Multiscale Analysis for Quantum Systems and Applications

Istituto Nazionale di Alta Matematica

Roma, October 24-26, 2007.

Programme

Wednesday, October 24

First session - Room INDAM.

- 13.45 - 14.15: Registration
- 14.15 - 14.30: Welcome
- Short Communications
  - 14.30 - 15.00: **D. Finco,** *Quantum graphs and quantum waveguides with Dirichlet boundary conditions.*
  - 15.00 - 15.30: **J. Wachsmuth,** *Effective dynamics for constrained quantum systems.*
  - 15.30 - 16.00: **V. Pierfelice,** *Global wellposedness and scattering results for nonlinear Schrödinger equations on hyperbolic spaces.*
  - 16.00 - 16.30: **A. Mantile,** *On the optimization of the fundamental eigenvalue of confining point interaction operators.*
- 16.30 - 17.00: Coffee Break

Second session - Room II, Dipartimento di Matematica.

- Short Communications
  - 17.00 - 17.30: **L. Tenuta,** *Quasi-static limits in Nonrelativistic Quantum Electrodynamics.*
  - 17.30 - 18.00: **L. Fanelli,** *Dispersion of the magnetic Dirac flow.*
  - 18.00 - 18.30: **R. Bertelle,** *A quasi-variational inequality model for semiconductor simulation.*
  - 18.30 - 19.00: **R. Carlone,** *Metastable states in a model of spin dependent point interactions.*

Thursday, October 25

"Giornata INDAM" - Room INDAM

- 9.00 - 9.15: Introduction to "Giornata INdAM"
- 9.15 - 10.15: **C. Le Bris,** *Some mathematical and algorithmic aspects of computational materials science.*
- 10.15 - 10.45: Coffee Break
- 10.45 - 11.45: **R. Resta,** *The insulating state of matter: a geometrical theory.*
- 11.45 - 12.45: **A. Gnudi,** *Numerical simulation of ballistic quantum transport in silicon nanowires accounting for full band effects.*
- 12.45 - 14.30: Lunch
- 14.30 - 15.30: **A. Ghetti,** *Electron and hole inversion layer mobility: theory and simulation.*
- 15.30 - 16.00: Coffee Break
- 16.00 - 17.00: **R. Schrader,** *Physics and mathematics of metric graphs.*

17.00 - 19.00: Informal discussion - Aula Picone, Dip. Matematica
Social dinner - meeting point: Piazzale Aldo Moro at 19.30 (sharp)

Friday, October 26

Morning session - Room INDAM.

- 9.00 - 10.00: **S. Pascazio,** *Statistical mechanics of multipartite entanglement.* - Room INDAM
- 10.00 - 10.30: Coffee Break
- Short Communications - Room INDAM
  - 10.30 - 11.00: **R. Adami,** *Computation of quantum de-coherence.*
  - 11.00 - 11.30: **C. Cacciapuoti,** *One dimensional approximations of the Laplacian on thin waveguides.*
  - 11.30 - 12.00: **C. De Falco,** *Coupling of quantum and electrothermal effects in semiconductor device simulation.*
  - 12.00 - 12.30: **C. Manzini,** *Fluid-dynamical models for quantum-driven semiconductor transport in high-field regime.*
- 12.40 - 13.15: Conclusione del progetto: rendiconto e discussione.

Invited Talks

The talks are listed in chronological order.

Some mathematical and algorithmic aspects of computational material science

Claude Le Bris (ENPC and INRIA, Paris, France).

The talk will overview some recent mathematical contributions to computational material science. First, the theoretical and challenging question of the passage from computational chemistry and microscopic solid state physics models (such as Hartree Fock type models) to continuum mechanics models for crystalline solids will be addressed. The discussion will be based upon a series of joint works with Xavier Blanc (Université Paris 6 and INRIA, Paris) and Pierre Louis Lions (College de France, Paris).

Second, some numerical aspects of the problem will be considered. Practical numerical approaches like the quasicontinuum method (a method coupling a discrete, atomistic description of matter, with a continuum mechanics description) will be examined from the perspective of numerical analysis. The second part of the talk is based on a series of works with Xavier Blanc and Frederic Legoll (LAMI-ENPC, Paris).

