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Some properties of the kinetic equation for electron transport in semiconductors

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Abstract

The paper studies the kinetic equation for electron transport in semiconductors. New formulas for the heat generation rate are derived by analyzing the basic scattering mechanisms. In addition, properties of the steady state distribution are discussed and possible extensions of the deviational particle Monte Carlo method to the area of electron transport are proposed.

Contents

1 Introduction

Kinetic theory is a common tool for modelling charge transport in semiconductors ([6, 10, 8]). The continued miniaturization of semiconductor devices leads to new challenges related to heat generation ([20, 12, 11, 16]). The direct simulation Monte Carlo (DSMC) method for the Boltzmann transport equation has been extended to cover the generation and distribution of heat in the device. The lattice heating rate is calculated on the basis of the exchange of phonons between the electrons and the lattice (see [19, 22, 13] and references therein).

The purpose of this paper is to contribute to the study of heat generation in semiconductor devices. New formulas for the heat generation rate are derived from the kinetic equation by analyzing the scattering mechanisms. In addition, some ideas for improving the existing stochastic algorithms are proposed. The paper is organized as follows. In Section 2 the basic kinetic equation is introduced. The underlying stochastic model is described in Section 3. Formulas for the heat generation rate are derived in Section 4. Finally, Section 5 contains comments concerning the Maxwellian steady state distribution and possible extensions of the deviational particle Monte Carlo method to the area of electron transport.

2 Kinetic equation

The kinetic equation

$$\left[\frac{\partial}{\partial t} + v(k)\cdot\nabla_x - \frac{q}{\hbar}\,E(t,x)\cdot\nabla_k\right] f(t,x,k) = (Q\,f)(t,x,k)\,, \tag{2.1}$$

is used to study electron transport in semiconductors ([6, 4, 8]). It determines the time evolution of the distribution $f(t,x,k)$ of electrons with respect to position $x \in D \subset \mathbb{R}^3$ (Euclidean space) and wave-vector $k \in \mathbb{R}^3$. The velocity $v(k)$ is defined as

$$v(k) = \frac{1}{\hbar}\,\nabla_k\,\varepsilon(k)\,, \tag{2.2}$$

where $\varepsilon(k)$ is the kinetic energy of an electron with wave-vector k . The electric field E depends on the electron distribution function f . It is defined as

$$E(t,x) = -\nabla_x\Phi(t,x)\,, \tag{2.3}$$

where the electric potential Φ satisfies the Poisson equation

$$\epsilon\,\Delta_x\Phi(t,x) = q\,[n(t,x) - n_D(x)]\,. \tag{2.4}$$

The function

$$n(t,x) = \int_{\mathbb{R}^3} f(t,x,k)\,dk \tag{2.5}$$

is the electron density and n_D denotes the donor density. Moreover, q is the absolute value of the electron charge, ϵ is the permittivity and $\hbar$ denotes Planck's constant divided by 2π . Boundary conditions will not be used in this paper.

The scattering collision operator has the form

$$(Q\,f)(t,x,k) = \int_{\mathbb{R}^3} S(k',k)\,f(t,x,k')\,dk' - f(t,x,k)\int_{\mathbb{R}^3} S(k,k')\,dk'\,. \tag{2.6}$$

The transition rate from a state k to a state k' is determined by the function

$$\begin{aligned} S(k,k') = {} & K_0\,\delta(\varepsilon(k')-\varepsilon(k)) + \\ & \sum_{i=1}^{6} K_i\Big[\delta(\varepsilon(k')-\varepsilon(k)+\hbar\omega_i)\,(\kappa_i+1)+\delta(\varepsilon(k')-\varepsilon(k)-\hbar\omega_i)\,\kappa_i\Big]. \end{aligned} \tag{2.7}$$

The coefficients K_0, K_i are physical constants and $\hbar\omega_i$ is the energy of a phonon with frequency ω_i . The function (2.7) represents the main scattering mechanisms in silicon, at room temperature, which are due to several electron-phonon interactions (see [7, Section III.D.1], [6, Section 2.2.5] for more details). Finally, the quantities

$$\kappa_i = \frac{1}{\exp\left(\frac{\hbar\omega_i}{k_B\,T_L}\right)-1} \tag{2.8}$$

are phonon occupation numbers, where k_B is Boltzmann's constant and T_L is the lattice temperature.

