# Preface

Downscaling of semiconductor devices, which is now reaching the nanometer scale, makes it mandatory for us to understand the quantum phenomena involved in charge transport. Indeed, for nanoscale devices, the quantum nature of electrons cannot be neglected. In fact, it underlies the operation of an increasing number of devices. Unlike classical transport, the intuition of the physicist and the engineer is becoming insufficient for predicting the nature of device operation in the quantum context—the need for sufficiently accurate and numerically tractable models represents an outstanding challenge in which applied mathematics can play an important role.

The CIME Session "Quantum Transport: Modelling, Analysis and Asymptotics", which took place in Cetraro (Cosenza), Italy, from September 11 to September 16, 2006, was intended both to present an overview of up-to-date mathematical problems in this field and to provide the audience with techniques borrowed from other fields of application.

It was attended by about 50 scientists and researchers, coming from different countries. The list of participants is included at the end of this book.

The school was structured into four courses:

- **Grégoire Allaire** (École Polytechnique, Palaiseau, France) *Periodic Homogeneization and Effective Mass Theorems for the Schrödinger Equation.*
- **Anton Arnold** (Technische Universität, Vienna) *Mathematical Properties of Quantum Evolution Equations.*
- **Pierre Degond** (Université Paul Sabatier and CNRS, Toulouse, France) *Quantum Hydrodynamic and Diffusion Models Derived from the Entropy Principle.*
- **Thomas Yizhao Hou** (Caltech, Los Angeles, USA) *Multiscale Computations for Flow and Transport in Heterogeneous Media.*

This book contains the texts of the four series of lectures presented at the Summer School. Here follows a brief description of the subjects of these courses.

The first course, titled *Periodic Homogeneization and Effective Mass Theorems for the Schrödinger Equation*, was given by Professor Grégoire Allaire, a renowned specialist in homegeneization theory, and introduced the audience to the theory of homogeneization, a powerful tool for mathematically analyzing the multiscale aspects which are encountered in mathematical physics. First, the heuristic method of two-scale asymptotic expansions is discussed, then an entire section is devoted to the rigorous aspects and the main theoretical results that are at the root of the two-scale convergence. Such a method can be applied to the homogeneization of partial differential equations with periodically oscillating coefficients, like the model problem of diffusion in a periodic medium. These tools are then used to derive rigorously the so-called effective mass approximation which justifies the averaging of the crystal lattice effect on the transport of electrons in solids.

The course *Mathematical Properties of Quantum Evolution Equations*, given by Professor Anton Arnold, was aimed at introducing the basic mathematical properties of quantum evolution equations, such as the Schrödinger equation, the von Neumann equation and the Wigner formalism, and also dealt with the modelling of electron injection from reservoirs into semiconductor nano-devices, and the mathematical and numerical analysis of open boundary conditions for such equations. For the Schrödinger–Poisson analysis Strichartz inequalities are presented. In the density matrix formalism, both closed and open quantum systems can be treated. Their evolution is discussed in the space of trace class operators and energy subspaces, employing Lieb–Thirring inequalities. For the analysis of the Wigner–Poisson–Fokker–Planck system, quantum kinetic dispersion estimates are derived for Wigner–Poisson systems, inspired by the Vlasov–Poisson case. In this course, standard dispersion inequalities for the Schrödinger equation and novel stability properties of discrete artificial boundary conditions obtained by Professor Arnold are shown.

The course *Quantum Hydrodynamic and Diffusion Models Derived from the Entropy Principle*, given by Professor Pierre Degond, presents a novel methodology for the derivation of quantum macroscopic equations from kinetic-type models which is based on a deep understanding of the analogy between classical and quantum dynamics. The entropy minimization strategy of Levermore is considered in the quantum context, and is shown to produce diffusion or hydrodynamic-type equations in which the quantum features appear in particular in the nonlocal character of the relationship between the macroscopic variables such as the particle density and the entropic ones such as the chemical potential. The ad hoc corrections of classical fluid equations, which are commonly used in engineering simulations, are clarified and corrected using this approach. They appear as expansions of the fully quantum models in powers of the Planck constant. A whole field of difficult mathematical problems is open for researchers.

The last course was dedicated to numerical issues. In this course, titled *Multiscale Computations for Flow and Transport in Heterogeneous Media* and given by Professor Thomas Hou, a leader in this field, multiscale finite element methods are presented, analysed and illustrated in various physical situations. The author presents an exhaustive review of the more important recent advances in developing multiscale finite element methods for flow and transport in strongly heterogeneous porous media. The applications targeted by this course are in domains other than quantum transport, but the methodology will be of great interest to researchers involved in quantum transport modelling. Indeed, one of the main features of the quantum transport problem is the existence of different scales: macroscopic scales which are related to electrostatic forces and microscopic scales connected to oscillations of single wave functions and at which interference effects take place. Standard numerical methods need mesh sizes at microscopic scales, thus leading to unnecessarily high numerical cost. The goal of the course is to present methods that capture the small-scale effect on the large scales, but do not require resolving all the small-scale features. The course presented novel numerical multiscale methods which allow the use of coarse meshes while succeeding in resolving the microscopic scales.

The school succeeded in introducing the basic mathematical techniques to analyze quantum transport, to present new models dealing with collisions in the quantum context and to enlarge the knowledge in the domain to multiscale techniques borrowed from other fields of applied mathematics. The choice of the courses and the speakers was suggested by the demand of exhaustively presenting the state of art of quantum transport modelling, proposing both the kinetic and the hydrodynamic models, as well as the analytical and numerical aspects of the more significant problems.

During the course, the Thursday afternoon was dedicated to a poster session, where some of the young participants had the opportunity to show their more recent research and to discuss it with all the participants. The contributors to the poster session were D. Finco, E. Kalligiannaki, O. Maj, C. Manzini, O. Morandi, J.P. Milišic, C. Negulescu, G. Panati, T. Ryabukha, M. Schulte, and V.O. Shtyk.

The directors of this course thank the members of the CIME Scientific Committee for their invitation to organize it, and the Director, Professor Pietro Zecca, and the Secretary, Professor Elvira Mascolo, for their continuous help in the organization.

A special thanks has to be addressed to the lecturers for their good presentations, which stimulated scientific discussions. A thanks has to be addressed also to the attending people, constantly animated with genuine interest. The presence of some participants specialist in quantum transport topics favoured interactions among the students, and we are grateful for the attention paid by a precise and careful audience.

We also like to thank MIP Toulouse for its financial support of the French participants.

Finally, we thank the Director and all the staff of Hotel San Michele in Cetraro for their warm hospitality, which greatly contributed to the friendly atmosphere among all the participants.

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