The insulating state of matter: A geometrical theory

Raffaele Resta (Università di Trieste and CNR-INFM DEMOCRITOS National Simulation Center, Trieste, Italy).

In a milestone paper appeared in 1964, W. Kohn showed that the insulating state of matter reflects a peculiar organization of the electrons in their ground state: the cause for the insulating behavior is electron localization [1]. Such localization, however, manifests itself in a very subtle way, fully elucidated much later. I will present the modern developments of the theory, which started in 1999. and continue to these days. The many-body wavefunction of an insulator is characterized by means of geometrical concepts. We consider a many-body system, whose most general Hamiltonian, includes both a “twist” (alias “flux”), and a vector potential $\mathbf{A}$ of magnetic origin:

$$\hat{H}(\mathbf{k}) = \frac{1}{2m} \sum_{i=1}^{N} (\mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i) + \hbar\mathbf{k})^2 + \hat{V},$$

where the potential $\hat{V}$ includes a one-body term (the external potential) and a two-body one (the electron-electron interaction). For any $\mathbf{k}$, and for any system size L, the ground wavefunction obeys periodic (toroidal) boundary conditions. The Provost-Vallee quantum metric tensor [2], is in our case:

$$g_{\alpha\beta}(\mathbf{k}) = \mathrm{Re}\,\langle \partial_\alpha \Psi_0(\mathbf{k}), \partial_\beta \Psi_0(\mathbf{k}) \rangle - \langle \partial_\alpha \Psi_0(\mathbf{k}), \Psi_0(\mathbf{k}) \rangle \langle \Psi_0(\mathbf{k}), \partial_\beta \Psi_0(\mathbf{k}) \rangle \,,$$

where $\partial_\alpha = \partial / \partial k_\alpha$. The corresponding many-body Berry curvature is

$$\Omega_{\alpha\beta}(\mathbf{k}) = i[\langle \partial_\alpha \Psi_0(\mathbf{k}), \partial_\beta \Psi_0(\mathbf{k}) \rangle - \langle \partial_\beta \Psi_0(\mathbf{k}), \partial_\alpha \Psi_0(\mathbf{k}) \rangle],$$

and vanishes for time-reversal invariant systems. The insulating state of matter is characterized by having $g_{\alpha\beta}(0)/N$ finite in the thermodynamic limit, at variance with metals where it diverges [3]. This quantity provides a measure of Kohn's localization in *any kind* of insulator, and has the physical meaning of the ground-state quantum fluctuation of macroscopic polarization. In the simple case of a crystalline system of noninteracting electrons, this same quantity sets a lower bound for the quadratic spread of the Wannier functions (which, again, diverges in the metallic case).

In 2d the Chern number is $C_1 = 4\pi^2 \Omega_{12}(0)/L^2$ in the large-L limit. For a quantum Hall fluid, the transverse conductivity is proportional to C_1, ergo to $\Omega_{12}(0)/N$. The system is indeed an insulator: in fact the longitudinal conductivity vanishes, and $g_{11}(0)/N$ is finite [4].

[1] W. Kohn, Theory of the insulating state, Phys. Rev. **133**, A171 (1964)

[2] J. P. Provost and G. Vallee, Commun. Math Phys. **76**, 289 (1980).

[3] R. Resta, Why are insulators insulating and metals conducting?, J. Phys.: Condens. Matter **14**, R625 (2002).

[4] R. Resta, Electron Localization in the Quantum-Hall Regime, Phys. Rev. Lett. **95**, 196805 (2005).

Numerical simulation of ballistic quantum transport in silicon nanowires accounting for full band effects

Antonio Gnudi (DEIS-ARCES, Università di Bologna, Italy).

