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Time dependent transport in 1D micro- and nanostructures: solving the Boltzmann and Wigner–Boltzmann equations

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Abstract. For many decades the Boltzmann distribution function has been used to calculate the non-equilibrium properties of mobile particles undergoing the combined action of various scattering mechanisms and externally applied force fields. When the latter give rise to the occurrence of inhomogeneous potential profiles across the region through which the particles are moving, the numerical solution of the Boltzmann equation becomes a highly complicated task. In this work we highlight a particular algorithm that can be used to solve the time dependent Boltzmann equation as well as its quantum mechanical extension, the Wigner–Boltzmann equation. As an illustration, we show the calculated distribution function describing electrons propagating under the action of both a uniform and a pronouncedly non-uniform electric field.

1. Introduction

In this paper we propose the method of characteristic curves as an alternative approach to solve the time dependent Boltzmann equation and other kinetic equations with a similar kernel structure, such as the Wigner–Boltzmann equation. In section 2 we briefly outline the corresponding algorithm which is thoroughly described in [1]. In section 3, we illustrate and discuss how the algorithm can be exploited most conveniently to calculate the Boltzmann distribution function for an electron gas moving in two different force field profiles, whereas section 4 provides the conclusions.

2. Characteristic curves of the Boltzmann equation

Consider an ensemble of mobile, charged particles with band mass m moving through a force field $\mathbf{F}(\mathbf{r})$. Providing a classical tool to quantify the probability of finding a particle with momentum \mathbf{p} at a position \mathbf{r} at an arbitrary time instant $t > 0$, the Boltzmann distribution function $f(\mathbf{r}, \mathbf{p}, t)$ satisfies the time-dependent Boltzmann transport equation (BTE)

$$\frac{\partial f(\mathbf{r}, \mathbf{p}, t)}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f(\mathbf{r}, \mathbf{p}, t) + \mathbf{F}(\mathbf{r}) \cdot \nabla_{\mathbf{p}} f(\mathbf{r}, \mathbf{p}, t) = Q_B[f(\mathbf{r}, \mathbf{p}, t)]. \quad (1)$$

Appearing as a functional of $f(\mathbf{r}, \mathbf{p}, t)$, the Boltzmann collision integral $Q_B[f(\mathbf{r}, \mathbf{p}, t)]$ incorporates the transition probabilities associated with all relevant, microscopic scattering

mechanisms that may affect the particle flow. A straightforward algorithm providing an iterative, numerical solution of Eq. (1) can be constructed by observing that the classical trajectories $\mathbf{R}(s)$ and $\mathbf{P}(s)$, traversed by a particle in phase space between the time instants $s = -t$ and $s = 0$ are in fact the characteristic curves of the BTE. Indeed, inserting Newton's equations

$$\frac{d\mathbf{R}(s)}{ds} = \frac{\mathbf{P}(s)}{m}, \quad \frac{d\mathbf{P}(s)}{ds} = \mathbf{F}[\mathbf{R}(s)], \quad (2)$$

together with the function $T(s) = t + s$ into Eq. (1), we may turn the left-hand side of the latter into a complete differential, reduce the BTE to an ordinary differential equation and integrate it formally while interpreting \mathbf{r} and \mathbf{p} as “initial” position and momentum,

$$f(\mathbf{r}, \mathbf{p}, t) = f_0(\mathbf{R}(-t), \mathbf{P}(-t)) + \int_0^t ds Q_B[f(\mathbf{R}(s-t), \mathbf{P}(s-t), s)], \quad (3)$$

where we need to specify the initial distribution function $f_0(\mathbf{r}, \mathbf{p})$. Requiring merely the history of the distribution function during the time interval $[-t, 0]$, Eq. (3) can easily be recast in a forward step algorithm

$$f(\mathbf{r}, \mathbf{p}, t_n) = f(\mathbf{R}(-\Delta t), \mathbf{P}(-\Delta t), t_{n-1}) + \Delta t Q_B[f(\mathbf{R}(-\Delta t), \mathbf{P}(-\Delta t), t_{n-1})], \quad (4)$$

by choosing an equidistant time grid $t_n = n\Delta t$, $n = 0, 1, 2, \dots, N$. The time step Δt should be small compared with the system's characteristic times such as dwell times, scattering times etc., whereas t_N represents the numerical onset of the steady state (if any), i.e. the time at which $f(\mathbf{r}, \mathbf{p}, t_N)$ does not appreciably differ from its previous values.

