

Effective quantum potentials are a relatively inexpensive way to rudimentarily incorporate quantum effects into Monte Carlo simulations of carrier transport in device structures. The basic concept is to replace the action of the Hamiltonian on wave functions in a Wigner formulation by the action of a classical Hamiltonian on particles with an appropriately modified potential, i.e. to use quantum corrected Coulomb forces. Such approaches, based on the Bohm potential, have been used successfully to model tunneling phenomena in quantum chemistry and semiconductor device modeling applications [WY99]. One of the major challenges in the use of Bohm potentials is the requirement to compute higher order derivatives of densities, which poses a difficult numerical problem, due to statistical noise. In addition, the Bohm potential depends still locally on densities and their derivatives, and therefore accounts for nonlocal interaction of electrons only through a gradient expansion. Several approaches have been introduced to represent the quantum interaction of wave packets more accurately, leading to smoothed quantum potentials [RF02].

We present a new form of effective quantum potential, based on thermodynamic considerations. The presented approach is based on a perturbation theory around thermodynamic equilibrium and leads to an effective potential which is dependent on the energy and wave vector of each individual electron, thus effectively lowering step function barriers for high energy carriers [GRV03]. The quantum potential is derived from the idea that the Wigner equation and the Boltzmann equation with the quantum corrected potential should possess the same steady states. Therefore the quantum mechanical thermal equilibrium should be expressed by a corresponding classical equilibrium via

$$W\{\exp(-\beta H[V])\} = \exp\left[-\frac{\beta \hbar^2 k^2}{2m_*} - e\beta V^Q(x, k, \beta)\right] \quad ,$$

where $H[V] = -\frac{\hbar^2}{2m_*}|\nabla_x|^2 + eV$ holds and $W\{\rho\}$ denotes the Wigner transform [WI32], i.e. the exponential on the left hand side is the exponential of a self adjoint operator, while 'exp' on the right hand side denote just the usual exponential function, and β denotes the inverse thermal energy.

The resulting quantum potential V^Q is in general two degrees smoother than the original Coulomb and barrier potential V , i.e. possesses two more classical derivatives, which essentially eliminates the problem of statistical noise. The computation of the quantum potential involves only the evaluation of pseudo differential operators, and can therefore be effectively facilitated using Fast Fourier Transform algorithms. This approach is quite general and can easily be modified to c.f. triangular quantum wells.

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