In ultra-scaled silicon-nanowire devices with small diameter, the transport problem can be formulated in terms of an open-boundary 1D Schrodinger equation for each subband in the longitudinal direction for electrons injected from the source and drain reservoirs. According to the equivalent Hamiltonian theorem, the kinetic operator is based on the subband energy dispersion relation $\varepsilon(k)$ of the 1D electron gas of the nanowire, which can be accurately computed by means of an atomistic model. Even though most of the I-V characteristics can be reasonably well calculated within the constant effective mass approximation, there are interesting aspects that are strictly related with the full subband structure. The numerical difficulties rising from the direct discretization of the high-order differential operator can be partly circumvented using a transfer matrix method (TMM) in combination with an expansion of $\varepsilon(k)$ in powers of k^2. However, the TMM fails when $\varepsilon(k)$ has relative extremes within the first Brillouin zone of the nanowire. A solution method is discussed based on the expansion of $\varepsilon(k)$ in Fourier series, which fully accounts for the finite energy extension as well as for the periodicity of the band structure. Results will be presented relative to test potential profiles and to simulations of realistic nanowire transistors as well.

Electron and hole inversion layer mobility: theory and simulation

Andrea Ghetti (ST Microelectronics, Italy).

This presentation would like to give an overview the current status about the modeling and simulation of MOSFET inversion layer effective mobility for both electrons and holes. First, the concept of effective mobility in MOSFET, and experimental evidences about its universal behavior for a given temperature and wafer orientation is briefly summarized. Next, current status about effective mobility physical modeling is overviewed. The peculiar feature of MOSFET inversion layer mobility is that, differently from bulk material, charge transport takes place in a narrow region at the interface where, free carriers form a 2D gas because of quantum mechanical effects. Thus, 2D full band structure calculation as a function of the electrical field and mechanical stress is illustrated. Finally, some numerical results about 2D full band structure and effective mobility calculation for both electrons and holes will be presented.

Physics and mathematics of metric graphs

Robert Schrader (Freie Universität Berlin, Berlin, Germany).

We discuss several contexts in physics and biology where the theory of metric graphs is used or might be used. This leads to a list of open mathematical problems.

Statistical mechanics of multipartite entanglement

Saverio Pascazio (Università di Bari, Bari, Italy).

Entanglement is one of the most intriguing features of quantum mechanics. It is widely used in quantum communication and information processing and plays a key role in quantum computation.

At the same time, entanglement is not fully understood and has many puzzling features. It is deeply rooted into the linearity of quantum theory and in the superposition principle and (for pure states) is essentially and intuitively related to the impossibility of factorizing the state of the total system in terms of states of its constituents.

Let us make an example: consider an ensemble of n spin-1/2 particles (qubits), whose Hilbert space $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$ has dimension $N = 2^n$, and divide this set in two *balanced* parts, A and $\bar{A}$, made up of n_A and $n_{\bar{A}}$ qubits respectively ($n = n_A + n_{\bar{A}}$, $n_A = \lfloor n/2 \rfloor \leqslant n_{\bar{A}}$ with no loss of generality). The total Hilbert space factorizes in the tensor product $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_{\bar{A}}$, with dimensions $N_A = 2^{n_A}$ and $N_{\bar{A}} = 2^{n_{\bar{A}}}$ respectively ($N = N_A N_{\bar{A}}$). A pure state

$$\mathcal{H} \ni |\psi\rangle = \sum_{j=0}^{N-1} z_j |j\rangle, \quad z_j \in \mathbb{C}, \quad \sum_{j=0}^{N-1} |z_j|^2 = 1 \tag{1}$$

can be conveniently written in terms of the so-called computational basis $\{|j\rangle\}_{j=0,\dots,N-1}$, that in turn can be naturally expressed in terms of binary sequences belonging to $\{0,1\}^n$ (whose decimal representation are the indices j). Each binary sequence is essentially the collection of the eigenvalues of third Pauli matrices $\sigma_3 = \mathrm{diag}(1,-1)$, each acting on a single qubit.

We shall say that the state is *separable* if it can be factorized:

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_{\bar{A}}\rangle, \qquad \text{with} \quad |\psi_A\rangle \in \mathcal{H}_A, \quad |\psi_{\bar{A}}\rangle \in \mathcal{H}_{\bar{A}}. \tag{2}$$

Otherwise $|\psi\rangle$ is *entangled.*

The characterization and quantification of entanglement is an open and challenging problem. It is possible to give a good definition of *bipartite* entanglement, namely when the original ensemble of qubits is divided in *two* parts, A and $\bar{A}$, like before. The problem of defining *multipartite* entanglement (whatever we mean by this expression) is more difficult and no unique definition exists.

