First Joint Meeting between the RSME and the AMS

Sevilla, June 18–21, 2003

Abstracts

Session 23

Mathematical aspects of semiconductor modeling and nano–technology

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The Boltzmann-Poisson system in semiconductors: Numerical simulations for Silicon and GaAs devices

María J. Cáceres (Universidad de Granada)

The Boltzmann-Poisson system modeling the electron flow in semiconductors is used to discuss the validity of the Child-Langmuir asymptotics. The scattering kernel is approximated by a simple relaxation time operator. The Child-Langmuir limit gives an approximation of the current-voltage characteristic curves by means of a scaling procedure in which the ballistic velocity is much larger that the thermal one. We discuss the validity of the Child-Langmuir regime by performing detailed numerical comparisons between the simulation of the Boltzmann-Poisson system and the Child-Langmuir equations in test problems (for Silicon and GaAs). On the other hand, we present numerical results for the kinetic system of charge transport in GaAs where the collision operator is obtained by means of the Fermi's golden rule. It takes in account various scattering mechanisms the electrons undergo in a semiconductor. In such way that, some of them leave the electrons in the same valley as they are before the collision, (intravalley transitions), while other scatterings can drive the electrons into a different valley (intervalley transitions).

The half space problem for kinetic relaxation under a strong force field scaling

Naoufel Ben Abdallah (Université Paul Sabatier, Toulouse)

Irene M. Gamba* (University of Texas)

Axel Klar (TU Darmstadt)

Half space problems of the linear Boltzmann equation with a constant driving force are considered. Such problems model boundary layers between kinetic zones and fluid zones described by a high field limit of the Boltzmann equation. Existence, uniqueness and asymptotic behaviour of solutions is studied for positive and negative driving forces. In the positive case, the electric force accelerate the particles and we show that the solution of the half space problem is only detemined by the inflow data. In contrast, for negative forces, the behaviour at infinity has to be prescribed in order to insure uniqueness. Due to the non vanishing forces, the problem does not posses any entropy. The existence and uniqueness issues are dealt with by supersolution techniques, while the asymptotic behaviour is analyzed by semi-explicit integration of the equations along the characterictics. For relaxation time approximation a fast numerical method for computing the asymptotic state method is presented and tested.

New Advances in Numerical Micromagnetics Simulations

Carlos J. García-Cervera* (University of California, Santa Barbara)

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Understanding the mechanisms of magnetization reversal in ferromagnetic samples of nanoscale size is of interest in the study of the magnetic recording process, in particular in computer disks and in computer memory cells, such as MRAMs. Most experimental studies coincide that the presence of magnetization vortices inside a ferromagnetic sample has a dramatic effect in the magnetization reversal process. It is therefore necessary to resolve numerically length scales comparable to the size of magnetic vortices in order to carry out realistic micromagnetics simulations. In this talk I will describe the *Gauss-Seidel Projection Method*, an implicit method for the Landau-Lifshitz equations, whose complexity is comparable to solving the scalar heat equation implicitly. This method allows us to carry out fully resolved calculations for the switching of the magnetization in micron-sized elements, even in the presence of thermal noise.

A direct solver for 2D non-stationary Boltzmann-Poisson Systems for Semiconductor Devices

Jose A. Carrillo (University of Granada)

Irene M. Gamba (University of Texas at Austin)

Armando Majorana* (University of Catania)

Chi-Wang Shu (Brown University)

The Boltzmann equation (BTE) describes electron transport in semiconductor devices. Solving it numerically is not an easy task because the BTE is an integro-differential equation with six dimensions in the phase space and one in time. Though one of the most popular method to model charge transport in such devices is the Monte Carlo method, it is very noisy at high energy regimes and inefficient for simulations of transients.
We consider the two-space, three-phase-velocity dimensional single-band Boltzmann equation describing electron flow in a MESFET devices. The collision operator models scattering processes between free electrons and phonons in thermal equilibrium, including terms modeling phonon absorption and emission rates. The doping profile and the self-consistent electric field are related by the Poisson equation relating the potential to total space charges under strong applied bias.
In this work we extend our recent one-dimensional simulation using a simple numerical scheme based on a splitting scheme where the advection part is treated WENO-solver and the time dependent by Runge-Kutta method, after a spherical coordinate transformation is performed in order to deal for the singular nature of the phonon-scattering processes.

Recent Progress in Quantum Hydrodynamis Models for Semiconductors

Ansgar Juengel (Universitaet Konstanz)

Hailiang Li (University of Vienna)

Peter A Markowich* (University of Vienna)

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Hydrodynamic models for semiconductors originate from the Madelung formulation of the Schroedinger equation and describe the flow of quantum particles in a form which is somewhat analogous to classical macroscopic gas dynamics (Euler equations). Challenging mathematical problems occur in the analysis (and numerical treatment) of these equations, typically stemming from their dispersive nature (inherited from the Schroedinger equation). We report on recent existence, uniqueness and semiclassical limit results.