We assume that the kinetic energy $\varepsilon(k)$ of an electron with wave-vector k has the form

$$\varepsilon(k) = g(|k|)\,, \tag{2.9}$$

where g is a strictly increasing and differentiable mapping of $[0,\infty)$ onto itself. It follows from (2.2) and (2.9) that

$$v(k) = \frac{g'(|k|)}{\hbar\,|k|}\,k\,. \tag{2.10}$$

Property (2.9) is fulfilled under the common assumption of analytic bands in the quasi-parabolic approximation. In this case, $\varepsilon(k)$ is determined by the relation

$$\varepsilon(k)\,[1+\alpha\,\varepsilon(k)] = \frac{\hbar^2|k|^2}{2m^*}\,, \tag{2.11}$$

where $\alpha \geq 0$ denotes the non-parabolicity factor and m^* is the effective electron mass. If $\alpha > 0$, then (2.11) implies

$$\varepsilon(k) = \frac{\sqrt{1+\frac{2\alpha\hbar^2|k|^2}{m^*}}-1}{2\alpha} \tag{2.12}$$

and (2.10) takes the form

$$v(k) = \frac{\hbar k}{m^*\sqrt{1+\frac{2\alpha\hbar^2|k|^2}{m^*}}} = \frac{\hbar k}{m^*[1+2\alpha\varepsilon(k)]}\,.$$

In the case $\alpha = 0$, which is called parabolic, one obtains

$$\varepsilon(k) = \frac{\hbar^2|k|^2}{2m^*} \qquad \text{and} \qquad v(k) = \frac{\hbar k}{m^*}\,. \tag{2.13}$$

3 Stochastic model

A common technique for the numerical treatment of equation (2.1) is the Monte Carlo method ([7, 6, 4]). This approach is based on a system of stochastic particles that mimic the time evolution of electrons. Their behaviour is determined by the electric field and the scattering mechanisms. A time step Δt is used to decouple the transport equation (2.1) and the Poisson equation (2.4). That is, each particle moves with its velocity (2.2), is accelerated according to a fixed electric field $\hat{E}(x)$ and performs scattering collisions according to the transition rate function (2.7). After Δt , the density (2.5) is measured and the field is re-calculated according to (2.3), (2.4).

For a fixed electric field $\hat{E}(x)$, equation (2.1) is a version of Kolmogorov's forward equation

$$\frac{\partial}{\partial t} f(t,x,k) = (A^* f)(t,x,k) \,, \tag{3.1}$$

with

$$(A^* f)(t,x,k) = \Big[-v(k)\cdot\nabla_x + \frac{q}{\hbar}\,\hat{E}(x)\cdot\nabla_k\Big]\, f(t,x,k) + (Q\,f)(t,x,k) \,,$$

where A^* denotes the adjoint operator. The generator A of the corresponding Markov process is (cf. [2])

$$(A\varphi)(x,k) = \Big[v(k)\cdot\nabla_x - \frac{q}{\hbar}\,\hat{E}(x)\cdot\nabla_k\Big]\,\varphi(x,k) + \int_{\mathbb{R}^3} S(k,k')\,[\varphi(x,k')-\varphi(x,k)]\,dk' \,, \tag{3.2}$$

where φ is a sufficiently smooth test function. The weak form of equation (3.1),

$$\frac{d}{dt}\int_D\int_{\mathbb{R}^3} \varphi(x,k)\,f(t,x,k)\,dk\,dx = \int_D\int_{\mathbb{R}^3} (A\varphi)(x,k)\,f(t,x,k)\,dk\,dx \,, \tag{3.3}$$

is called Dynkin's formula. Boundary conditions are taken into account via restrictions on the class of test functions.

The generator (3.2) determines a piecewise deterministic Markov process $(x(t),k(t))$ in the sense of [2]. Its time evolution is as follows.

- During the *free flight*, the particle moves according to Newton's equations of motion,

  $$\frac{d}{dt}\,x(t) = v(k(t)) \,, \qquad \frac{d}{dt}\,k(t) = -\frac{q}{\hbar}\,\hat{E}(x(t)) \,. \tag{3.4}$$

  Equations (3.4) are solved with a numerical scheme up to the next scattering time, or up to Δt , if no scattering occurs. Note that $v(k)$ is given in (2.10).

- The distribution function of the random *scattering time* τ is

  $$\text{Prob}(\tau < s) \;=\; 1-\exp\left(-\int_0^s \lambda(k(t))\,dt\right), \qquad s>0\,, \tag{3.5}$$

  where

  $$\lambda(k) = \int_{\mathbb{R}^3} S(k,k')\,dk' \tag{3.6}$$

denotes the total scattering rate. With probability

$$\text{Prob}(\tau \geq \Delta t) \quad = \quad \exp\left(-\int_0^{\Delta t} \lambda(k(t))\, dt\right),$$

the particle does not scatter during the time interval $[0, \Delta t]$. Various acceptance-rejection techniques have been introduced to increase the efficiency of this step (see the survey in [14]).

