Programme blanc 2007

B - Description du projet

QUATRAIN : QUAntum TRAnsport In Nanostructures

Acronyme ou titre court du projet : QUATRAIN

B-1 – Objectives and context

B-1.1 – Objectives, methodology and applications

In order to comply with the growing needs of ultra fast, low consumption and high functionality operation, it is no secret information that microelectronics industry produces highly miniaturized devices with very small characteristic length scales. In such devices, quantum effects such as interferences or tunneling effect become important and more and more predominant. Consequently, since the standard numerical tools used in the industry are based on classical physics, a wide field of research is open in order to design suitable quantum transport models and corresponding efficient numerical methods.

Numerical simulations based on the Schrödinger equation in the context of nanoelectronics have to face difficulties due to the specific properties of this equation: oscillatory behavior of the solutions, presence of resonances, many particles effects and scattering phenomena. The contribution of mathematics is then required at several levels. The understanding of the qualitative properties of the equations enables to identify different regimes and, coupled to asymptotic analysis, is a powerful tool to derive new models adapted to various situations. The design of numerical schemes is also deeply dependent of the identification of the different scales that can be exhibited.

This project proposes to explore several directions of research linked to the mathematical and numerical issues raised by applications from emerging fields of nanoelectronics and physics at the nanometer scale. Let us list here a few target applications which will guide the mathematical questions raised in this project. The first ones concern nanostructures where the charges are transported while strongly confined in one or several directions. A first example is the double-gate MOSFET, where the transport is along a plane, a second one is the nanowire, where the transport is along a line. The very promising technology of carbon nanotubes is also interesting from this point of view since it induces transport along curved lines. More generally, we will consider bio-inspired nanostructures (DNA), molecular electronics (Carbon nanotubes and organic molecules). Another emerging field of electronics is the field of spintronics, which is based on the manipulation of the spin of electrons rather than their charge. Finally, an application from another field of physics will also be concerned by this project: the Bose-Einstein condensates, which is a special state of matter condensate in a coherent quantum state.

In the core of the document, the description of this project is organized according to the common methodologies that will be set up to deal with some problems raised by these applications. The first part concerns the interactions between quantum effects − such as oscillations − and nonlinearities modeling selfconsistent electrostatic interactions. The second one is about the treatment of collisions and hierarchies of quantum transport models that can be designed for regimes driven by collisions. The third part is about the specific mathematical and numerical problems raised by the fact that devices are connected to the outside: quantum models have to be set on open domains.

B-1.2 – State of the art of quantum transport models

In the quantum framework, taking simultaneously into account out of equilibrium phenomena, scattering processes and confinement is a difficult task both from the modeling and numerical points of

view. The current approaches can only partially conciliate these issues. We have classified them into three types.

The first class of models consists in ballistic modeling based on the Schrödinger equation or on the quantum Liouville equation. The numerical resolution can be done, equivalently, either by considering directly the system in open domain with transparent boundary conditions, or by the mean of the so-called non equilibrium Green functions (NEGF). This approach is currently followed in the United States around M. Lundstrom, S. Datta and M. P. Anantram. These models have two drawbacks: they are very expensive numerically due to a large number of equations, and collisions are difficult to take into account.

The second class of models consists in considering the phase-space counterpart of the Schrödinger equation, the Wigner equation. By exploiting the analogy between this equation and classical kinetic models, collisional Wigner equations can be written (like by W. Frensley [1] in the 90's). Such models were studied mathematically by several authors in the European network Hyke (www.hyke.org), like P. A. Markowich [2], A. Arnold [3], J. A. Carrillo [4] and coauthors. However, the Wigner function at the basis of this approach is not a distribution function and numerical simulations can lead to unphysical results such as negative densities.

Quantum macroscopic models such as quantum hydrodynamics or the density gradient model are also very popular. This approach, followed for instance by C. Gardner and C. Ringhofer [5] in Tempe or by A. Jüngel [6] in Mainz, relies on an analogy between the Schrödinger equation and the pressureless Euler system corrected by the so-called Bohm potential (which is obtained by writing the equations for the phase and the amplitude of the wavefunction). Quantum macroscopic model can be written in a phenomenological manner by adding this Bohm potential to classical hydrodynamic or drift-diffusion models [7]. The advantage of such models is that collisional effects seem to be reasonably taken into account, but their justification is far from obvious. Moreover, this Bohm potential reads as the second derivative of a nonlinear function of the density, so this high order term changes dramatically the mathematical nature of the equations and is difficult to handle numerically.