Non-linear transport in semiconductor multiquantum wells doped with magnetic impurities

Manuel Béjar (Instituto de Ciencia de Materiales (CSIC))

A. H. MacDonald (University of Texas at Austin)

Gloria Platero* (Instituto de Ciencia de Materiales (CSIC))

David Sánchez (Instituto de Ciencia de Materiales (CSIC))

Magnetic dc-biased semiconductor superlattices (SLs) have very interesting non-linear physical properties because of the giant spin splitting produced by the exchange interaction between the conduction band electrons and the magnetic impurities local spin, at low magnetic field [1]. We have studied n-doped II-VI ZnSe/(Zn,Cd,Mn)Se multiple quantum wells in which the elements on the group II have been substituted by Mn^{+2} magnetic ions. We observe that the formation of electric field domains proven theoretically and experimentally in non-magnetic heterostructures is strongly changed by Mn distribution in the SL. We observe interesting new features in the transport properties due to the presence of impurities: changes in the typical branch structure of the density current, substantial modification of spin polarization in the magnetic wells in the superlattice with respect to their value in the isolated magnetic quantum wells and induced spin polarization in the non-magnetic ones.

[1] D. Sánchez et al., Phys. Rev. B,**65**, 035301 (2002).

[2] M. Béjar et al., Phys. Rev. B,**67**, 045324 (2002).

Quantum collisons in the Boltzmann equation via local extensions to Fermi's Golden Rule

Christian Ringhofer (Arizona State University)

It is generally accepted that the dominant collision mechanism for electron transport in solid state materials is given by Fermi's Golden Rule (FGR), describing the interaction of electrons with the phonon lattice. The FGR can be derived from a complete quantum description of the open system via the Schroedinger equation for the Froehlich Hamiltonian. In this talk we first give an overview of the general methodology to introduce dissipative terms into open quantum systems with a non-constant number of particles leading to the Levinson or the Barker-Ferry equation. We then proceed to present a perturbation theory around this procedure which yields in zero order the FGR and in first order a non-local correction to the semiclassical phonon collision operator. This correction will enable us to study effects such as collisional broadening and the intra-collisional field effect in the framework of existing Boltzmann solvers.

Low-field limit for a nonlinear discrete drift-diffusion model

Luis L. Bonilla (Universidad Carlos III de Madrid an CSIC)

Thierry Goudon (Université Nice-Sophia Antipolis)

Oscar Sánchez* (Universidad de Granada)

Juan Soler (Universidad de Granada)

Charge transport in semiconductor superlattices can be described through a discrete drift-diffusion model. In this model, we identify some small parameter $h > 0$, by means of physically relevant dimensionless quantities. Precisely, we investigate a regime where the length of the superlattice period is small while the doping profile is high. In the limit $h \to 0$, we are led to a nonlinear drift diffusion model, coupled to the Poisson equation.

Quantum device simulations by Wigner Equations

Irena Gamba (The University of Texas at Austin)

Jing Shi* (The University of Texas at Austin)

We present a new numerical solver for Wigner Type equations, which model the evolution of Wigner functions that gives the distribution density in the phase space. High order numerical discretization is employed in the simulation and contributes in an essential way in order to capture the dispersive behavior of the model.

We shall discuss some benchmark cases. In particular we present a numerical simulation of quantum resonant tunnelling diode. The resulting Wigner equation coupling with quantum Fokker-Planck term and relaxation time term are presented and compared. This work is part of a project in collaboration with Peter Markowich and Christian Ringhofer.

A WENO solver for the transients of Boltzmann-Poisson system

Jose A. Carrillo (University of Granada)

Irene M. Gamba (University of Texas at Austin)

Armando Majorana (University of Catania)

Chi-Wang Shu* (Brown University)

In this talk we describe our recent work in developing a deterministic high order accurate finite difference weighted essentially non-oscillatory (WENO) solver to the solution of the Boltzmann-Poisson system for semiconductor devices. Weformulate the Boltzmann-Poisson system in a spherical coordinate system using the energy as one of the coordinate variables, thus reducing the computational complexity to two dimensions in phase space when the device is one dimensional in physical space, and dramatically simplifying the evaluations of the collision terms. The solver is accurate in time hence useful also for time dependent simulations. The high order accuracy and non-oscillatory properties of the solver allow us to use very coarse meshes to get a satisfactory resolution, thus making it feasible to develop a two dimensional solver (which is five dimensional plus time when the phase space is discretized). The computational results in one physical space dimension have been compared with those by a Monte Carlo simulation and excellent agreements have been found. The advantage of the current solver over a Monte Carlo solver includes its faster speed, noise-free resolution, and easiness for arbitrary moment evaluations. This solver is a useful benchmark to check on the physical validity of various moment models.

Stochastic and Determinstic Switching Dynamics in Semiconductor Superlattices

Sthephen Teitsworth (Duke University)

This talk focuses on switching dynamics between different current states in semiconductor superlattices (SL's) under conditions of electric-field domain formation and bistability in the current-voltage (I-V) relationship. For such systems, current switching events correspond directly to the relocation — from one quantum well of the SL to another — of the charge monopole that separates the low- and high-field regions. Depending on the polarity and magnitude of the applied voltage pulse, the switching dynamics may be purely stochastic or may involve a combination of complex deterministic and stochastic mechanisms. In terms of the stochastic switching properties, the statistical distribution of the relocation times has a Gaussian form with small variance when the final voltage is far from a region of current bistability. As the bistable region is approached, the mean switching time increases dramatically, and the distribution shifts to a first-passage-time (FPT) form with large variance. The connection between the FPT switching time distribution and current bistability can be interpreted in terms of appropriate Fokker-Planck equations.