- If $\tau < \Delta t$, then a *scattering mechanism* is chosen randomly, according to its relative probability, and a new state k' is generated from the differential cross section of this mechanism. Details of this step will be given in the next section.

4 Heat generation

In this section we study the problem of heat generation. First a detailed description of the scattering mechanisms is provided. Then the notion of the heat generation rate is introduced. Finally, some properties of this quantity are established.

4.1 Scattering mechanisms

The transition rate function (2.7) has a probabilistic interpretation in terms of random jumps determined by various scattering mechanisms. It takes the form

$$S(k,k') = S_0(k,k') + \sum_{i=1}^{6} \Big[S_i^+(k,k') + S_i^-(k,k')\Big], \tag{4.1}$$

where

$$S_0(k,k') = K_0\, \delta(\varepsilon(k') - \varepsilon(k))\,, \tag{4.2}$$

$$S_i^+(k,k') = K_i\, \delta(\varepsilon(k') - \varepsilon(k) + \hbar\omega_i)\,(\kappa_i + 1) \tag{4.3}$$

and

$$S_i^-(k,k') = K_i\, \delta(\varepsilon(k') - \varepsilon(k) - \hbar\omega_i)\,\kappa_i\,. \tag{4.4}$$

The transition rate function (4.2) corresponds to elastic (acoustic) scattering, which means that the electron just gets a new orientation, while its energy is preserved. The transition rate functions (4.3), (4.4) correspond to inelastic (optical) scattering, which means that the electron either looses energy (interpreted as emission of a phonon, sign "$+$") or gains energy (interpreted as absorption of a phonon, sign "$-$") and gets a new orientation. The quantities $\hbar\omega_i$ are phonon energies. Emission of a phonon is only possible if $\varepsilon(k) > \hbar\omega_i$, otherwise the electron does not have enough energy. Relative frequencies of various scattering events are determined by the corresponding rates

$$\frac{\lambda_0(k)}{\lambda(k)}\,, \qquad \frac{\lambda_i^{\pm}(k)}{\lambda(k)}\,, \qquad i=1,\ldots,6\,, \tag{4.5}$$

where

$$\lambda_0(k)=\int_{\mathbb{R}^3} S_0(k,k')\,dk'\,, \qquad \lambda_i^{\pm}(k)=\int_{\mathbb{R}^3} S_i^{\pm}(k,k')\,dk' \tag{4.6}$$

and λ is defined in (3.6).

4.2 Heat generation rate

The sum over all phonon emission minus phonon absorption events per unit time (multiplied with the corresponding phonon energies) was used in the electrothermal Monte Carlo method (cf. [19, 20, 22]) as an approximation to the rate of heat generation. It was shown in [13] that a better (in the sense of lower variance) estimate of the heat generation rate is obtained by calculating the functional

$$H(t,x)=\int_{\mathbb{R}^3} G(k)\,f(t,x,k)\,dk\,, \tag{4.7}$$

where

$$G(k)=\sum_{i=1}^{6}\hbar\omega_i\,[\lambda_i^{+}(k)-\lambda_i^{-}(k)]\,. \tag{4.8}$$

Here we derive a result concerning the heat generation rate in the spatially homogeneous (bulk) case. Equation (2.1) takes the form

$$\left[\frac{\partial}{\partial t}-\frac{q}{\hbar}\,\hat{E}\cdot\nabla_k\right] f(t,k)=(Q\,f)(t,k)\,. \tag{4.9}$$

In this situation, the electric field E is independent of f . It is determined by an external field $\hat{E}$, which does not depend on t .

Theorem 4.1 *Assume (2.9). Let $f(\infty,k)$ be any steady state solution of equation (4.9). Then*

$$\int_{\mathbb{R}^3} G(k)\,f(\infty,k)\,dk \;=\; -q\,\hat{E}\cdot\int_{\mathbb{R}^3} v(k)\,f(\infty,k)\,dk\,. \tag{4.10}$$

In the parabolic case (2.13), the function f satisfies

$$\int_{\mathbb{R}^3} v(k)\,\lambda(k)\,f(\infty,k)\,dk=-\frac{q}{m^*}\,\hat{E}\int_{\mathbb{R}^3} f(\infty,k)\,dk\,. \tag{4.11}$$

According to (4.10), one obtains

$$H(\infty) := \int_{\mathbb{R}^3} G(k)\, f(\infty,k)\, dk = 0\,, \qquad \text{if} \quad \hat{E} = 0\,. \tag{4.12}$$

Moreover, relation (4.10) implies

$$H(\infty) > 0\,, \qquad \text{if} \quad \hat{E} \neq 0\,, \tag{4.13}$$

since the average velocity and $-\hat{E}$ are parallel. This property is a (heuristic) consequence of the probabilistic description of the trajectory of an electron. Indeed, in the jump moments, the orientation of k is uniform, according to (4.2)–(4.4). Between the jump moments, there is a drift into the direction $-\hat{E}$, according to (3.4). Thus, in the steady state, the average wave-vector and, according to (2.10), the mean velocity are proportional to $-\hat{E}$. A related property is (4.11).