As mentioned above, the objective of our project is to combine the above three descriptions in order to obtain accurate enough, numerically tractable and rigorously justified models, then to develop sound numerical methods to discretize the obtained models and apply them to the simulation of "realistic" devices. To will be done, by looking at reduced dimensionality models for strongly confined electron ensembles, by including and justifying an asymptotic description of resonances which reduces even more the dimensionality of the problem, by pursuing the effort in deriving hybrid models coupling quantum and classical transport equations, by thoroughly studying the quantum fluid models derived from entropy principles, and by defining and implementing novel multiscale numerical schemes for quantum transport. The extension of the approaches to spin polarized transport opens a new research direction to be mathematically developed with a promising interplay of transport and micromagnetism phenomena.

B-1.3 – Experience of the partners and previous collaborations

The group which constitutes this project has a leading position in applied quantum transport modelling at the national level and is one of the few internationally recognized groups (together with the Vienna and Berlin groups for instance).

Most of the members of both teams have contributed to several parts of the research projects and are used to work together on transport problems (Ben Abdallah, Degond, Méhats, Castella, Negulescu, Pinaud, Puel). They have complementary expertise in the field ranging from mathematical modelling and scientific computing to non linear analysis, scattering and operator theory and semiclassical analysis.

Some of them have been involved in two projects (ACINIM MOQUA and ACI, Modèles dispersifs vectoriels) where an interdisciplinary collaboration with M. Mouis from the Institut de Microélectronique, Electromagnétisme et Photonique (IMEP, Grenoble) on the simulation of nano-transistors was developed. During this collaboration, numerical multiscale tools for quantum transport (the Schrödinger equation in open geometries) have been successfully developed and applied essentially to the so-called double gate Mosfet. Various mathematical models have been deduced and rigorously analyzed, like kinetic and diffusion models for partially quantized systems, strongly confined quantum systems, etc.

The question of spin transport arised from a beginning collaboration of the MIP partner with the team of X. Marie and T. Amand (Laboratoire de Physique et Chimie des Nano Objets, LPCNO, INSA Toulouse). Newly hired assistant professor E. Fouassier is involved in developing this collaboration. The implication of another newly hired assistant professor D. Sanchez is in particular fully justified by his skills in micromagnetism analysis and simulations, which is of primary importance in spin polarized transport. Cooperation with the project SICOMAF (ANR 2006) to which D. Sanchez belongs will be naturally sought. On the other hand, the participation of Francis Nier and V. Bonnaillie-Noël will be highly profitable to the project, in view of the expertise they bring in the theoretical treatment of resonances.

In order to keep a reasonable size, the project is purely centered on mathematical and numerical issues and does not formally include interdisciplinary interactions. However, cross collaborations with the IMEP and LPCNO will be naturally developed and new common projects at various levels (national, local) will be lead.

B-2 – Description of the project and expected results

B-2.1 – Oscillations and nonlinearities

In order to take advantage of specificities of electronic devices, several asymptotics are usually applied to the Schrödinger equation by physicists in order to get simplified systems, with less expensive numerical costs [8,9,10]. Let us briefly list a few well-known approximations, which we further describe more in detail.

In the case of the bidimensional electron gas (2DEG), consider the 3D Schrödinger equation with a potential that strongly confines particles in one direction. It is natural to write the solution of this system as the product of eigenfunctions of the transversal confinement operator by a solution of the Schrödinger equation in the two remaining directions. This mode-space approximation presents the advantage to reduce the dimensionality of the equations. If we go further, in situations where the length scales are such that the longitudinal transport can by considered as classical while the confined direction remains quantum, one can perform an analogue of the Born-Oppenheimer approximation and obtain the subband models. A third well-known example is the effective mass approximation, which replaces advantageously the Schrödinger with a periodic potential. A last example is the case of electronic transport in devices subject to strong applied magnetic fields, where the so-called edge-state model has been successfully used to explain many experiments in connection with the quantum Hall effect.