Though being devised originally to tackle the BTE, one may as well use the algorithm defined in Eq. (4) to investigate the Wigner–Boltzmann distribution function $f_W(\mathbf{R}, \mathbf{p}, t)$ obeying the Wigner–Boltzmann transport equation (WBTE) [1, 5, 6, 7]

$$\frac{\partial f_W(\mathbf{R}, \mathbf{p}, t)}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{R}} f_W(\mathbf{R}, \mathbf{p}, t) = Q_B[f_W(\mathbf{R}, \mathbf{p}, t)] + Q_W[f_W(\mathbf{R}, \mathbf{p}, t)] \quad (5)$$

that may be considered a pragmatic quantum mechanical extension of the BTE where \mathbf{r} is replaced with \mathbf{R} , the so-called “center-of-mass” coordinate. As such, it borrows the Boltzmann collision integral Q_B from the BTE to include decoherent scattering processes while non-locality effects are described by the Wigner kernel

$$W(\mathbf{R}, \mathbf{p}) = -\frac{i}{\hbar} \int d^3x \left[U\left(\mathbf{R} + \frac{\mathbf{x}}{2}\right) - U\left(\mathbf{R} - \frac{\mathbf{x}}{2}\right) \right] \exp\left(-\frac{i\mathbf{p} \cdot \mathbf{x}}{\hbar}\right). \quad (6)$$

Entering the Wigner collision term

$$Q_W[f_W(\mathbf{R}, \mathbf{p}, t)] = \int \frac{d^3p'}{(2\pi\hbar)^3} f(\mathbf{R}, \mathbf{p}', t) W(\mathbf{R}, \mathbf{p} - \mathbf{p}'), \quad (7)$$

the kernel $W(\mathbf{R}, \mathbf{p})$ accumulates all non-local contributions arising from the potential energy function $U(\mathbf{r})$ which is related to the force field by $\mathbf{F}(\mathbf{r}) = -\nabla U(\mathbf{r})$. In contrast to earlier works [5, 7] relying as well on classical paths to solve the WBTE, we follow an alternative approach and rewrite the WBTE such that its left-hand side is identical to that of the BTE. Accordingly, the right-hand side consists of an effective collision term, given by

$$Q[f_W(\mathbf{R}, \mathbf{p}, t)] = Q_B[f_W(\mathbf{R}, \mathbf{p}, t)] + Q_W[f_W(\mathbf{R}, \mathbf{p}, t)] + \mathbf{F}(\mathbf{R}) \cdot \nabla_{\mathbf{p}} f_W(\mathbf{R}, \mathbf{p}, t), \quad (8)$$

with $\mathbf{F}(\mathbf{R}) = -\nabla_{\mathbf{R}} U(\mathbf{R})$. In spite of its internal complexity $Q_W[f_W]$ shares at least one feature with its classical counterpart $Q_B[f_W]$, namely the mere dependence on times prior to the time instant t appearing in the left-hand side of the WBTE. Consequently, the forward step algorithm introduced in Eq. (4) can be usefully invoked to solve the time dependent WBTE as well.

3. Examples

As an illustration, we calculate the distribution function of electrons moving through a simple semiconductor device.

3.1. *n-i-n diode*

First, we consider an intrinsic semiconductor layer being sandwiched between two n^+ -doped reservoirs to form a n-i-n diode. For the sake of simplicity, we treat this structure as a 1D device with density and field profiles merely depending on the z coordinate and we discard any inelastic scattering events ($Q_B = 0$). On the other hand, as the force field $F(z)$ turns out to be strongly localized inside the intrinsic region and the adjacent junction areas, it proves convenient to rephrase the Wigner collision integral in terms of the Fourier transform $\tilde{F}(k)$ of the force field:

$$Q_W(Z, p, t) = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dk \tilde{F}(2k) e^{2ikZ} \cdot \frac{f(Z, p - \hbar k, t) - f(Z, p + \hbar k, t)}{k}. \quad (9)$$

Starting from an initial distribution with an empty intrinsic region, we reach a steady state after about 300 time steps. The corresponding distribution function revealing the particle diffusion into the central layer is shown in Fig. (1).

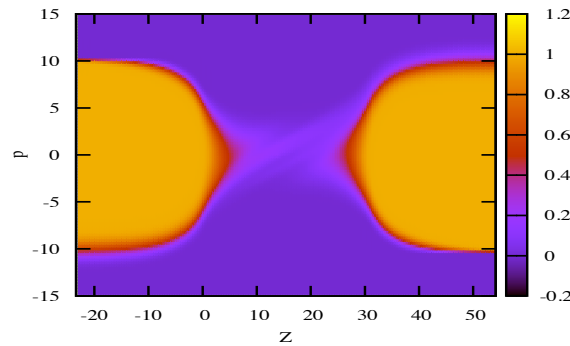


Figure 1. Wigner-Boltzmann distribution for a n-i-n diode after 300 time steps. The intrinsic region extends along the interval $0 \leq Z \leq 31.1$. All quantities are expressed in atomic units.