4.3 Proof

The proof of (4.10) is based on the following lemma.

Lemma 4.2 *Assume (2.9) and denote*

$$J(y) = \frac{[g^{-1}(y)]^2}{g'(g^{-1}(y))}\,. \tag{4.14}$$

Let F be any continuous function on $[0,\infty)$. Then

$$\begin{aligned} &\int_{\mathbb{R}^3} \delta(\varepsilon(k)-\varepsilon(k'))\, F(\varepsilon(k'))\, dk' = \\ &\qquad 4\pi\, F(\varepsilon(k))\, J(\varepsilon(k)) = F(\varepsilon(k)) \int_{\mathbb{R}^3} \delta(\varepsilon(k')-\varepsilon(k))\, dk'\,, \end{aligned} \tag{4.15}$$

$$\begin{aligned} &\int_{\mathbb{R}^3} \delta(\varepsilon(k)-\varepsilon(k')+\hbar\omega_i)\, F(\varepsilon(k'))\, dk' = \\ &\qquad 4\pi\, F(\varepsilon(k)+\hbar\omega_i)\, J(\varepsilon(k)+\hbar\omega_i) \\ &\quad = \quad F(\varepsilon(k)+\hbar\omega_i) \int_{\mathbb{R}^3} \delta(\varepsilon(k')-\varepsilon(k)-\hbar\omega_i)\, dk' \end{aligned} \tag{4.16}$$

and

$$\begin{aligned} &\int_{\mathbb{R}^3} \delta(\varepsilon(k)-\varepsilon(k')-\hbar\omega_i)\, F(\varepsilon(k')\, dk' = \\ &\qquad 4\pi\, F(\varepsilon(k)-\hbar\omega_i)\, J(\varepsilon(k)-\hbar\omega_i)\, 1_{(0,\infty)}(\varepsilon(k)-\hbar\omega_i) \\ &\quad = \quad F(\varepsilon(k)-\hbar\omega_i) \int_{\mathbb{R}^3} \delta(\varepsilon(k')-\varepsilon(k)+\hbar\omega_i)\, dk'\,. \end{aligned} \tag{4.17}$$

The notation $1_{(0,\infty)}(x)$ is used for the step function taking the values 1, for $x > 0$, and 0, otherwise.

Proof. Consider the substitution $g(r) = y$ so that

$$g'(r)\,dr = dy \qquad \text{and} \qquad r = g^{-1}(y)\,. \tag{4.18}$$

Using spherical coordinates, one obtains (for any $a \neq 0$ and $b \in \mathbb{R}$)

$$\int_{\mathbb{R}^3} \delta(a\,\varepsilon(k) + b)\, F(\varepsilon(k))\, dk =$$
$$4\pi \int_0^\infty \delta(a\,g(r) + b)\, F(g(r))\, r^2\, dr = 4\pi \int_0^\infty \delta(a\,y + b)\, F(y)\, J(y)\, dy$$

and

$$\int_{\mathbb{R}^3} \delta(\varepsilon(k) - b)\, F(\varepsilon(k))\, dk = \int_{\mathbb{R}^3} \delta(-\varepsilon(k) + b)\, F(\varepsilon(k))\, dk = 4\pi\, F(b)\, J(b)\, 1_{(0,\infty)}(b)$$

so that the assertions (4.15)–(4.17) follow. ■

According to Lemma 4.2, one obtains (cf. (4.1)–(4.4), (4.6), (4.8))

