
Analysis of Coupled Quantum-Classical Models for the Electron Transport in Nanostructures

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We are interested in the modelling of the transport and interaction of electrons partially confined in a nanostructure. The particles are assumed to have a wave behaviour in the confinement directions (z) and to behave like point particles in the directions parallel to the electron gas (x). This leads to a coupling between Quantum and Classical models in the momentum variable.

For each fixed x and at each time t , the eigenfunctions χ_p and the eigenenergies ϵ_p of the Schrödinger operator (2) in the z are computed. The occupation number of each eigenfunction is calculated through the resolution of a Vlasov equation (1) in the x direction, the force field being the gradient of the eigen-energy. The whole system is coupled to the Poisson (3) equation for the electrostatic interaction. In the case of a bounded domain, the whole system writes

$$\partial_t f_p + v \cdot \nabla_x f_p - \nabla_x \epsilon_p \cdot \nabla_v f_p = 0, \quad (1)$$

$$\begin{cases} -\frac{1}{2} \partial_{zz} \chi_p + V \chi_p = \epsilon_p \chi_p, \\ \chi_p(t, x, \cdot) \in H_0^1(0, 1), \quad \int_0^1 \chi_p \chi_q dz = \delta_{pq}, \end{cases} \quad (2)$$

$$-\Delta V = \sum_{p \geq 1} \left(\int_{\mathbb{R}^2} f_p dv \right) |\chi_p|^2, \quad (3)$$

with Cauchy data $f_p(0, x) = f_p^0$ and suitable boundary conditions.

In a first part, existence of weak solutions will be shown for boundary value problems in the stationary and time dependent regimes. The proofs rely on the one hand on the study of quasistatic Schrödinger-Poisson systems and on the other hand on an energy estimate (for the time dependent case) and on supersolution techniques (for the stationary case).

Then the adaptation to the case of the whole space will be presented. The existence of a unique classical solution is shown, the proof being based on an iterative scheme.