All these approximations are usually fully justified for the linear Schrödinger equation, by using appropriate asymptotic analysis. It is also worth noticing that, due to the fact that the Schrödinger equation is involved in these problems, fast oscillating terms are usually present in the systems. Nevertheless, the point is that these models have to be used in practice in nonlinear situations. Indeed, the electrostatic interactions between particles themselves are described through the mean field theory (or Hartree approximation) thanks to the Poisson selfconsistent potential. In this project, we are interested in the interactions between the above “linear” approximations and the nonlinearity induced by the Poisson equation. The question will be in each case: to which extent can the asymptotic analysis and the nonlinearity be decoupled?

a) The strong confinement approximation

In the work [11], the Schrödinger-Poisson system was analyzed in the situation where a potential of strong confinement on a plane is applied. Two asymptotic models were exhibited in the framework of adiabatic theorems: the wavefunction can be decomposed on the eigenfunctions of the transversal confinement operator. The difficulty was to prove that the fast time oscillations generated by the strong confinement remain decoupled after the action of nonlinearities. This property indeed occurs due to regularizing effects of the Poisson equation. The same asymptotics was analyzed in [12,13] in the case of the cubic nonlinear Schrödinger equation applied to strongly anisotropic Bose-Einstein condensates (this system is also called the Gross-Pitaevskii in this context). In this case, the nonlinearity being local, the phenomenology is thoroughly different and one has to treat the presence of resonances between some of the oscillating terms. Specific tools had to be developed for that, based in particular on almost periodicity.

These works will be the basis of developments proposed in the present project. A work in progress [14] concerns the confinement on a line, with an application to nanowires, where the system is expected to converge towards the one dimensional cubic nonlinear Schrödinger equation. The confinement on a curved surface (starting with a sphere) for Schrödinger-Poisson will also be considered, the challenge being to understand the effects of the geometry. On the other hand, for the nonlinear Schrödinger equation with local nonlinearities, we only treated the case of smooth solution. It will be interesting to investigate the case of solutions in the energy space. Other questions related to blow up solutions arise in the case of focusing interactions. For instance: for the averaged system, what is the critical power for nonlinearities? Is it the one corresponding to the two dimensional Schrödinger equation, or to the three dimensional equation?

b) The subband models

In [15], the partial semiclassical limit of the linear Schrödinger equation in dimension three was analyzed by Wigner technique. The limit model reads as a hybrid classical-quantum system, coupled in momentum space: a Vlasov equation (classical) along two directions and a Schrödinger equation (thus quantum) in the remaining one. Then, the limit system was analyzed, coupled to the Poisson equation in [16,17]. The special case of data polarized on the first eigenmode enables to go further in the analysis. The important open question is now to perform the semiclassical limit directly on the nonlinear Schrödinger-Poisson system.

c) The mean field approximation

A topic related to the strong confinement presented above concerns the effective mass approximation for the Schrödinger equation. It consists of the homogenization of a strong periodic potential created by the crystal. At the limit, the dispersion relation given by the Bloch waves for small wave vectors is replaced by its tangent quadratic form. The dynamics is given by a Schrödinger equation with an effective mass. This result is known formally since the paper of Kohn and Luttinger in the 50's. A rigorous proof has been proven by Poupaud and Ringhofer in the 90's [18] indirectly by means of Wigner functions. Recently, G. Allaire et al. [19] proved the same result by using homogenization techniques. In collaboration with L. Barletti, N. Ben Abdallah has started to tackle the problem by following the approach of Kohn and Luttinger, who decomposed the wave function on a modified Bloch basis. This leads to an envelope function decomposition of the wave function which reduces the effective mass approximation to a perturbation problem of point spectrum. Fourier type methods and adiabatic decoupling theorems lead to the effective mass approximation. As an intermediate step, the so-called K-P interaction Hamiltonians are obtained. We hope that this method can be adapted to tackle the nonlinear problems. Attempts towards the justification of the position-dependent effective mass will also be done in this direction.

d) Transport in a strong magnetic field

Many magnetotransport experiments in two-dimensional electron systems have been explained in recent years within the so-called edge-state model. It describes asymptotically a two-dimensional electron gas in a high transversal magnetic field as a one-dimensional transport along the edge of the device. The asymptotic techniques developed for the analysis of strong confinement problem should apply to this kind of problems. We will study the case of a Schrödinger equation with a strong applied magnetic field and coupled to the Poisson equation. This topic is a part of the subject of the thesis of F. Fendt (Rennes, started in 2006, advisor: F. Méhats). A related subject that will be considered concerns the derivation of asymptotic models for fast rotating Bose-Einstein condensates. Indeed, writing the Schrödinger operator in a rotating frame amounts to introduce a fictitious constant magnetic field in the equation.

