Homogenization of a nonlinear transport equation

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Abstract

In this paper, we investigate the homogenization of a nonlinear kinetic equation modeling electron transport in semiconductors. We compute effective scattering coefficients for medium with periodic inhomogeneities.

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1 Introduction

This paper is devoted to the homogenization of a kinetic equation modeling electron transport in semiconductor devices. We recall that the purpose of homogenization is to understand how perturbations arising at a small (microscopic) scale in the properties of the medium (due to inhomogeneities) will affect the particles behavior at a large (macroscopic) scale. Mathematically, it amounts to study the asymptotic behavior of the solutions of an equation involving fastly oscillating coefficients.

There is a large body literature dealing with the periodic homogenization of partial differential equations. The cases of elliptic and parabolic equations (linear, quasi linear or fully nonlinear) and that of Hamilton-Jacobi equations, in particular, have been extensively investigated, and it is beyond the scope of this paper to review those results. Homogenization of transport

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phenomena has also received some interests before. In the context of neutron transport theory, many results have been obtained by G. Allaire and G. Bal ([AB97], [AB99]) and G. Allaire et al. ([AC00], [ABS02]). The models in consideration in those paper are some spectral problems for diffusion equations.

In the present paper, we consider a kinetic equation with scattering terms modeling the collisions of particles with the background medium. Inhomogeneities arising in the medium are taken into account via fast oscillations with respect to the space variables in the scattering coefficients.

Several authors have considered the homogenization of such equations in their diffusion regimes: When the mean free path of the particles is of the same order as the characteristic length of the inhomogeneities, homogenization and diffusion limit arise at the same scale. In that case, the oscillations are affecting the particles at the microscopic level (in the transport equation), but their effects are being investigated at the macroscopic level (in a diffusive regime) (see T. Goudon, F. Poupaud [GP01], [GP05] and T. Goudon, A. Mellet [GM01], [GM03]).

To our knowledge, the only result concerning the homogenization of kinetic equations at the microscopic level is due to L. Dumas and F. Golse (see [DG00]) and is restricted to the case of a linear transport equation. Their proof relies on velocity averaging results for transport equations (see [GLPS88]), which provide some compactness of some integrated quantities (such as the density) and allow for a compensated compactness type method. They derive effective scattering coefficients for particles transport in periodic or random media.

In this paper, we will be dealing with scattering terms modeling the collisions of a population of electrons with the semiconductor lattice. In nondegenerate situation, the Pauli exclusion principle has to be taken into account, leading to a nonlinear collision operator. Because of the quadradic terms, the method of Dumas-Golse can no longer be used. Our approach is very different and can be summarized as follows: Let f^ε and g be solutions of

$$Lf^\varepsilon = Q^\varepsilon(f^\varepsilon)\,, \qquad Lg = \overline{Q}(g)$$

where L is a transport operator and Q^ε and $\overline{Q}$ are two integral operators. We write

$$L(f^\varepsilon - g) = \big[Q^\varepsilon(f^\varepsilon) - Q^\varepsilon(g)\big] + \big[Q^\varepsilon(g) - \overline{Q}(g)\big], \tag{1}$$

Using the usual L^p estimates for transport operators and a Gronwall argument, (1) will give the strong convergence of f^ε to g if we can prove

1. that the Q^ε is continous in L^p,
2. that $Q^\varepsilon(g)$ converges to $\overline{Q}(g)$ in L^p,
3. that the initial datum converges in L^p strong.

In particular, we only have to consider the convergence of Q^ε when it is evaluated against a fixed function g, so the nonlinearity of the operator does not matter anymore. However, even with g smooth, there is no hope of getting the strong convergence of $Q^\varepsilon = Q(x/\varepsilon)$ with spatialy oscillating coefficients.

The idea is thus to integrate (1) along the characteristic curves. In the force-free case, when the characteristic curves are straight lines, we are led to prove that

$$\int_0^t Q(\frac{x+vs}{\varepsilon})(\tilde{g}) - \overline{Q}(\tilde{g})\, ds$$

goes to zero in L^p as $\varepsilon \to 0$. In particular, the oscillations with respect to the space variable are now oscillations with respect to the time variable and are being integrated. Note that the effective coefficients will be obtained by averaging $Q(x/\varepsilon)$ along the path followed by the particles. It turns out that for almost all direction v, the average along the characteristic lines is nothing but the standard average of the coefficients (this is a consequence of standard ergodic theorems).

