Numerical methods for Bloch-Poisson type equations

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Abstract
We present numerical methods for a rather new model to calculate quantum steady states of electrons in thermal equilibrium. The well known Bloch equation is generalized to arbitrary distribution functions (Fermi-Dirac) and appropriately coupled to the Poisson equation. A rational approximation of the distribution function yields an iterative algorithm.

I Introduction

We present and discuss algorithms to calculate quantum steady states of thermally equilibrated electrons in a semiconductor device. We consider a one–electron approximation with a self–consistent potential describing the Coulomb interaction of the electrons with each other and with the background of (positive) ions.

The most evident model is the Schrödinger-Poisson approach which has been widely used (see e.g [1], [2], [3], [4], [5]). However, the solution of the eigenvalue problem in an iterative loop is numerically rather expensive, such that it might be interesting to look for alternatives.

It is well known that under the assumption of Boltzmann statistics the steady state density matrix can be obtained from the so called Bloch equation (see e.g [6], [7], [8]). 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 ([8], [9]).

We present the generalization of the linear Bloch equation to a self-consistent model for arbitrary occupation probabilities. A rational approximation of the distribution function yields an iteration in the temperature variable, the position variable can be discretized e.g. by spectral methods. Due to the specific coupling to the Poisson equation Bloch-type equations give the steady state density matrix only for one, fixed temperature.

II Modeling

In the usual approach the state of the system is described by one–particle wave functions in some L^2–space (e.g. [1], [2], [3], [4], [5]). One has to calculate the eigenfunctions of the stationary Schrödinger equation

$$H\psi_i(r) = E_i\psi_i(r), \quad \|\psi_i\|_{L^2} = 1, \quad i \in N_0 \tag{II.1}$$

The Hamilton operator reads

$$H = -\frac{\hbar^2}{2m}\Delta + V(r) \tag{II.2}$$

with some local potential $V(r)$ taking into account the direct Coulomb interaction of the electrons. Additional terms like an applied external potential, heterojunction discontinuities, exchange-correlation terms etc. can be included without changing the algorithms. The (electron) density is given by

$$n(r) = \sum_{i \in N_0} f(E_i - F, \beta) \overline{\psi}_i(r) \psi_i(r) \tag{II.3}$$

where $f(E_i - F, \beta)$ 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 $V(r)$ as a function of $n(r)$ by simply solving the Poisson equation. Note that this direct coupling yields a β-dependence of all quantities.

For electrons we should use Fermi - Dirac (FD) statistics :

$$f_{FD}(E_i - F, \beta) = \frac{1}{e^{\beta(E_i - F)} + 1} \tag{II.4}$$

which are approximated by Boltzmann statistics for high temperatures (small β)

$$f_B(E_i - F, \beta) = e^{\beta(E_i - F)} = Z e^{-\beta E_i}. \tag{II.5}$$

The "Fermi energy F" and Z are (β-dependent) normalization constants :

$$\int n(x) dx = 1 \tag{II.6}$$

As an alternative to the Schrödinger–Poisson equation the (charge) density $n(x)$ for a given temperature β can be expressed using what we call "Bloch-ansatz" :

$$n(x) = Tr\ f(H - F \cdot id) \tag{II.7}$$

Here we mean "trace" in the following sense :

$$n(x) \ = \ \rho(r = x,\ s = x,\ \beta^*) \ \equiv \ \rho(x,\ x) \tag{II.8}$$

where $\rho(r,\ s,\ \beta^*)$ is the (normalised) density matrix, i.e. the integral kernel of the density operator $f(H - F \cdot id, \beta^*)$. We have

$$\rho(r,\ s,\ \beta^*) = f(H - F \cdot id,\ \beta^*) \delta(r - s) \tag{II.9}$$

or

$$\rho(r,\ s,\ \beta^*) = \sum_{j=1}^{\infty} f(E_j - F,\ \beta^*) \overline{\psi}_j(r) \psi_j(s) \tag{II.10}$$

which shows the equivalence of the Bloch-ansatz to the Schrödinger approach.

For the Boltzmann distribution (II.7) yields the "classical" Bloch equation [6] as an evolution equation (in β) for the unnormalized density matrix.

$$\frac{\partial}{\partial \beta} \rho(r, s, \beta) = -H_r \rho(r, s, \beta); \quad \beta \in (0, \beta^*] \tag{II.11}$$

where H_r means acting on the r varibable only.

(II.12) $$\rho(r,s,\beta=0)=\delta(r-s)$$

(II.13) $$n(r)=\frac{\rho(r,r,\beta^*)}{\int\rho(y,y,\beta^*)dy},\quad \beta^*\ fixed$$

We had to fix β^* since the coupling to the Poisson equation requires attention : A direct coupling for temperature dependent $n(x,\ \beta)\ :=\ \rho(x,\ x,\ \beta)$ yields a β-dependent Hamiltonian and the Bloch equation is not valid. Only $\rho(r,\ s,\ \beta^*)$ has a physical meaning for the selfconsistent Bloch equation ([8], [9]).

For other than the Boltzmann distribution no such parabolic evolution equations can be derived. However, we can still derive iterations for the density matrix without solving the eigenvalue problem (II.1), (II.2).