A good bipartite entanglement measure is the so-called *purity* of subsystem A, which is defined in terms of the reduced density operator of A, $\rho_A = \mathrm{tr}_{\bar{A}}\, \rho$ ($\rho = |\psi\rangle\langle\psi|$ being the total density operator):

$$\pi_A = \mathrm{tr}_A\, \rho_A^2. \tag{3}$$

It is easy to see that $\pi_A = \mathrm{tr}_{\bar{A}}\, \rho_{\bar{A}}^2$ and that

$$\frac{1}{N_A} \leq \pi_A \leq 1. \tag{4}$$

Purity $\pi_A = 1$ if and only if ρ_A and $\rho_{\bar{A}}$ are projectors, that is, if the state is separable as in (2). Otherwise, if $\pi_A < 1$, $|\psi\rangle$ is entangled. Moreover, π_A saturates its minimum $N_A^{-1} = 2^{-n_A} = 2^{-\lfloor n/2 \rfloor}$ if and only if the reduced density operator of the (smaller) balanced partition A is proportional to the identity matrix $\rho_A = \mathbb{I}/N_A$. In such a case $|\psi\rangle$ is said to be endowed with *maximal bipartite entanglement* [at fixed bipartition $(A, \bar{A})$].

After a preceptive summary of the idea of entanglement, we introduce the notion of *maximally multipartite entangled* (pure) *states* (MMES) of n qubits as a generalization of the bipartite case. These states are minimizers of the following cost function

$$\pi_{\mathrm{ME}} = \begin{pmatrix} n \\ n_A \end{pmatrix}^{-1} \sum_{|A| = n_A} \pi_A, \tag{5}$$

that we shall call *potential of multipartite entanglement*. The quantity π_{ME} measures the average bipartite entanglement over all possible balanced bipartition and thus inherits property (4), i.e.

$$\frac{1}{N_A} \leq \pi_{\mathrm{ME}} \leq 1. \tag{6}$$

Some examples of MMES for small n are investigated, both analytically and numerically. If for some given n the lower limit in (6) is saturated, the bipartite entanglement of MMES is maximal for all possible balanced bipartitions and therefore does not depend on the bipartition.

Short communications

The talks are listed in chronological order.

Quantum graphs and quantum waveguides with Dirichlet boundary condition.

Domenico Finco (Università di Roma “La Sapienza”, Rome, Italy).

We analyze the problem of approximating a smooth quantum waveguide with a quantum graph. We consider a planar curve with compactly supported curvature and a strip of constant width around the curve. We rescale the curvature and the width in such a way that the strip can be approximated by a singular limit curve, consisting of one vertex and two infinite, straight edges, i.e. a broken line. We discuss the convergence of the Laplacian, with Dirichlet boundary conditions on the strip, in a suitable sense and we obtain two possible limits: the Laplacian on the line with Dirichlet boundary conditions in the origin and a non trivial family of point perturbations of the Laplacian on the line. The first case generically occurs and corresponds to the decoupling of the two components of the limit curve, while in the second case a coupling takes place.

Effective dynamics for constrained quantum systems

Jakob Wachsmuth (Tübingen Universität, Tübingen, Germany).

We consider Schrödinger dynamics under the assumption that the potential approximately confines the wave function to a certain submanifold C. The problem to deduce effective dynamics on the submanifold has been considered several times in the past. But in all results up to now the confining potential had to be constant along C up to rotations. I explain how adiabatic perturbation theory allows to deal with varying potentials. Furthermore I give an overview of the resulting effective dynamics. This is joint work with Stefan Teufel.

Global wellposedness and scattering results for nonlinear Schroedinger equations on hyperbolic spaces

Vittoria Pierfelice (Université d’Orleans, Orleans, France).