$$\int_{\mathbb{R}^3} S(k,k')\,[\varepsilon(k') - \varepsilon(k)]\, dk' =$$
$$\sum_{i=1}^{6} K_i \Bigg[(\kappa_i + 1) \int_{\mathbb{R}^3} \delta(\varepsilon(k') - \varepsilon(k) + \hbar\omega_i)\,[\varepsilon(k') - \varepsilon(k)]\, dk' +$$
$$\kappa_i \int_{\mathbb{R}^3} \delta(\varepsilon(k') - \varepsilon(k) - \hbar\omega_i)\,[\varepsilon(k') - \varepsilon(k)]\, dk'\Bigg]$$
$$= \sum_{i=1}^{6} K_i \Bigg[(\kappa_i + 1)\,(-\hbar\,\omega_i) \int_{\mathbb{R}^3} \delta(\varepsilon(k') - \varepsilon(k) + \hbar\omega_i)\, dk' +$$
$$\kappa_i\,\hbar\,\omega_i \int_{\mathbb{R}^3} \delta(\varepsilon(k') - \varepsilon(k) - \hbar\omega_i)\, dk'\Bigg]$$
$$= \sum_{i=1}^{6} \Bigg[(-\hbar\,\omega_i) \int_{\mathbb{R}^3} S_i^+(k,k')\, dk' + \hbar\,\omega_i \int_{\mathbb{R}^3} S_i^-(k,k')\, dk'\Bigg]$$
$$= \sum_{i=1}^{6} \hbar\,\omega_i \Big[\lambda_i^-(k) - \lambda_i^+(k)\Big] = -G(k)\,. \tag{4.19}$$

In terms of the probabilistic interpretation of the scattering mechanisms given in Section 4.1, property (4.19) is related to the expected jump size.

In the spatially homogeneous case, equation (3.3) takes the form

$$\frac{d}{dt} \int_{\mathbb{R}^3} \varphi(k)\, f(t,k)\, dk = \tag{4.20}$$
$$\int_{\mathbb{R}^3} \Bigg[-\frac{q}{\hbar}\,(\hat{E} \cdot \nabla_k)\,\varphi(k) + \int_{\mathbb{R}^3} S(k,k')\,[\varphi(k') - \varphi(k)]\, dk'\Bigg] f(t,k)\, dk\,.$$

With $\varphi(k) = \varepsilon(k)$, equation (4.20) implies (cf. (2.2), (4.19))

$$\frac{d}{dt} \int_{\mathbb{R}^3} \varepsilon(k)\, f(t,k)\, dk = -q\,\hat{E} \cdot \int_{\mathbb{R}^3} v(k)\, f(t,k)\, dk - \int_{\mathbb{R}^3} G(k)\, f(t,k)\, dk \tag{4.21}$$

so that (4.10) follows.

Next we prove (4.11). According to (2.7), (2.9) and (2.10), one obtains (using spherical coordinates)

$$\int_{\mathbb{R}^3} S(k,k')\, v(k')\, dk' = 0\,. \tag{4.22}$$

Thus, with $\varphi(k) = v_i(k)$, equation (4.20) takes the form (cf. (3.6))

$$\frac{d}{dt}\int_{\mathbb{R}^3} v_i(k)\, f(t,k)\, dk = \int_{\mathbb{R}^3}\Big[-\frac{q}{\hbar}(\hat{E}\cdot\nabla_k)\, v_i(k) - v_i(k)\,\lambda(k)\Big]\, f(t,k)\, dk\,. \tag{4.23}$$

Since (cf. (2.2))

$$v_i(k) = \frac{1}{\hbar}\,\frac{\partial}{\partial k_i}\,\varepsilon(k)\,,$$

one obtains

$$\begin{aligned}(\hat{E}\cdot\nabla_k)\, v_i(k) = \hat{E}_1\,\frac{\partial}{\partial k_1}\, v_i(k) + \hat{E}_2\,\frac{\partial}{\partial k_2}\, v_i(k) + \hat{E}_3\,\frac{\partial}{\partial k_3}\, v_i(k) =\\ \frac{\partial}{\partial k_i}\Big(\hat{E}_1\, v_1(k) + \hat{E}_2\, v_2(k) + \hat{E}_3\, v_3(k)\Big) = \frac{\partial}{\partial k_i}\,(\hat{E}\cdot v(k))\end{aligned}$$

so that (4.23) implies

$$\begin{aligned}&\frac{d}{dt}\int_{\mathbb{R}^3} v(k)\, f(t,k)\, dk = \\ &\quad -\frac{q}{\hbar}\int_{\mathbb{R}^3}\nabla_k\,(\hat{E}\cdot v(k))\, f(t,k)\, dk - \int_{\mathbb{R}^3} v(k)\,\lambda(k)\, f(t,k)\, dk\,.\end{aligned} \tag{4.24}$$

In the parabolic case (2.13), one obtains

$$\nabla_k\,(\hat{E}\cdot v(k)) = \frac{\hbar}{m^*}\,\nabla_k\,(\hat{E}\cdot k) = \frac{\hbar}{m^*}\,\hat{E}$$

and (4.11) follows from equation (4.24).