B-2.2 – Quantum transport models for collisional regimes

a) Quantum Hydrodynamic models

Quantum hydrodynamics [20,21,24] and Quantum diffusive models [22,23,25] based on entropy minimization represent a new and very promising way to describe, at a macroscopic scale, quantum systems in strong interaction with their environment. These models can be derived starting from microscopic quantum systems, by writing the systems of moments and applying a closure procedure

based on an entropy minimization principle “à la Levermore”. They can be written as classical-like transport equations for the evolution of the moments (particle density, current density ...) coupled to constitutive equations which take the form of quantum quasi-equilibrium systems. These systems can be seen as generalization of Bohmian dynamics to mixed-states. A particular feature, but spectacular, is that from these models it has been possible to justify formally, thanks to semiclassical expansions, the well-known density-gradient model. Recall that the latter had only been obtained by phenomenological considerations. Moreover, in dimension one, preliminary numerical simulations shows that these models can catch quantum effects such as tunneling. Parts of these results have been obtained during the thesis of S. Gallego (Toulouse, started in 2004, advisors: P. Degond and F. Méhats).

Numerical schemes for quantum hydrodynamics and related models

To go further in this direction of research, there is a need of validation and calibration of these models. To this aim, it is necessary to be able to simulate bidimensional domains and open geometries. We propose developments in these two directions. In the case of the double-gate MOSFET, which is one of the target applications, quantum effects appear mainly in the transversal direction. It should be then interesting to adapt the subband decomposition method [28] to reduce the bidimensional constitutive equations –the quantum core of the model– to a collection of monodimensional spectral problems. An argument of adiabatic decomposition could be set up in order to justify this approach. Another interest of this approach could be to draw a link between quantum hydrodynamics and hybrid quantum classical models derived and analyzed in [29,30, 42], based on subbands, among which there is a drift-diffusion Schrödinger-Poisson system studied in the PhD thesis of N. Vauchelet (Toulouse 2003-2006, advisors: N. Ben Abdallah and F. Méhats).

New applications

Potential applications for these models concern of course nanoelectronics, but we have in mind to enlarge the application fields to quantum chemistry and some biological systems, in order to describe the evolution of quantum molecules in strong interaction with a solvent. We are in contact with I. Burghardt at the ENS of Paris, who works on this thematic with her coauthors [26,27].

b) Spintronics

Spintronics is an emerging field of electronics based on the use of the spin-polarized particle. The spin, as a quantum degree of freedom, can be an additional element of control inside the device and an instrument for selecting particles at both sides of the device [31]. We have started a few years ago to work on the modeling of the transport of spin-polarized systems. The models one can find in the literature [32] are either too expensive numerically (like systems of Boltzmann equations), or two simple and heuristic (drift-diffusion [33]), and our project is to derive a hierarchy of well understood models for spin systems. This field is the subject of the thesis of R. El Hajj (Toulouse, started in 2004, advisor: N. Ben Abdallah).

Coupling with ferromagnetism

Ferromagnetic metals are of primary importance in spintronics. Understanding and quantitatively simulating the interplay between magnetization dynamics and charge and spin transport is one of the motivations of this project. Indeed, contrary to the subject of micromagnetism which is widely studied, few efforts have been made in the mathematical community in the direction of modelling spin transport in semi-conductors or ferromagnetic metals. In a purely quantum context, electrons with spin are modeled by the spinor wave function which is a 2 component complex vector. Spin-orbit coupling, spin relaxation, and precession along the magnetization are the important terms to be included in the Schrödinger equation. In the classical context, the unknown is a 2 x 2 hermitian matrix. It is then with values in a four dimensional space. One of the components is the standard particle distributions while the three others are interpreted as the components of spin distribution. The dynamics of spin is influenced not only by electrostatic forces and collisions, but also by spin relaxation phenomena and precession along the magnetization. The injection of spins in thin ferromagnetic material involves an additional torque effect in the Landau-Lifschitz equation which governs the dynamics of the magnetization, and which might considerably change the dynamics of the magnetization, resulting in what is called the magnetization reversal phenomenon. In all these applications, arise questions related to modelling, analysis and numerical simulations of classical and quantum transport models.