We study the dispersive properties of the Schroedinger equation on hyperbolic spaces, obtaining the Strichartz estimates for a broader family of admissible pairs. As a first consequence, we obtain considerably stronger wellposedness results for NLS. In particular, in contrast with the flat case, we prove the L^2 and H^1 global wellposedness for any subcritical nonlinearity without the assumption of gauge invariance. Also the usual distinction between short range and long range nonlinearity is modified: the geometry of the hyperbolic space makes every power-like nonlinearity short range. A second important application of our global Strichartz estimates is to prove "scattering" for NLS both in L^2 and in H^1, without any assumption of symmetry or gauge invariance. Notice that, in the euclidean case, this is only possible for the critical power $\gamma = 1 + \frac{4}{n}$ and can be false for subcritical powers, while on the hyperbolic space global existence and scattering of small L^2 solutions holds for all powers $1 < \gamma \leq 1 + \frac{4}{n}$. This is a direct effect of the negative curvature.

On the optimization of the fundamental eigenvalue of confining point interaction operators.

Andrea Mantile (Czech Technical University, Prague, Czech Republic).

We consider the relations between geometrical properties and spectral quantities related to confining point interaction potentials de.ned on bounded domains of $\mathbb{R}^d$, $d \leq 3$. This class of interactions is suitably defined in terms of selfadjoint extensions of symmetric operators. In particular, it turns out that their spectral properties can be explicitly expressed in terms of the integral kernel of the operator $(-\Delta + z)^{-1}$, where Dirichlet conditions on the boundary are assumed for the Laplacean operator. Our aim is to study the behavior of the spectral points of a point interaction Hamiltonian depending on the position of its scattering center and on the shape of the interaction domain. In particular we investigate how to place the scattering center in order to maximize or minimize the fundamental eigenvalue.

Quasi-static limits in Nonrelativistic Quantum Electrodynamics.

Luca Tenuta (Tübingen Universität, Tübingen, Germany).

We consider a system of N nonrelativistic particles of spin $1/2$ interacting with the quantized Maxwell field (mass zero and spin one) in the limit when the particles have a small velocity.

Two ways to implement the limit are considered: $c \to \infty$ with the velocity v of the particles fixed and $v \to 0$ with c fixed. The second case can be rephrased as the limit of heavy particles, $m_j \to \varepsilon^{-2} m_j$, observed over a long time, $t \to \varepsilon^{-1} t$, $\varepsilon \to 0^+$, with kinetic energy $E_{\mathrm{kin}} = \mathcal{O}(1)$.

Focusing on the second approach we construct subspaces which are invariant for the dynamics up to terms of order $(v/c)\sqrt{\log(v/c)^{-1}}$ and describe effective dynamics, *for the particles only*, inside them. At the lowest order, $(v/c)^0$, the particles interact through Coulomb potentials. At the second one, $(v/c)^2$, the mass gets a correction of electromagnetic origin and a velocity dependent interaction, the Darwin term, appears. Contrary to the case $c \to \infty$, the effective dynamics are independent of the spin of the particles.

Dispersion of the magnetic Dirac flow.

Luca Fanelli (Università di Roma " La Sapienza ", Rome, Italy).

In this talk we will present an overview of recent results on dispersive, Strichartz and Kato-Yajima smoothing estimates for the Dirac equation with a magnetic field. We are interested in potentials which can be singular at points and decay at ∞. The physical interest for the "dispersivity" of these equations is followed by the aim of using the above estimates to treat nonlinear problems from a mathematical point of view.

A quasi-variational inequality model for semiconductor simulation.

Roberto Bertelle (Università di Padova, Padova, Italy).

From a theoretical point of view, the QuasiŨVariational Inequality Model (QVIM) can be fruitfully applied in the semiconductor field to compute the electrostatic potential inside an abrupt, reverse biased, p-n junction diode. With the present work we extend the previous QVIM to treat arbitrarily doped p-n junctions under both reverse and forward bias. We also show that the model is capable to give a solution for the electric potential as well as for the free carrier concentrations. Furthermore, the algorithm based on this kind of model takes low computational time and exhibits good robustness property. Some numerical examples are given to show the last features, namely the condition number of the problem compared with other cases.

Metastable states in a model of spin dependent point interactions.

Raffaele Carlone (Università di Napoli, Napoli, Italy).

