QUANTUM STEADY STATES VIA
SELFCONSISTENT BLOCH-TYPE EQUATIONS

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Abstract

We present the Bloch–Poisson model describing quantum steady states of electrons in thermal equilibrium. A comparison to the Schroedinger-Poisson model and a discussion of the used statistic (Boltzmann or Fermi-Dirac) correlated to the choice of the effective local potential is given. The use of the Bloch–equation for the Fermi-Dirac case is sketched. A short introduction to analytical and numerical features of the Bloch-Poisson system and its classical limit is given.

1. Introduction. Our goal is the calculation of quantum steady states of an electron ensemble in thermal equilibrium. We consider a one-electron approximation with a self-consistent potential describing the Coulomb interaction of the electrons with each other and with a background of (positive) ions.

The most evident way of setting up this model is to consider the eigenvalue problem for the Schrödinger equation directly coupled to the Poisson equation (e.g. [1], [2]). The electron density then is defined as a sum over the squares of the modulus of the eigenfunctions weighted by occupation probabilities.

Under the assumption of Boltzmann statistics, the computationally expensive eigenvalue problem can be avoided using the Bloch equation for the density matrix ([3], [4], [5], [6]). The Bloch equation is a parabolic equation in which the role of the time is played by the reciprocal of the temperature. The spatial operator is the negative Hamiltonian and the initial datum is a delta-distribution. The charge density is obtained by evaluating the density matrix at the normalized diagonal. The appropriate coupling to the Poisson equation leads to a non–standard evolution problem ([6]).

The thermal equilibrium density matrix or its Fourier transform, the Wigner function, can be used as an initial condition for modelling time dependent problems. Recently relevant numerical results for the resonant tunneling diode have been obtained using a relaxation time ansatz for the collision term in the Quantum Liouville equation ([7]).

2. The Schrödinger-Poisson model. In this approach the state of the system is described by one-particle wave functions in an L^2-space (e.g. [1], [2]). We have to calculate the eigenfunctions of the stationary Schrödinger equation

$$(2.1) \qquad H\psi_i(r) = E_i\psi_i(r), \quad \|\psi_i\|_{L^2} = 1, \quad i \in \mathsf{N}_0,$$

The Hamiltonian reads

$$(2.2) \qquad H = -\frac{\hbar^2}{2m}\Delta + V_{\text{eff}}(r).$$

with some local effective potential $V_{\text{eff}}(r)$ taking into account the Coulomb interaction of the (large number of) electrons. We omit additional terms like an applied external potential, heterojunction discontinuities, etc.

The (electron) density is given by

$$(2.3) \qquad n(r, \beta) = \sum_{i \in \mathbf{N}_0} f(E_i, \beta) \overline{\psi}_i(r) \psi_i(r)$$

where $f(E_i, \beta)$ is the probability of finding an electron in the state ψ_i. Thermodynamics enter via the reciprocal temperature $\beta = 1/kT$, where k is the Boltzmann constant and T the temperature.

In order to achieve self–consistency we calculate $V_{\text{eff}}(r)$ as a function of $n(r)$. The most common way is by simply solving the Poisson equation (q is the (positive) unit charge):

$$(2.4) \qquad V_{\text{eff}}(r, \beta) = V_{\text{Coulomb}}(r) = -\frac{q}{4\pi} \int \frac{1}{|r - r'|} n(r') dr'.$$

3. Effective potential vs. occupation probabilities.

It is well known that electrons obey Fermi–Dirac $(F - D)$ statistics:

$$(3.1) \qquad f_{FD}(E_i, \beta) = \frac{1}{e^{\beta(E_i - F)} + 1}$$

and that Boltzmann statistics are the high temperature approximation of $F - D$ statistics:

$$(3.2) \qquad f_B(E_i, \beta) = Z e^{-\beta E_i}.$$

The "Fermi energy" F and the "partition function" Z are β–dependent normalization constants.

The choice of the statistics used in (2.3) cannot be regarded independently of the choice of the effective potential $V_{\text{eff}}(r)$. For consistency with the underlying antisymmetrized (Hartree–Fock) ansatz in the reduction of the many body problem, the use of $F - D$ statistics should be combined with the inclusion of an exchange–correlation term $V_{XC}(r)$.

This potential has the opposite sign of $V_{\text{Coulomb}}(r)$ and it takes into account the Pauli principle and the Coulomb repulsion of the electrons ("exchange–correlation hole").

A frequently used expression is given by the so-called $X\alpha$ exchange term:

$$(3.3) \qquad V_{XC}(r) = \alpha e^2 \left(\frac{3}{\pi}\right)^{\frac{1}{3}} (n(r))^{\frac{1}{3}}, \quad \alpha \in \left[\frac{2}{3}, 1\right].$$

It is a very good choice as long as no spin dependence is introduced. (For a discussion and more references, see [8], [9].)

On the other hand, the sole use of $V_{\text{Coulomb}}(r)$ linked with the use of Boltzmann statistics is consistent with a Hartree–ansatz for the many body wave function.