We stress out the fact that this method works with linear as well as nonlinear collision operators. In particular, it provides a new proof of the result of [DG00] that does not use averaging lemmas. However, it relies on the fact that the characteristic curves are straight lines, and could not be easily generalized to a model with electric field. Also, the method require more hypotheses on the initial datum. Finally, we point out that it is not clear what would happen in the case of a random inhomogeneous medium with this approach.

2 Model and results.

In the framework of semiconductors, the distribution function depends on the position $x \in \mathbb{R}^N$, the wave vector $k \in \mathbb{R}^N$ and the time t. The wave vector k varies in the reciprocal lattice of the crystal. We denote by B the reduced zone of that lattice (B is a n-torus, called the first Brillouin zone). A particle with wave vector k has an energy $\mathscr{E}(k)$, where $\mathscr{E}$ is a given (smooth) function defined on B. The velocity of the particle is then given by

$$v(k) = \nabla_k \mathscr{E}(k).$$

The evolution of $f(x,k,t)$ is described by the following Boltzmann equation:

$$\partial_t f + v(k) \cdot \nabla_x f = Q(x)(f), \tag{2}$$

where the operator $Q(x)$ takes into account the interactions between the electrons and the semiconductor crystal. Those interactions involve several phenomena: Collisions with impurities, interactions with phonons... The general form of this operator is

$$Q(f) = \int_B \sigma(x,k',k) f(k')(1-f(k)) - \sigma(x,k,k') f(k)(1-f(k'))\, dk',$$

where $\sigma(x,k,k')$ is a non negative function defined on $\mathbb{R}^N \times B \times B$ (periodic with respect to k and k'). It represents the probability for a particle to change its wave vector k into another k' during an interaction at position x. The terms $(1-f)$ take into account the Pauli exclusion principle. Note that with this operator, Equation (2) satisfies a natural maximum principle that guarantees that

$$0 \leq f(x,k,t) \leq 1.$$

The dependence on the position variable x of Q takes into account the fact that the repartition of the scattering sources is not in general homogeneous.

The cross section σ usually satisfies the following symmetry property (the so-called detailed balance principle):

$$\sigma(x,k,k') e^{-\mathscr{E}(k)/k_B T} = \sigma(x,k',k) e^{-\mathscr{E}(k')/k_B T}.$$

However such an assumption is not necessary to our purpose.

We recall the following existence result due to F. Poupaud [Pou90]:

Proposition 2.1 *Under the following hypothesis:*

$$0 \leq \sigma(x,k,k') \leq C \tag{3}$$

$$0 \leq f_o(x,k) \leq 1 \qquad f_o \in W^{1,1}(\mathbb{R}^N \times B), \tag{4}$$

equation (2) has a unique smooth solution $f(x,k,t)$ such that

$$0 \leq f(x,k,t) \leq 1 \tag{5}$$

$$f \in W^{1,1} \cap W^{1,\infty}([0,T] \times R^N \times B). \tag{6}$$

and satisfying the initial condition

$$f(x,k,0) = f_o(x,k).$$

Next, we assume that the medium presents some inhomogeneities of length l, in a periodic manner. This is taken into account by assuming that the cross-section σ takes the form

$$\sigma(\frac{x}{l}, k, k'),$$

where

$$y \mapsto \sigma(y,k,k')$$

is $[0,1]^N$-periodic. Equivalently, we'll assume that σ is defined on $\mathbb{T}^N \times B \times B$ where $\mathbb{T}^N$ denotes the torus $\mathbb{R}^N/\mathbb{Z}^N$. We make the following assumption:

$$\sigma \in \mathcal{C}^0(\mathbb{T}^N, L^\infty(B \times B)) \qquad \textbf{(H1)}$$

(in particular (3) is satisfied). We could also take into account the dependence of σ on the macroscopic variable x, and work with $\sigma(x,y,k,k')$ defined on $\Omega \times \mathbb{T}^N \times B \times B$. However, for the sake of clarity, we shall assume that σ is independent on x.