In a recent paper we characterized a family of selfadjoint hamiltonians generating the dynamics of a quantum particle interacting, via zero range forces, with an array of localized quantum system with a finite number of energy levels. Those results are used to investigate the spectral properties of the system made of a localized quantum bit (a model-atom) in interaction with a non relativistic quantum particle. We show that starting with an unperturbed system with a ground state and an upper energy level embedded in the continuous spectrum the interaction make the ground state move slightly in energy and the upper energy level turn into a metastable state.

Computation of quantum decoherence.

Riccardo Adami (Università di Milano Bicocca, Milano, Italy).

According to the common explanation of quantum decoherence, superposition states can be destroyed even by a weak interaction with an external environment. In this talk we show how decoherence emerges and evolves in the dynamics of an electron interacting with a phonon bath. A key role in our analysis is played by the separation of scales of the wave packet profile and the interference pattern. The result has been obtained in collaboration with L. Erdos (Munich).

One dimensional approximations of the Laplacian on thin waveguides

Claudio Cacciapuoti (Doppler Institute, Czech Technical University, Prague, Czech Republic).

We discuss one dimensional approximations of the Laplacian defined on a thin waveguide. Our analysis is restricted to a two dimensional, planar, waveguide of constant width, obtained by fattening a curve with compactly supported curvature. The waveguide is squeezed by introducing a scaling parameter. The main point is to show that suitable scalings of width and curvature can produce limit operators on the line involving point interactions. The problem strongly depends on the conditions assumed on the boundary of the waveguide. We consider several boundary conditions and describe the related techniques.

Coupling of quantum and electrothermal effects in semiconductor device simulation

Carlo de Falco (Dublin City University, Ireland and Joseph W. Jerome Northwestern University, Evanston, IL, USA).

According to the ITRS predictions, self-heating and mutual-heating effects will gain increasing importance in the near future especially in emerging SOI and thin-film CMOS technologies, where single device cooling is going to become a serious limitation. Furthermore, due to off-state leakage currents caused by quantum electrostatic effects, even steady-state power consumption will become an important factor affecting device and chip performance. This scenario imposes severe requirements on the development of mathematical models and numerical simulation methods. On the one hand, simulation tools capable to deal with both quantum and heating effects are in order. On the other hand, the increasing complexity of the device geometries and the demand for the concurrent simulation of larger chip areas require models with low computational cost to achieve reasonable efficiency. In this communication, we present a hierarchy of models including quantum electrostatic and self–heating effects for semiconductor device simulation. We adapt the functional iteration and computational techniques used for isothermal Quantum Corrected Drift Diffusion (QCDD) models to the non isothermal case, and we describe an approach for multiscale thermal coupling of neighbouring devices. The degree of accuracy and computational complexity of the members of the hierarchy are compared in extensive numerical experiments.

Fluid-dynamical model for quantum-driven semiconductor transport in high-field regime.

Chiara Manzini (Università di Firenze, Florence, Italy).

In some applications semiconductor devices operate at drift-collision balance regimes. In these regimes, the applied electric field and the interaction with the environmnet have comparable order of magnitude and are dominant with respect to the transport. We start from Wigner equation with an additional BGK term containing the $\mathcal{O}(\hbar^2)$-correction of the classical thermodynamical equilibrium function, describing the state to which the system shall be driven by the interaction with the environment. We consider a scaled version of this equation with advection and relaxation terms of the same order in ϵ. Via a Chapman-Enskog procedure, we solve the scaled equation at order $\mathcal{O}(1)$ and at $\mathcal{O}(\epsilon)$. Then we derive closures and constitutive relations for the terms appearing in the hydro-dynamical system obtained by taking moments of the scaled Wigner equation. The closed system shall contain drift terms of $\mathcal{O}(1)$ in ϵ, while classical and $\mathcal{O}(\hbar^2)$ diffusive terms shall appear as corrections of $\mathcal{O}(\epsilon)$. Additional $\mathcal{O}(\epsilon)$–drift and diffusive terms shall appear to be referred to the high-field regime. Moreover, the equation for the energy-density shall contain *quantum–high-field* corrections due to the use of the pseudo-differential operator in Wigner equation.