4. The Bloch-Poisson model.
Using Boltzmann statistics we can describe the system by the unnormalized density matrix [3]:

$$(4.1) \qquad \rho(r, s, \beta) = \sum_i e^{-\beta E_i} \overline{\psi}_i(r) \psi_i(s).$$

Differentiation with respect to β gives the Bloch equation [3], [4], [5], [6]:

$$(4.2) \qquad \rho_\beta(r, s, \beta) = -H_r \rho(r, s, \beta); \quad \beta \in (0, \beta^*]$$

$$(4.3) \qquad \rho(r, s, \beta = 0) = \delta(r - s)$$

with the Hamiltonian (2.2) acting on the r–variable only. β^* denotes the (fixed) temperature of the device. The electron density now reads

(4.4)
$$n(r) = \frac{\rho(r,r,\beta^*)}{\int \rho(y,y,\beta^*)dy}, \quad \beta^* \text{ fixed.}$$

According to our discussion in Section 3 we take the direct Coulomb term only as $V_{\text{eff}}(r)$:

(4.5)
$$\Delta V_{\text{eff}}(r) = \frac{q}{\varepsilon_s}(n(r) - C(r))$$

where ε_s is the permittivity and $C(r)$ is the doping profile of the considered semiconductor.

We remark that $\rho(\beta)$, described by the system (4.1)–(4.5) represents the density matrix in thermal equilibrium only for $\beta = \beta^*$, and $\rho(\beta)$ is just an auxiliary quantity for $\beta \neq \beta^*$. This situation contrasts the linear Bloch equation [3], [5], where $\rho(\beta)$ represents the correct density matrix for any temperature. Note that a direct coupling of the Bloch and the Poisson equation for all β is not correct, since the Hamiltonian would then be β–dependent via the potential, and additional terms in (4.2) occur.

5. Boundary conditions (BC) and mathematical analysis.

The Bloch–Poisson model has been analyzed with homogeneous Dirichlet BC and periodic BC on a bounded domain as well as for the whole space case [6], [10], [11].

Of course, other, more realistic boundary conditions are desirable (e.g. [12]), but one should be aware that due to the Fourier transformation in the Wigner–Weyl transformation, the equivalence of the Schrödinger and the Wigner picture gets lost.

In [5], [6], [10], [11] existence of a solution of the Bloch Poisson system has been proven using semigroup theory in Sobolev spaces with a negative index. Due to the specific coupling at $\beta = \beta^*$ uniqueness cannot be achieved by contraction arguments, but ([2]) using a monotonocity property of the charge density n according to the equilibrium potential V and a perturbation ΔV.

(5.1)
$$\int (n[V + \Delta V](r) - n[V](r))\Delta V(r)dr \geq 0.$$

It reflects the tendency of the electrons to occupy states of low (potential) energy ([13]).

6. Numerical ideas and classical limit.
In [6], [11] an iteration over the potential V was used: For given V_n the Bloch equation (4.2), (4.3) is solved for $\beta \in (0, \beta^*]$, the density (4.4) is evaluated for fixed $\beta = \beta^*$ and the Poisson equation (4.5) yields a new potential V_{n+1}. Since this mapping $V_{n+1} = F(V_n)$ is in general no contraction this iteration should be replaced by an underrelaxed fixed point iteration:

(6.1)
$$V_{n+1} = (1 - \omega)V_n + \omega F(V_n), \quad 0 < \omega < 1.$$

In [6] convergence of this algorithm (for ω sufficiently small) was proved based on the monotonocity property (5.1). As a first iterate for (6.1) we can use the potential V^0 of the according classical problem obtained by the limit $\hbar \to 0$ ([6], [11])

(6.3)
$$\Delta V^0 = \frac{\exp(\beta^* V^0(x))}{\int \exp(\beta^* V^0(y))dy} - C(x).$$

Note that the classical limit cannot be performed directly for the density matrix but for Wigner transformed quantities.

7. Generalized Bloch equation ($F - D$ statistics).

For Fermi–Dirac statistics (cp. [5]) the Bloch equation (4.2), (4.3) has to be replaced by:

$$(7.1) \qquad \rho(r,s,\beta^*) = \left(1 + e^{\beta^*(H_r - F)}\right)^{-1} \delta(r - s)$$

with the effective Hamilton operator (H_r acting on the r–variable) according to Section 3:

$$(7.2) \qquad H = -\tfrac{\hbar^2}{2m}\Delta_r + V_{\text{Coulomb}}(r) + V_{XC}(r).$$

The Fermi–energy results from the normalization

$$(7.3) \qquad \int \rho(r,r,\beta^*)dr = 1 \Rightarrow F.$$

Hence the charge density is given by

$$(7.4) \qquad n(r) = \rho(r,r,\beta^*).$$

The following fixed point iteration $\rho_k(r,s) \rightarrow \rho_{k+1}(r,s)$ allows for Bloch–type parabolic equations again [14] and requires no determination of the Fermi–energy F:

$$(7.5) \qquad n_k(r) = \rho_k(r,r)$$

$$(7.6) \qquad \Delta(V_{\text{Coulomb}}(r))_k = \tfrac{q}{\varepsilon_s}(n_k(r) - C(r)).$$

$$(7.7) \qquad \tilde{\rho}_{k+1}(r,s) = e^{-\beta^* \frac{1}{2}(H_r + H_s)}(\delta(r - s) - \rho_k(r,s)).$$

$$(7.8) \qquad \rho_{k+1}(r,s) = \frac{\tilde{\rho}_{k+1}(r,s)}{\int \tilde{\rho}_{k+1}(y,y)dy}.$$

Note that (7.7) has the form of the Bloch equation with a different initial condition. Again we have to use an underrelaxation iteration like (6.1) to assure convergence.

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