III Numerical methods

For the Boltzmann statistics case the following relaxed iteration for the potential has been proven to be convergent in [8] : For given V_k the Bloch equation (II.11), (II.12) is solved for $\beta\in(0,\beta^*]$, the density (II.13) is evaluated for fixed $\beta=\beta^*$ and the Poisson equation yields a potential $\tilde{V}_{k+1}$ which gives the new potential

(III.14) $$V_{k+1}\ (x)=(1-\omega)V_k\ (x)+\omega\tilde{V}_{k+1}\ (x),\quad \omega<1$$

For Fermi–Dirac statistics it is possible to use an analogous iteration which avoids the explicit calculation of the Fermi-level [10] :

(III.15) $$\rho_k\ (r,\ s,\ \beta)$$

$$\Downarrow$$

(III.16) $$n[\rho_k]\ (x)=\rho(x,\ x,\ \beta^*)$$

$$\Downarrow$$

(III.17) $$\Delta V_k[\rho_k]\ (x)\ =\ -n[\rho_k](x)$$
$$H_k[\rho_k]\ =\ -\Delta\ +\ V_k[\rho_k]$$

$$\Downarrow$$

(III.18) $$\frac{\partial}{\partial\beta}\tilde{\rho}=e^{-\beta\frac{1}{2}(H_r+H_s)},\quad \beta\in\ (0,\beta^*]$$

(III.19) $$\tilde{\rho}(\beta=0)=\delta(r-s)-\rho_k(r,\ s,\ \beta=0)$$

$$\Downarrow$$

(III.20) $$\rho_{k+1}(r,\ s,\beta)=\frac{\tilde{\rho}(r,\ s,\ \beta)}{\int\tilde{\rho}(y,\ y,\ \beta)dy}$$

Like in the Boltzmann case the iteration has to be appropriately underrelaxed to assure convergence. Underrelaxed iterations have been used for the Schrödinger –Poisson equation ([4], [5]).

However, the numerical results of Nier [4] show that the optimal underrelaxation parameter ω depends heavily on the Debye length λ_d of the considered device and that ω has to be extremely small for realistic values of λ_D. On the other hand, the iteration (III.15) - (III.20) applies only for F-D statistics as given by (II.4), which looks different for the 2-D case (see e.g. [1]).

The method we propose is based on a rational (Padé)-approximation of an arbitrary distribution function $f(\beta(E_i - F))$:

$$f(z) \simeq \tilde{f}(z) = \prod_{\ell=1}^{N} \frac{a_\ell z + b_\ell}{z + c_\ell} \tag{III.21}$$

To understand the idea we take the Boltzmann case $f(z) = e^{-\beta z}$ and solve the Bloch equation (II.11), (II.12) with an implicit Euler-scheme :

$$(I + \Delta\beta H_r)\rho_{\ell+1} = \rho_\ell, \quad k = 0, \ldots, N-1, \quad N \cdot \Delta\beta = \beta^* \tag{III.22}$$

$$\rho_0 = \delta(r - s) \tag{III.23}$$

Hence we see that the numerical iteration corresponds to the approximation

$$f(z) = e^{-\beta^* z} \simeq (1 + \frac{\beta^*}{N} z)^{-N} = \tilde{f}(z) = \prod_{\ell=1}^{N} \frac{\frac{N}{\beta^*}}{z + \frac{N}{\beta^*}} \tag{III.24}$$

In general we have

$$\tilde{f}(\beta^*(H - F)) = \prod_{\ell=1}^{N} (H - F \cdot id + c_\ell \cdot id)^{-1}(a_\ell H - a_\ell F \cdot id + b_\ell) \tag{III.25}$$

where β^* is contained in the coeffizients a_ℓ, b_ℓ, c_ℓ which have to be determined once from the (Padé) - approximation.

Hence we use the following iteration for the potential V and the Fermi-level F:

$$V_k(x),\ F_k \quad (F_{k-1}) \tag{III.26}$$

$$\Downarrow$$

$$H_k = -\Delta + V_k$$

$$(a_\ell H_k - a_\ell F_k \cdot id + b_\ell)(H_k - F_k \cdot id + c_\ell \cdot id)^{-1} z_{\ell+1} = z_\ell, \quad \ell = 0, \ldots, N-1 \tag{III.27}$$

$$z_0 = \delta(r - s) \tag{III.28}$$

$$\rho_k[V_k,\ F_k](r,\ s,\ \beta^*) := z_{N-1}(r, s) \tag{III.29}$$

$$\Downarrow$$

$$n_k[V_k,\ F_k]\,(x) = \rho_k(x,\ x, \beta^*) \tag{III.30}$$

$$\Downarrow$$

$$C_k[V_k,\ F_k] := \int n_k[V_k,\ F_k](x)dx \tag{III.31}$$

$$\Downarrow$$

(III.32) $V_{k+1}(x)$ *solving* $-\Delta V_{k+1}(x) = \dfrac{n_k[V_k, F_k](x)}{C_k[V_k, F_k]}$

$$\Downarrow$$

(III.33) F_{k+1} *is given implicitly by the normalization* (II.6)

A secant scheme using C_k and also F_{k-1}, C_{k-1} gives :

(III.34) $$F_{k+1} = F_k - (C_k - 1)\frac{F_k - F_{k-1}}{C_k - C_{k-1}}$$

Note that in general the iteration (III.26)–(III.33) does not correspond to any differential equation like the Bloch equation for Boltzmann statistics.

The above iteration has been tested for a 1-D model. The discretization in x has been done both with finite differences on an equidistant grid and with a spectral collocation method using trigonometric basic functions. Homogenous Dirichlet boundary conditions have been used.

First results have shown a good convergence with a moderate number (below 10) of iterates. Indeed, the Padé-approximation with $N = 6$ is basically indistinguishable from the exact FD-distribution. The implementation of a 2-D code using the spectral method is ongoing.

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