Computing the steady states for an asymptotic model of quantum transport in resonant heterostructures

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We propose a rapid method to compute the steady states, including bifurcation diagrams of resonant tunneling heterostructures in the far from equilibrium regime. Those calculations are made on a simplified model which takes into account the characteristic quantities which arise from an accurate asymptotic analysis of the nonlinear Schrödinger-Poisson system. After a summary of the existing theoretical results, the asymptotic model is explicitly adapted to some physically realistic situations and numerical results are shown in various cases.

1-Introduction

We focus on the purely quantum models like Schrödinger-Poisson system to describe accuretaly the quantum transport. It is quite easy to recover the negative differential resistance typical of resonant tunneling diode but hysteresis phenomena are more difficult to catch : an accurate treatment of the tunnel effect through the barrier has to be taken into account. We have to overcome difficulties related with the out of equilibre regime and the complexity of a rough numerical treatment due to the presence of resonant states.

2-Model and scaling

We present the nonlinear Schrödinger-Poisson system with the Landauer-Büttiker approach wich involves the stationary scattering states. In order to make precisely the connection with the theoretical analysis and for a more flexible numerical treatment, the Schrödinger-Poisson system is written here with dimensionless quantities and unknowns. The small parameter h is well identified with this writting as the scaled Fermi length (with respect to the size of the device).

The analysis carried out by the third author on the specific asymptotic model of quantum wells in a semiclassical island was developed in order to elucidate the role of the geometry of the barriers in these nonlinear phenomena. It has been done in a general enough framework in order to cover several heterostructure problems. In doing so, he provided the right quantities which govern the nonlinear phenomenon with an accurate treatment of the tunnel effect :

- the dimenlionless small parameter h,
- the position of the well,
- the energy levels of resonant states,
- the Agmon distance (i. e. the action).

3-Implementation

Here we present an adaptation of the theoretical asymptotic analysis which leads to a very rapid determination of bifurcation diagrams.

On complete numerical computations for the original model, we check that the theoretical model in the limit $h \to 0$ is relevant. As a consequence of the scaling of the wells as quantum wells in a semiclassical island, for wich the classically permitted region is asymptotically reduced to a single point, the nonlinear potential is restricted to the classs of piecewise affine potential and it is the key point which permits to reduce the complexity of the full nonlinear system. Then the Agmon distance admit an explicit algebraic expression. As the constraints which involve the Agmon distance in the theoretical result have no obvious convexity properties, the simplest and robut way to take them into account is a penalization method. For several devices (GaAs, Si), we show how our numerical approach is flexible and catches accurately in many different cases the nonlinear phenomena.

4-Conclusion

We obtain in a short time quantitative results which allow to observe non linear phenomena like hysteresis, and more complex bifurcation diagrams in the presence of multiple wells. These computed asymptotic solutions can be used as initial data for a Newton algorithm in the numerical treatment of the complete quantum model. Alternatively this simple model gives also a good insight of the dependence of the bifurcation diagram with respect to some quantitative data : geometry of the barriers and wells, donor density and the applied bias.

Références

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