

ON THE FORMULATION OF ENTROPY FOR A PARTIALLY QUANTIZED ELECTRON SYSTEM IN SEMICONDUCTORS

V. Dario Camiola*, Giovanni Mascali**, Vittorio Romano*

*Dipartimento di Matematica e Informatica, Università di Catania, viale A. Doria 6, 95125 Catania, Italy,
E-mail: camiola@dmi.unict.it, romano@dmi.unict.it

**Dipartimento di Matematica, Università della Calabria and INFN-Gruppo c. Cosenza, 87036 Cosenza, Italy,
E-mail: g.mascali@unical.it

EXTENDED ABSTRACT

In the formulation of hydrodynamic subband models for charge carriers in semiconductors in presence of confinement effects in one or two directions, a crucial problem, in order to apply the maximum entropy principle (MEP), is an appropriate assumption on the entropy for a 2D or 1D electron gas which combines a semiclassical description in the transport direction and quantum effects in the transversal direction. The attempts already known in the literature are based on the quantum formulation of the maximum entropy principle, as proposed in the pioneering work of Jaynes [1] and its more recent revisitation in [2; 3; 4]. However the technical difficulties in solving the constraints in the quantum case are a very complex and daunting task because the algebraic relations are now operatorial ones. Even the expansion in powers of \hbar does not circumvent the problem since only low order terms can be retained otherwise the presence of too high order derivatives makes the resulting equations practically impossible to solve numerically.

When confined structures, like those arising in double-gate MOSFET's or standard MOSFET's are considered, one can take advantage from the symmetry of the problem which allows one to make a geometrical splitting in quantized direction and longitudinal direction. In [5; 6] we have proposed a hybrid expression for the entropy of the system under consideration where in each subband the semiclassical entropy, arising as the limit of the Fermi-Dicac one, is weighted by the square modulus of the envelope functions obtained by solving the Schroedinger-Poisson equations. Summing up the contribution of each subband, the resulting form of the entropy contains both semiclassical information, intended in the usual sense of statistical mechanics or information theory, and a quantum aspect which weights the importance of the single subband, giving more relevance to those associated with a lower energy.

Examples of applications of such an approach have been presented in [7; 8] where the simulations of nanoscale double gate MOSFET's show a good accuracy of the models.

REFERENCES

- [1] Jaynes, E. T.: Information Theory and Statistical Mechanics. Phys. Rev. B vol. 106, pp. 620–630, 1957.
- [2] Degond, P., Ringhofer, C., Quantum moment hydrodynamics and the entropy principle, J. Stat. Phys. vol.112, pp. 587-628, 2003.
- [3] Degond, P., Gallego, S., Méhats, F., Ringhofer, C. , Quantum hydrodynamic and diffusion models derived from the entropy principle, in *Quantum Transport: modelling, analysis and asymptotics - lectures given at the CIME summer school held in Cetraro (Italy), September 11-16, 2006* (N. Ben Abdallah & G. Frosali (eds.)), Lectures Notes in Mathematics vol. 1946, Springer, 2008, pp. 111-168.
- [4] Ben Abdallah, N., Méhats, F., Vauchelet, N.: Diffusive transport of partially quantized particles: existence, uniqueness and long-time behaviour. Proc. Edinb. Math. Soc. vol. 2, pp. 513–549, 2006.
- [5] Mascali, G., Romano, V.: Hydrodynamic subband model for semiconductors based on the maximum entropy principle. IL NUOVO CIMENTO C vol. 33, pp. 155–163, 2010.
- [6] Mascali, G., Romano, V.: A non parabolic hydrodynamical subband model for semiconductors based on the maximum entropy principle. Mathematical and Computer Modeling vol. 55, pp. 1003-1020, 2012.
- [7] Camiola V.D., Mascali G., Romano V. "Numerical simulation of a double-gate MOSFET with a subband model for semiconductors based on the maximum entropy principle. Continuum Mechanics and Thermodynamics" vol. 24, pp. 417–436, 2012.
- [8] Camiola V.D., Mascali G., Romano V. "Simulation of a double-gate MOSFET by a non-parabolic energy-transport model for semiconductors based on the maximum entropy principle ", to appear in MCM (2012)