5 Deviational particle Monte Carlo

In this section we propose an extension of the deviational particle Monte Carlo method to the area of electron transport. This method has been developed by Hadjiconstantinou and co-workers [1, 5, 24, 21] for the Boltzmann equation in rarefied gas dynamics. Recently it has been applied to phonon transport [17, 18]. The basic idea is to approximate the deviation of the solution from a given function (e.g., a local steady state) by particles. This approach is particularly successful in applications with a small signal-to-noise ratio, where it leads to significant variance reduction compared to standard DSMC.

5.1 Steady state

Theoretical results concerning convergence to equilibrium for the solution of equation (4.9) were obtained in [9]. A related numerical study was performed in [15]. Here we derive some properties of a specific steady state by applying techniques from the previous section. In physical terms, the results are related to the Maxwell-Boltzmann distribution, which is an approximation to the Fermi-Dirac distribution (see [8, Remark 1.12], [6, Section 2.5]).

Theorem 5.1 *Assume (2.9). The function*

$$f_M(k) = A\,\exp\left(-\frac{\varepsilon(k)}{k_B\,T_L}\right), \qquad \textit{where} \quad A > 0\,, \tag{5.1}$$

satisfies (cf. (2.6))

$$Q f_M = 0 \tag{5.2}$$

so that it is a steady state of equation (4.9) with zero external field. Moreover, the function (5.1) has the following properties.

- *The heat generation rate satisfies (cf. (4.7), (4.8))*

$$\int_{\mathbb{R}^3} G(k)\, f_M(k)\, dk = 0\,, \tag{5.3}$$

in accordance with (4.12).

- *The mean velocity satisfies (cf. (2.2))*

$$\int_{\mathbb{R}^3} v(k)\, f_M(k)\, dk = 0\,. \tag{5.4}$$

- *In the parabolic case (2.13), the mean energy satisfies*

$$\frac{\int_{\mathbb{R}^3} \varepsilon(k)\, f_M(k)\, dk}{\int_{\mathbb{R}^3} f_M(k)\, dk} = \frac{3}{2}\, k_B\, T_L\,. \tag{5.5}$$

In this case the function (5.1) is a Maxwellian density.

Proof. Introduce the function

$$\tilde{f}_M(\varepsilon) = A\,\exp\left(-\frac{\varepsilon}{k_B\,T_L}\right)$$

and note the identity (cf. (2.8))

$$\kappa_i\,\exp\left(\frac{\hbar\omega_i}{k_B\,T_L}\right) = \kappa_i + 1\,. \tag{5.6}$$

It follows from Lemma 4.2 and (5.6) that (cf. (4.2)–(4.4))

$$\int_{\mathbb{R}^3} S_0(k', k)\, f_M(k')\, dk' = f_M(k) \int_{\mathbb{R}^3} S_0(k, k')\, dk'\,, \tag{5.7}$$

$$\int_{\mathbb{R}^3} S_i^+(k',k)\, f_M(k')\, dk' = \tag{5.8}$$
$$K_i\,(\kappa_i+1)\,\tilde{f}_M(\varepsilon(k)+\hbar\omega_i)\int_{\mathbb{R}^3}\delta(\varepsilon(k')-\varepsilon(k)-\hbar\omega_i)\,dk'$$
$$= \quad K_i\, f_M(k)\,\kappa_i\int_{\mathbb{R}^3}\delta(\varepsilon(k')-\varepsilon(k)-\hbar\omega_i)\,dk' = f_M(k)\int_{\mathbb{R}^3} S_i^-(k,k')\,dk'$$

and

$$\int_{\mathbb{R}^3} S_i^-(k',k)\, f_M(k')\, dk' = \tag{5.9}$$
$$K_i\,\kappa_i\,\tilde{f}_M(\varepsilon(k)-\hbar\omega_i)\int_{\mathbb{R}^3}\delta(\varepsilon(k')-\varepsilon(k)+\hbar\omega_i)\,dk'$$
$$= \quad K_i\, f_M(k)\,(\kappa_i+1)\int_{\mathbb{R}^3}\delta(\varepsilon(k')-\varepsilon(k)+\hbar\omega_i)\,dk' = f_M(k)\int_{\mathbb{R}^3} S_i^+(k,k')\,dk'\,.$$

According to (5.7)–(5.9), one obtains (cf. (4.1))

$$\int_{\mathbb{R}^3} S(k',k)\, f_M(k')\, dk' = f_M(k)\int_{\mathbb{R}^3} S(k,k')\,dk'$$

so that (5.2) follows from (2.6).