Quantum hydrodynamics for spins

In collaboration with L. Barletti, F. Méhats has started to derive quantum macroscopic models for spin systems, by applying the strategy of entropy minimization described above. This approach should enable to obtain a quantum drift-diffusion system for spin transport, analogous to the well-known density-gradient system, which does not exist yet.

c) Surface roughness

The question of modeling surface roughness in nanotransistors is extremely important for electrical engineers, who want to predict the impact on performances of surface irregularities between Silicon and the oxide. The interesting scale is not the one of the surface roughness, but the one of the transport, which is larger. We will thus seek homogenized transport models, and eventually analyze such models. Several routes will be investigated to study such homogenized Schrödinger systems, from deterministic to stochastic methods.

B-2.3 – Quantum transport in open domains

An electronic device is by essence an open system: electrons are injected from a reservoir (the source), they travel through the active region (channel of a Mosfet, double barrier of a resonant tunneling diode, etc.) and leave the device towards another reservoir (the drain). Let us describe the most popular approach, the Landauer-Büttiker method, for modeling (stationary) open Schrödinger systems. In the reservoirs, scattering phenomena drive the electrons ensemble towards a thermal equilibrium: the electrons are in a mixed state with the statistics of the reservoirs. Hence, the system to be solved inside the active region is a set of Schrödinger equations indexed by their energy.

Each state exhibits strong variations in the position variable for high energy. Besides, in the case of transversal transport in heterostructures, like the resonant tunneling diode (RTD), the variation of the state with respect to the energy variable shows extremely sharp variations around energies called resonant energies. Because of these two facts, the spatial variable and the energy variable have to be discretized in an unnecessarily refined way. We propose here several strategies in order to accelerate the numerical simulations.

a) Asymptotic model for the steady states of resonant heterostructures

In [34, 35], a rapid method was built to compute an approximation of steady states of resonant tunneling heterostructures in the far from equilibrium regime. Those calculations are made on a simplified model, which originates from a previous work of C. Presilla and J. Sjöstrand and which takes into account characteristic quantities arising from an accurate asymptotic analysis of the Schrödinger-Poisson system: the regime of quantum wells in semiclassical islands. An interesting point is that this work enables to draw bifurcation diagrams and exhibit hysteresis phenomena, which strongly depends on the geometry of the device. This method does not give an exact solution of the system, but present the advantage to be very rapid. It can thus be used as a support for complete Schrödinger-Poisson calculations. For instance, it can provide an initial guess, especially in cases where there are multiple steady states. It can also be a very useful tool to predict the localization in energy of resonances, in order to design well-adapted non uniform energy grids. In this project, we will implement these ideas. In a second step, we will consider a more ambitious sequel of this work which consists in investigating the dynamical case through similar asymptotic analysis.

b) Multiscale numerical schemes for the Schrödinger-Poisson system

In [36, 37, 38], numerical methods were designed in order to allow the use of coarse grids, both in the spatial and energy variables. For the spatial variable, the idea consisted in using a well-adapted shape functions based on WKB expansions which predict the form of the oscillations near the semiclassical regime, i.e. for the highest energies. For the energy variable, the idea consists in a numerical adaptation of the asymptotic model introduced by C. Presilla and J. Sjöstrand to account for resonances and which has been rigorously justified in [34,35] (see the above paragraph). The wave function can be split into an exterior part which lives outside the double barrier, and is slowly varying with

respect to the energy, and an interior part which lives in the well between the barriers and is strongly varying. But the latter can be well approached by its projection on the resonant state, which is not difficult to compute. The generalization of these ideas to the time-dependent case will be done in this project, in particular with the thesis of A. Faraj (Toulouse, started in 2005, advisor: N. Ben Abdallah). Strong links with item a) will naturally be further developed

