Simulation of a Resonant Tunneling Diode using an Entropic Quantum Drift-Diffusion Model

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PRESENTATION OF THE MODEL

We present a new quantum diffusive model derived in [1], [2] and studied in [3]: the entropic Quantum Drift-Diffusion model (eQDD) is a quantum fluid model describing the evolution of the electron density $n(t,x)$ subject to the electrical potential $V(t,x)$ and interacting with a thermal bath of fixed temperature T. The first equation is the equation of mass conservation and reads:

$$e\partial_t n - \mathrm{div} j = 0, \tag{1}$$

where e is the positive electron charge and j is the current defined as follows:

$$j = e\mu n \nabla(A - V). \tag{2}$$

In this equation, μ is the electron mobility. We call $A(t,x)$ the quantum chemical potential which is linked to the density of electrons by a relation which is non local in space and which is the key of this quantum model:

$$n[A] = \sum_{p\geq 1} \exp\left(-\frac{\lambda_p[A]}{k_B T}\right) |\psi_p[A]|^2. \tag{3}$$

Here k_B is the Boltzmann constant and $(\lambda_p, \psi_p)_{p\geq 1}$ are the eigenvalues and the normalized eigenfunctions of the following modified Hamiltonian:

$$H[A] = -\frac{\hbar^2}{2}\mathrm{div}\left(\frac{1}{m(x)}\nabla\right) - eA, \tag{4}$$

where $\hbar$ is the Planck constant and m is the effective mass of an electron.

We show in the presentation some formal links between the eQDD model and several other models. Indeed, the limit of the eQDD model as the dimensionless Planck constant goes to zero is the Classical Drift-Diffusion model, while the leading order correction term is the Bohm potential appearing in the Density-Gradient model.

NUMERICAL RESULTS

The 1D transient eQDD model coupled to the Poisson equation is discretized in time using a semi-implicit Euler scheme and we discretize the space variable using finite-differences. This scheme is solved with the Newton algorithm and we check that we can capture some well known features of the resonant tunneling diode: fig.1 shows the time evolution of the density from the peak to the valley. To obtain this figure, we apply a voltage of $0.25V$ and wait for the electrons to achieve the stationary state. Then we suddenly change the value of the applied bias to $0.29V$ and we record the evolution of the density. As expected, the density inside the well grows significantly. Fig.2 shows the evolution of the current density at the left contact and we can observe one oscillation before the stationary state is achieved.

Fig.3 shows the influence of the effective mass on the current voltage characteristics. As noted for the Density-Gradient model, this parameter must be artificially increased to obtain resonance but this figure shows also the importance of the effective mass inside the barriers, where the notion of effective mass is questionable.

We also show in the presentation some qualitative and quantitative comparisons with the Density-Gradient model and some interesting and unexpected differences are pointed out.

REFERENCES

[1] P. Degond, F. Méhats and C. Ringhofer, *Quantum Energy-Transport and Drift-Diffusion models*, J. Stat. Phys., **118**, 3/4 (2205)

[2] P. Degond, F. Méhats and C. Ringhofer, *Quantum hydrodynamic models derived from the entropy principle*, Contemporary Mathematics, **371** (2005)

[3] S. Gallego and F. Méhats, *Entropic discretization of a Quantum drift-diffusion model*, SIAM journal on numerical analysis, **43**, 5 (2005)

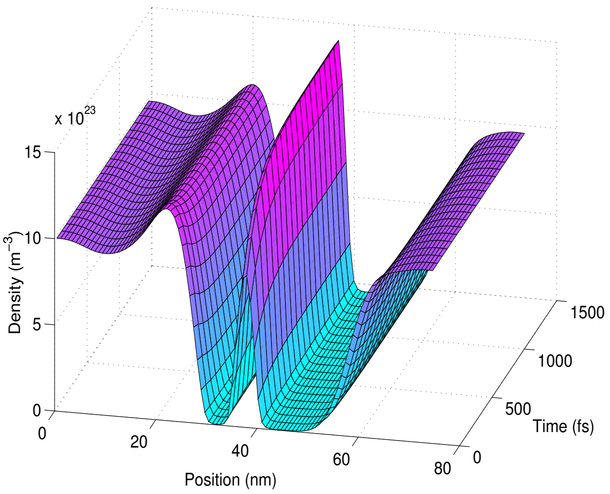

Fig. 1. Evolution of the density from the peak to the valley.

