space. The resulting dynamical scheme is fully adaptive both with respect to the temporal and spatial discretization.

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