Introducing the small parameter $\varepsilon = l/L$, where L denotes the characteristic macroscopic length, we are led to consider the following equation:

$$\partial_t f_\varepsilon + v(k) \cdot \nabla_x f_\varepsilon = Q_\varepsilon(f_\varepsilon) \qquad (7)$$

$$f_\varepsilon(x,k,0) = f_o(x,k). \qquad (8)$$

with

$$Q_\varepsilon(f) = \int_B \sigma(x/\varepsilon, k', k) f(k')(1-f(k)) - \sigma(x/\varepsilon, k, k') f(k)(1-f(k'))\, dk'. \qquad (9)$$

Proposition 2.1 gives the existence of a solution f_ε provided that f_o satisfies (4).

Finally, we need to make the following technical assumption:

$$\mu(\{k \setminus v(k) \in \cup_{a \in S, z \in \mathbb{R}} (az, z)\}) = 0, \qquad \textbf{(H2)}$$

where μ denotes the Lebesgue measure on B and S is the set of vectors $(a_1 \cdots a_{N-1}) \in \mathbb{R}^{N-1}$ whose coordinates are rationally dependent of 1. That is S is the set of vectors such that there exists $(m_0, \cdots, m_{N-1}) \in \mathbb{Z}^{N-1}$ satisfying

$$m_0 + m_1 a_1 + \cdots + m_{N-1} a_{N-1} = 0, \qquad (m_0, \cdots, m_{N-1}) \neq (0, \cdots, 0)$$

Note that the set $\cup_{a\in S, z\in\mathbb{R}}(az, z)$ is of measure 0 in $\mathbb{R}^N$, so this hypothesis is satisfied, for example, if we have $\det(D^2\mathscr{E}(k)) \neq 0$ for all $k \in B$. Hypothesis **H2** will be essential in the use of ergodic theorem; It says that almost all characteristic curves have nice averaging properties.

Our main result reads as follows

Theorem 2.1 *If hypothesis* **H1** *and* **H2** *hold, then, as ε goes to zero, the solution $f_\varepsilon(x,k,t)$ of Equation (7) converges in $L^\infty([0,T], L^1(\Omega \times B))$ to $g(x,k,t)$, solution of:*

$$\partial_t g + v(k)\cdot\nabla_x g = \overline{Q}(g) \tag{10}$$

$$g(x,k,0) = f_o(x,k). \tag{11}$$

where the asymptotic collision operator is given by

$$\overline{Q}(g) = \int \overline{\sigma}(k', k)g(k')(1-g(k)) - \overline{\sigma}(k,k')g(k)(1-g(k'))\,dk',$$

with an effective scattering coefficient satisfying

$$\overline{\sigma}(k,k') = \int_{\mathbb{T}^N} \sigma(y,k,k')\,dy.$$

3 Proof of Theorem 2.1

1- An integral formulation for (2).
Integrating the transport equation (2) along characteristic lines, we obtain:

$$f_\varepsilon(t, x+v(k)t, k) = f_0(x,k) + T_\varepsilon(f_\varepsilon) \tag{12}$$

where $T_\varepsilon(f_\varepsilon)$ is equal to:

$$\int_0^t \int \sigma\left(\frac{x+v(k)s}{\varepsilon}, k', k\right) f_\varepsilon(x+v(k)s, k')(1 - f_\varepsilon(x+v(k)s,k))$$
$$-\sigma\left(\frac{x+v(k)s}{\varepsilon}, k, k'\right) f_\varepsilon(x+v(k)s, k)(1 - f_\varepsilon(x+v(k)s,k'))dk'ds.$$

Similarly, we can write:

$$g(t, x+v(k)t, k) = f_0(x,k) + \overline{T}(g), \tag{13}$$

with

$$\overline{T}(g) = \int_0^t \int \overline{\sigma}\left(k',k\right) g(x+v(k)s,k')(1-g(x+v(k)s,k)) \\ -\overline{\sigma}\left(k,k'\right) g(x+v(k)s,k)(1-g(x+v(k)s,k'))\,dk'\,ds.$$