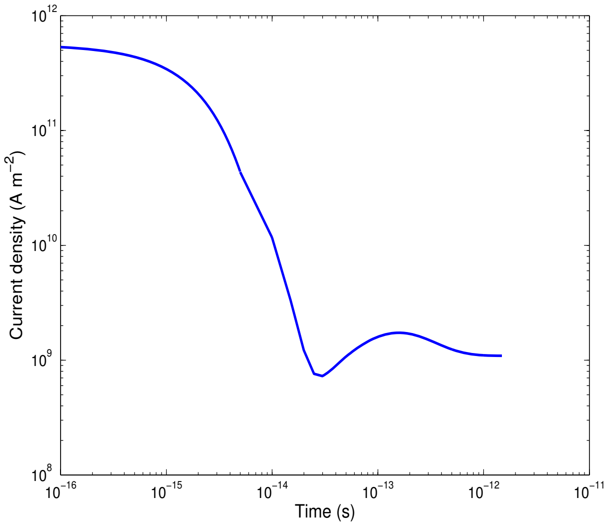

Fig. 2. Evolution of the current density at the left contact

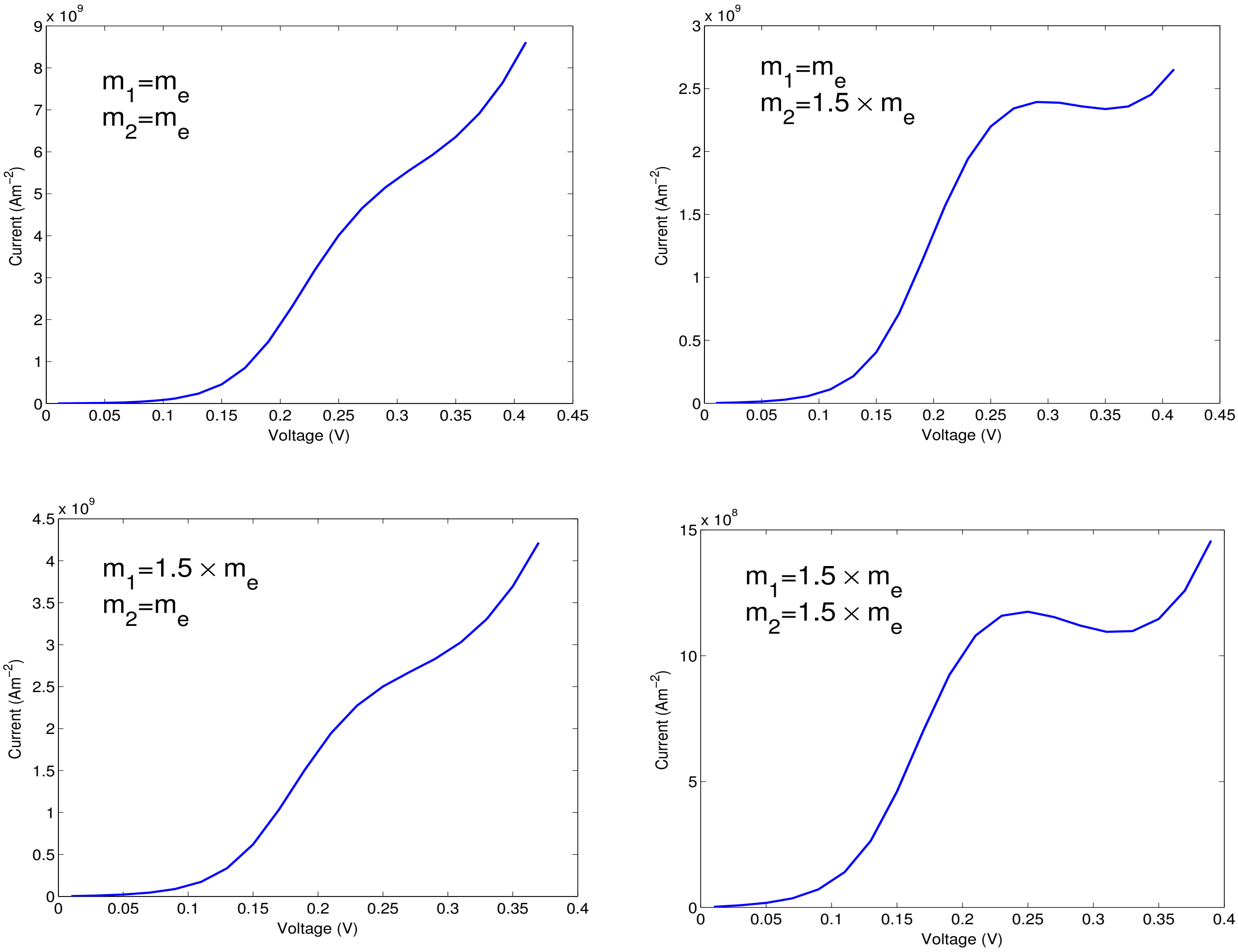

Fig. 3. Influence of the effective mass on the IV curve, m_1 being the mass outside the barriers and m_2 the mass inside.