c) Integration of hybrid models in a simulator

For several years, hybrid models were studied by members of the project team, involving the coupling of models of different nature in various ways: spatial coupling in [39, 40, 41] or coupling in momentum space in [16,29,30,42]. The plan now is to design an integrated simulator, fed with these hybrid models and the various numerical methods presented above. The basis for this simulator already exists: it is called superNESSIE (see a snapshot of the interface on Fig. 1 below) and is an evolution of a numerical code inherited from the thesis of Eric Polizzi (Toulouse, 1998-2001, advisor: N. Ben Abdallah). The final aim is to design this simulator as a tool for interdisciplinary research, with a pleasant ergonomics, in to order to be directly used by the physicists we have been collaborating with for several years, like M. Mouis and her team at the IMEP, Grenoble (see [37,43,44]).

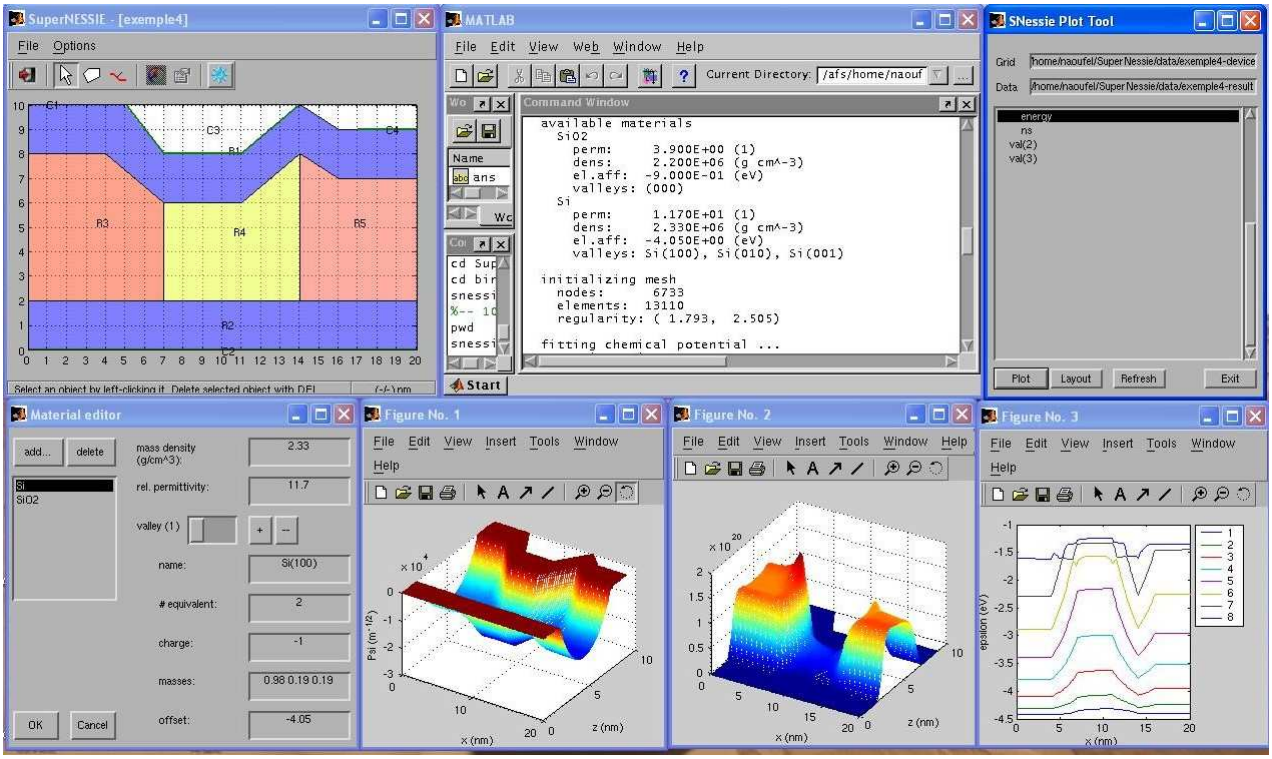

Fig. 1: the simulator superNESSIE

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