Finally, equations (12) and (13) yield

$$\int\int |(f_\varepsilon - g)(t, x+v(k)t, k)|\,dx\,dk \\ \leq \int\int |T_\varepsilon(f_\varepsilon) - T_\varepsilon(g)|\,dx\,dk + \int\int \left|T_\varepsilon(g) - \overline{T}(g)\right|\,dx\,dk. \quad (14)$$

This equality is the corner stone of the proof. To show the convergence of f_ε to g, we will show that the first term is controlled by the L^1 norm of $|f_\varepsilon - g|$ and that the second term goes to zero as ε goes to zero. A Gronwall argument will then give the result. Note that the convergence of T_ε to the homogenized operator $\overline{T}$ is only needed when T_ε is evaluated at the function g. Since g is a given function independent on ε we do not have to take a limit in nonlinear terms.

2- Continuity of the collision operator.
The first part is a straightforward computation: Thanks to Hypothesis (**H1**), we have

$$\int_{\mathbb{R}^N}\int_B |T_\varepsilon(f_\varepsilon) - T_\varepsilon(g)|\,dk\,dx \\ \leq C\int_{\mathbb{R}^N}\int_B\int_0^t\int_B |f_\varepsilon(s,x+v(k)s,k') - g(s,x+v(k)s,k')|\,dk'\,ds\,dk\,dx \\ +C\int_0^t\int_{\mathbb{R}^N\times B\times B} f_\varepsilon(s,x+v(k)s,k')|f_\varepsilon(s,x+v(k)s,k) - g(s,x+v(k)s,k)| \\ +C\int_0^t\int_{\mathbb{R}^N\times B\times B} g(s,x+v(k)s,k)|f_\varepsilon(s,x+v(k)s,k') - g(s,x+v(k)s,k')|.$$

Using the fact that $f_\varepsilon \leq 1$, we deduce

$$\int_{\mathbb{R}^N}\int_B |T_\varepsilon(f_\varepsilon) - T_\varepsilon(g)|\,dk\,dx \\ \leq C|B|\int_0^t\int_B\int_{\mathbb{R}^N} |f_\varepsilon(s,x,k) - g(s,x,k)|\,dx\,dk\,ds. \quad (15)$$

3- Homogenization along the characteristic lines.
It remains to prove that $T_\varepsilon(g)$ converges to $\overline{T}(g)$ as ε goes to zero. It will be a consequence of the following lemma:

Lemma 3.1 *Assume that (***H2***) holds. Then, for every test function ϕ depending on t, k, k', the quantity:*

$$\int_0^t \int_B \sigma\left(\frac{x+v(k)s}{\varepsilon}, k', k\right) \phi(t,k,k')\, dk'\, ds$$

converges for almost every x and k to:

$$\int_0^t \int_B \overline{\sigma}(k,k')\left(k', k\right) \phi(t,k,k')\, dk'\, ds.$$

First, we check that the Lemma indeed completes the proof of Theorem 2.1: Applying Lemma 3.1 with $\phi(t,k,k') = g(x+v(k)s,k')(1-g(x+v(k)s,k))$, shows that the gain term in $T_\varepsilon(g)$

$$\int_0^t \int \sigma\left(\frac{x+v(k)s}{\varepsilon}, k', k\right) g(x+v(k)s,k')(1-g(x+v(k)s,k))\, dk'\, ds$$

converges for almost every x and k to

$$\int_0^t \int \overline{\sigma}(k,k') g(x+v(k)s,k')(1-g(x+v(k)s,k))\, dk'\, ds.$$

We proceed similarly with the loss term and deduce that

$$T_\varepsilon(g) \longrightarrow \overline{T}(g)$$

as ε goes zero for almost every x and k. By Lebesgue's dominated convergence theorem, we deduce that the convergence holds in L^1.