3.2. *Polaron scattering*

Next, we consider an electron gas moving in a bulk, polar semiconductor and being driven by a uniform electric field F applied along the z -direction. Consequently, the Wigner kernel reduces to the Boltzmann force term with $f(\mathbf{r}, \mathbf{p}, t) = f(p_z, p_\perp, t)$ and $p_\perp \equiv \sqrt{p_x^2 + p_y^2}$, while Q_B describes the interaction of the electrons with longitudinal optical (LO) phonons having a dispersion free energy $\hbar\omega_{LO}$ [9] or an equivalent temperature $\Theta = \hbar\omega_{LO}/k_B$. Given the lattice temperature T , the corresponding transition probabilities read

$$\Pi(\mathbf{p} \rightarrow \mathbf{p}') = \frac{1}{|\mathbf{p} - \mathbf{p}'|^2} \left[A_e \delta\left(\frac{p^2}{2} - \frac{p'^2}{2} - 1\right) + A_a \delta\left(\frac{p^2}{2} - \frac{p'^2}{2} + 1\right) \right], \quad (10)$$

where the absorption(emission) coefficients $A_a(A_e)$ are proportional to the Fröhlich coupling constant α ,

$$A_e = \frac{\alpha}{\pi\sqrt{2}}(1 + \nu), \quad A_a = \frac{\alpha}{\pi\sqrt{2}}\nu, \quad \nu = \frac{1}{e^{\Theta/T} - 1}, \quad (11)$$

and all quantities are expressed in polaronic units ($\hbar = m = \omega_{LO} = 1$). Fig. (2) compares the

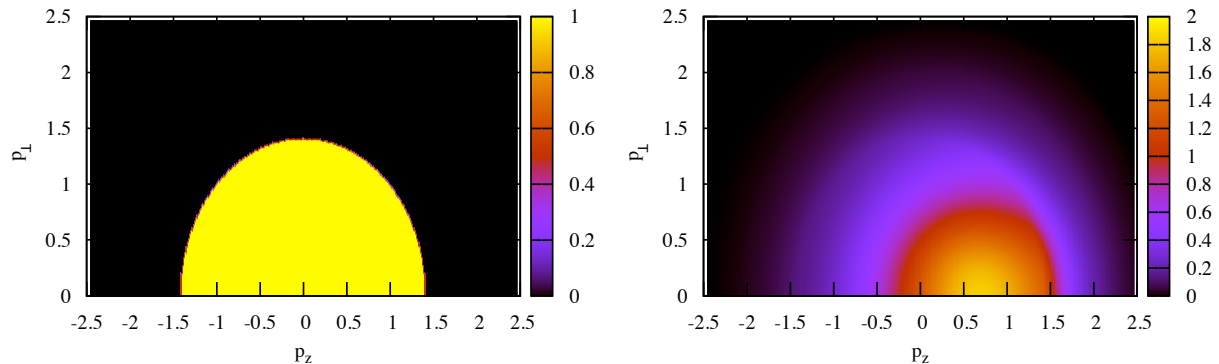


Figure 2. Polaron distribution function in equilibrium (left) and in the presence of a uniform electric field after 500 time steps (right). The following parameters have been used: $A_a = 0.2$, $A_e = 1.0$ and $F = 1.0$. All quantities are expressed in polaronic units ($\hbar = m = \omega_{LO} = 1$).

initial distribution $f_0(\mathbf{p})$ with the steady-state distribution attained after 500 time steps. The former describes a configuration with all electrons gathering inside the sphere $|\mathbf{p}| = \sqrt{2}$ while the latter develops an sharp maximum shifting to positive p_z -values due to the action of the uniform electric field. It should be noted that the same steady state distribution is found when $f_0(\mathbf{p})$ is chosen otherwise, e.g. a simple Maxwellian.

4. Conclusion

The characteristic curves method provides a natural computational framework to evaluate the time-dependent Wigner and Wigner–Boltzmann distribution functions. Accordingly, only an initial distribution function needs to be specified and no artificial boundary conditions directly impinging on the steady state (such as fixing the chemical potentials of the contacts) need to be imposed.

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