The maximum entropy principle in a quantum mechanical approach

Lino Reggiani and Jeremy Pousset [1]

[1]Dipartimento di Matematica e Fisica, Ennio De Giorgi, Università del Salento, Italy

We review the state of the art of the maximum entropy principle (MEP) in its classical and quantum (QMEP) formulation. Within the classical MEP we overview a general theory able to provide, in a dynamical context, the macroscopic relevant variables for carrier transport in the presence of electric fields of arbitrary strength. For the macroscopic variables the linearized maximum entropy approach is developed including full-band effects within a total energy scheme. Under spatially homogeneous conditions, we construct a closed set of hydrodynamic equations for the small-signal (dynamic) response of the macroscopic variables. The coupling between the driving field and the energy dissipation is analyzed quantitatively by using an arbitrary number of moments of the distribution function. The theoretical approach is applied to n-Si at 300 K and is validated by comparing numerical calculations with ensemble Monte Carlo simulations and with available experimental data. Within the quantum MEP we introduce a quantum entropy functional of the reduced density matrix, the principle of quantum maximum entropy is then asserted as *fundamental principle of quantum statistical mechanics*. Accordingly, we have developed a comprehensive theoretical formalism to construct rigorously a closed quantum hydrodynamic transport within a Wigner function approach. The theory is formulated both in thermodynamic equilibrium and nonequilibrium conditions, and the quantum contributions are obtained by only assuming that the Lagrange multipliers can be expanded in powers of $\hbar^2$, being $\hbar$ the reduced Planck constant. In particular, by using an arbitrary number of moments, we prove that: (i) on a macroscopic scale all nonlocal effects, compatible with the uncertainty principle, are imputable to high-order spatial derivatives both of the numerical density n and of the effective temperature T; (ii) the results available from literature in the framework both of a quantum Boltzmann gas and a degenerate quantum Fermi gas are recovered as particular cases; (iii) the statistics for the quantum Fermi and Bose gases at different levels of degeneracy are explicitly incorporated; (iv) a set of relevant applications admitting exact analytical equations are explicitly given and discussed; (v) the quantum maximum entropy principle keeps full validity in the classical limit, when $\hbar \to 0$. Future perspectives of the MEP, including many body effects, relativistic invariance and fractional statistics are briefly addressed.

REFERENCES

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