It follows from (5.8) and (5.9) that (cf. (4.6))

$$\int_{\mathbb{R}^3}\lambda_i^+(k)\, f_M(k)\,dk = \int_{\mathbb{R}^3}\left[\int_{\mathbb{R}^3} S_i^+(k,k')\,dk'\right] f_M(k)\,dk = \tag{5.10}$$
$$\int_{\mathbb{R}^3}\left[\int_{\mathbb{R}^3} S_i^+(k,k')\, f_M(k)\,dk\right] dk' = \int_{\mathbb{R}^3} f_M(k')\,\lambda_i^-(k')\,dk'\,.$$

Property (5.3) is a consequence of (4.8) and (5.10). Property (5.4) follows from (2.10), due to rotational symmetry. It remains to establish property (5.5). Using spherical coordinates and the substitution $g(r)=y$, one obtains (cf. (4.14), (4.18))

$$\int_{\mathbb{R}^3} F(\varepsilon(k))\,dk = 4\pi\int_0^\infty F(g(r))\,r^2\,dr = 4\pi\int_0^\infty F(y)\,J(y)\,dy\,, \tag{5.11}$$

for any non-negative function F such that the integrals are finite. In particular, it follows from (5.11) that

$$\int_{\mathbb{R}^3}\varepsilon(k)^i\, f_M(k)\,dk = 4\pi\,A\int_0^\infty y^i\,\exp\left(-\frac{y}{k_B\,T_L}\right) J(y)\,dy = \tag{5.12}$$
$$4\pi\,A\,(k_B\,T_L)^{i+1}\int_0^\infty y^i\,\exp(-y)\,J(k_B\,T_L\,y)\,dy\,, \qquad i=0,1,2,\ldots\,.$$

In the parabolic case (2.13), one obtains (cf. (2.9), (4.14))

$$J(y) \quad = \quad \left(\frac{m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{2\,y}\,. \tag{5.13}$$

It follows from (5.12) and (5.13) that

$$\begin{aligned}\int_{\mathbb{R}^3} \varepsilon(k)^i\, f_M(k)\, dk &= 4\pi\, A\, (k_B\, T_L)^{i+1} \left(\frac{m^*}{\hbar^2}\right)^{\frac{3}{2}} \int_0^\infty y^i\, \exp(-y)\, \sqrt{2\, k_B\, T_L\, y}\, dy \\ &= 2\pi\, A \left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}} (k_B\, T_L)^{i+\frac{3}{2}}\, \Gamma\left(i+\frac{3}{2}\right),\end{aligned}$$

which implies (5.5). ■

5.2 Deviational particles

Here we discuss some basic steps towards an application of the deviational particle Monte Carlo method to the numerical treatment of equation (2.1). Introduce the function

$$\bar{f}(t,x,k) = f(t,x,k) - f_M(k)\,, \tag{5.14}$$

where f is a solution of (2.1) and f_M is defined in (5.1). Note that (cf. (2.2))

$$\nabla_k\, f_M(k) = -\frac{\hbar}{k_B\, T_L}\, f_M(k)\, v(k)\,. \tag{5.15}$$

According to Theorem 5.1 and (5.15), the function (5.14) satisfies the equation

$$\begin{aligned}\left[\frac{\partial}{\partial t} + v(k)\cdot\nabla_x - \frac{q}{\hbar}\, E(t,x)\cdot\nabla_k\right] \bar{f}(t,x,k) = \\ (Q\,\bar{f})(t,x,k) - \frac{q}{k_B\, T_L}\, f_M(k)\, E(t,x)\cdot v(k)\,.\end{aligned} \tag{5.16}$$

Equation (5.16) is similar to (2.1), but contains an additional source term. Equations (2.3)–(2.5) are applied to the original function f .

Functionals of the solution f are calculated as

$$\begin{aligned}&\int_D \int_{\mathbb{R}^3} \varphi(x,k)\, f(t,x,k)\, dk\, dx = \\ &\quad \int_D \int_{\mathbb{R}^3} \varphi(x,k)\, f_M(k)\, dk\, dx + \int_D \int_{\mathbb{R}^3} \varphi(x,k)\, \bar{f}(t,x,k)\, dk\, dx\,.\end{aligned}$$

Functionals with respect to f_M are either known explicitly (cf. (5.3)–(5.5)), or can be calculated by some deterministic method. Functionals with respect to $\bar{f}$ are calculated using a system of particles. The basic stochastic model described in Section 3 has to be extended by jumps corresponding to the creation of particles. This is covered by the general theory of stochastic particle systems related to kinetic equations (cf., e.g., [3]). However, slight modifications are needed, since the source term in (5.16) takes both positive and negative values. Thus, a system of particles with positive and negative weights is used.

