Signed Particle Interpretation for Wigner-Quantum Electron Evolution

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The Wigner formulation of quantum mechanics retains many concepts and relations developed in classical statistical mechanics: Quantum states and observables are represented by functions defined in phase space. Expectation values of the physical quantities are obtained by the same statistical notion, with the only difference that the Wigner state function replaces the classical distribution function.

Historically the formalism has been established on top of the operator mechanics (E.Wigner, 1932). This fact raises in particular the questions whether the formalism can be considered as an independent formulation of quantum mechanics and what differentiates classical from quantum behavior in phase space. It took almost twenty years to address these questions. The modern Wigner theory is formulated independently in terms of the Moyal bracket and the Groenewold star-product. Furthrmore, it is shown that this formulation recovers the operator mechanics, which proves the logical equivalence between the two formalisms. Rules establishing the correspondence between wave mechanics' operators and phase space functions, and when a real function is an admissible Wigner function, have been developed. This provides an intuitive way to formulate models of quantum systems, such as the electron evolution in nanoelectronic structures.

We show that for such systems the analogy between the classical Boltzmann and the Wigner-quantum electron evolution pictures can become even closer. The Wigner-Boltzmann equation is derived in a manner, which ensures a seamless transition between quantum coherent and scattering dominated evolution regimes. Most interestingly, this equation allows for a particle interpretation. Quantum point-like particles drift over Newtonian trajectories and are scattered from them due to interactions with the environment (e.g. lattice vibrations) just like Boltzmann electrons. Quantum behavior is characterized by additional attributes: Particles carry a positive or a negative sign, they are generated by the electric potential, and can annihilate each-other, if they meet in the phase space. Such *signed particles* evolution models provide the means for computer simulations and thus enable deep insight into the complicated interplay of coherent phenomena with processes of de-coherence characterizing the nanometer and femtosecond world. Although introducing considerable computational challenges, signed particle evolution models are amenable for highly parallel Monte Carlo simulation approaches, significantly reducing the simulation runtimes.