Kinetic and Diffusive Models for Partially Quantized Systems

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Classical motion of charged particles (say electrons) can be described by kinetic equations (Vlasov, Boltzmann) coupled to the Poisson equation for the electrostatic forces. For ultrasmall electron systems, like nanostructures, quantum effects are important and are well described by the Schrödinger–Poisson model. In partially confined electron systems like two-dimensional electron gases (2DEG), nanotubes or nanowires, both quantum and classical effects are present. Indeed, the width of a two-dimensional electron gas lying at a heterojunction is a few nanometers. As this length is comparable to the electron de Broglie length, the description of transport phenomena necessitates the use of the Schrödinger equation. In the direction parallel to the heterojunction, the length scale is usually several times higher, and a classical description for electron transport is suitable. This leads to a coupling between classical and quantum models in momentum space (which are obtained in the Born–Oppenheimer approximation).

The aim of this presentation is the study of a kinetic subband model coupled to the Poisson equation as well as a diffusion model in the same framework. In the sequel, the confined direction is denoted by $z \in (0,1)$ while the non-confined direction is called $x \in \omega \subset \mathbb{R}^d$. The problem consists in finding, for $t \in (0,T)$, $x \in \omega$, $z \in (0,1)$ and $v \in \mathbb{R}^d$, the unknowns $V(t,x,z)$, $(\epsilon_p(t,x), \chi_p(t,x,z), f_p(t,x,v))_{p\in\mathbb{N}^*}$ solving

$$\partial_t f_p + v \cdot \nabla_x f_p - \nabla_x \epsilon_p \cdot \nabla_v f_p = 0\,, \tag{1}$$

$$-\frac{1}{2}\partial_{zz}\chi_p + (V + V_{\text{ext}})\chi_p = \epsilon_p \chi_p\,, \tag{2a}$$

$$\chi_p(t,x,\cdot) \in H_0^1(0,1)\,, \quad \int_0^1 \chi_p \chi_q \, dz = \delta_{pq}\,, \tag{2b}$$

$$-\Delta V = \sum_{p\geq 1} |\chi_p|^2 \int_{\mathbb{R}^d} f_p \, dv\,. \tag{3}$$

Existence and uniqueness results are shown in the bounded domain and whole space case. Energy estimates as well as relative entropy inequalities are shown for the above model as well as for the diffusive subband model. The results have been obtained jointly with Florian Méhats, Géraldine Quinio and Nicolas Vauchelet (MIP Laboratoire CNRS, Toulouse).