In the following we sketch this algorithm in the spatially homogeneous case. Note that $v(k)$ is given in (2.10) and the external field $\hat{E}$ does not depend on t .

- **Initialization.** The particle system is initialized according to a density proportional to

$$|f_0(k) - f_M(k)|\,,$$

where f_0 is the initial state of equation (4.9). Particles get weights determined by the sign of the function $f_0 - f_M$.

If $f_0 = f_M$, then the algorithm starts with an empty particle system.

- **Creation.** Particles with wave-vector k are created according to a density proportional to

$$f_M(k)\,|\hat{E}\cdot v(k)|\,.$$

They get weights determined by the sign of the expression $\hat{E}\cdot v(k)$. This choice of constant weights ± 1 corresponds to the original deviational particle Monte Carlo method. Alternatively, particles can be created according to $f_M(k)$ getting variable weights proportional to $\hat{E}\cdot v(k)$.

If $f_0 = f_M$ and $\hat{E} = 0$, then the particle system stays empty, in accordance with Theorem 5.1.

- **Acceleration.** Particles are accelerated according to (cf. (3.4))

$$\frac{d}{dt}\,k(t) = -\frac{q}{\hbar}\,\hat{E}\,.$$

- **Scattering.** Particles are scattered as in the standard case (cf. (3.5), (4.1)–(4.5)).

According to Lemma 4.2, the scattering probabilities (4.5) take the form

$$\lambda_0(k) = \tilde{\lambda}(\varepsilon(k)) \qquad \text{and} \qquad \lambda_i^{\pm}(k) = \tilde{\lambda}_i^{\pm}(\varepsilon(k))\,,$$

where

$$\tilde{\lambda}_0(\varepsilon) = 4\pi\,K_0\,J(\varepsilon)\,,$$

$$\tilde{\lambda}_i^{+}(\varepsilon) = 4\pi\,K_i\,(\kappa_i+1)\,J(\varepsilon-\hbar\omega_i)\,1_{(0,\infty)}(\varepsilon-\hbar\omega_i)$$

and

$$\tilde{\lambda}_i^{-}(\varepsilon) = 4\pi\,K_i\,\kappa_i\,J(\varepsilon+\hbar\omega_i)\,.$$

The quasi-parabolic case (2.12) has the form (2.9) with

$$g(r) = \frac{\sqrt{1+\beta\,r^2}-1}{2\alpha}\,, \qquad \beta = \frac{2\alpha\hbar^2}{m^*}\,.$$

One obtains

$$g^{-1}(y) = \sqrt{\frac{(2\alpha\,y+1)^2-1}{\beta}}\,, \qquad g'(r) = \frac{\beta\,r}{2\alpha\,\sqrt{1+\beta\,r^2}}$$

and (cf. (4.14))

$$
\begin{aligned}
J(y) &= \frac{g^{-1}(y)}{\beta}\, 2\alpha\, \sqrt{1+\beta\,[g^{-1}(y)]^2} = \sqrt{\frac{(2\alpha\, y+1)^2-1}{\beta}}\, \frac{2\alpha\,(2\alpha\, y+1)}{\beta} \\
&= \left(\frac{2\alpha}{\beta}\right)^{\frac{3}{2}} \sqrt{2\, y\,(\alpha\, y+1)}\,(2\alpha\, y+1) \\
&= \left(\frac{m^*}{\hbar^2}\right)^{\frac{3}{2}} \sqrt{2\, y\,(\alpha\, y+1)}\,(2\alpha\, y+1)\,. \qquad (5.17)
\end{aligned}
$$

Note that (5.17) holds with $\alpha \geq 0$ (cf. (5.13)).

5.3 Comments

In the deviational particle approach sketched in Section 5.2 there is permanent creation of particles. In order to run the algorithm for large times, the growth of the system has to be controlled. This blow-up control is a common problem when dealing with “artificial” weighted particle systems instead of “natural” direct simulation systems (cf. [23, Section 3.4]). In [17, 18] particles are skipped, when they have had a sufficiently large number of scattering collisions. The argument is that those particles have reached a certain equilibrium and do not add any new information. A similar idea might be useful in our context, where the steady state for the deviation $\bar{f}$ is a combination of “old” particles (that have experienced enough scattering and acceleration) and “new” particles (permanently incepted by the source term). Beside the control issue, further work is needed to develop the details of an extension of the deviational particle approach to the spatially inhomogeneous case.

There is another interesting aspect related to stochastic weighted particle systems. Once the algorithm is based on weighted particles, it should be possible to provide alternatives for the simulation of scattering processes. This might be helpful in order to study effects of rare events, which do not happen frequently enough in the direct simulation algorithm in order to gather reliable statistics.

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