Finally, (14) and (15) give

$$\begin{aligned}\int_B \int_{\mathbb{R}^N} & |f_\varepsilon(t,x,k) - g(t,x,k)|\, dx\, dk \\ & \leq C|B| \int_0^t \int_B \int_{\mathbb{R}^N} |f_\varepsilon(s,x,k) - g(s,x,k)|\, dx\, dk\, ds \\ & \quad + \int_{\mathbb{R}^N} \int_B |T_\varepsilon(g) - \overline{T}(g)|\, dk\, dx,\end{aligned}$$

and Gronwall's Lemma implies

$$\int_0^t \int_B \int_{\mathbb{R}^N} |f_\varepsilon(s,x,k) - g(s,x,k)|\, dx\, dk\, ds$$
$$\leq \int_0^t e^{C|B|(t-s)} \int_{\mathbb{R}^N} \int_B |T_\varepsilon(g) - \overline{T}(g)|\, dk\, dx\, ds \qquad (16)$$

Since $|T_\varepsilon(g) - \overline{T}(g)|$ converges strongly to 0 in $L^1([0,T]\times\mathbb{R}^N\times B)$, we deduce that f_ε converges to g in $L^1([0,T]\times\mathbb{R}^N\times B)$. In turn, (14) implies that the convergence holds in $L^\infty([0,T], L^1(\mathbb{R}^N\times B))$, so the proof of Theorem 2.1 is complete.

Proof of Lemma 3.1: It is enough to show that for almost every x, k, k' and every $\alpha < \beta$:

$$\int_\alpha^\beta \sigma\left(\frac{x+v(k)t}{\varepsilon}, k', k\right) dt \longrightarrow \overline{\sigma}\left(k', k\right)(\beta-\alpha).$$

Throughout the proof, k and k' are given vectors in B, and we decompose the position variable $x = (\underline{x}, x_N) \in \mathbb{R}^N$, with $\underline{x} \in \mathbb{R}^{N-1}$ and $x_N \in \mathbb{R}$.

Let's denote $\gamma = \beta - \alpha$ and fix $y = (\underline{y}, y_N) \in \mathbb{R}^N$; we start by proving that:

$$\int_0^\gamma \sigma\left(y + v\frac{t}{\varepsilon}, k', k\right) dt \longrightarrow \gamma\overline{\sigma} \quad \text{as } \varepsilon \to 0. \qquad (17)$$

To that purpose, let t_0 be such that

$$v_N(k)t_0 = 1.$$

For $\varepsilon > 0$, let n be such that

$$\gamma/((n+1)t_0) \leq \varepsilon \leq \gamma/(nt_0),$$

then we have:

$$
\begin{aligned}
&\int_0^{\gamma} \sigma(y + vt/\varepsilon, k', k)\, dt \\
&\quad = \varepsilon \int_0^{\gamma/\varepsilon} \sigma(y + vt, k', k)\, dt \\
&\quad = \frac{\gamma}{nt_0} \int_0^{nt_0} \sigma(y + vt, k', k)\, dt + \mathcal{O}(\varepsilon) \\
&\quad = \frac{\gamma}{nt_0} \sum_{j=0}^{n-1} \int_{jt_0}^{(j+1)t_0} \sigma(y + vt, k', k)\, dt + \mathcal{O}(\varepsilon) \\
&\quad = \frac{\gamma}{nt_0} \sum_{j=0}^{n-1} \int_0^{t_0} \sigma((\underline{y} + j\underline{v}(k)t_0, y_N + jv_N t_0) + v(k)t, k', k)\, dt + \mathcal{O}(\varepsilon) \\
&\quad = \frac{\gamma}{nt_0} \sum_{j=0}^{n-1} \int_0^{t_0} \sigma((\underline{y} + j\underline{v}(k)t_0, y_N) + v(k)t, k', k)\, dt + \mathcal{O}(\varepsilon).
\end{aligned}
$$

Denoting by $T_{\underline{a}}$ the translation $\underline{y} \mapsto \underline{y} + \underline{a}$ on the torus $\mathbb{R}^{N-1}/\mathbb{Z}^{N-1}$, and introducing

$$
F(\underline{y}, y_N) = \int_0^{t_0} \sigma((\underline{y}, y_N) + v(k)t, k', k)\, dt,
$$

we deduce

$$
\int_0^{\gamma} \sigma(y + vt/\varepsilon, k', k)\, dt = \frac{\gamma}{nt_0} \sum_{j=0}^{n-1} F(T_{\underline{a}}^j(\underline{y}), y_N) + \mathcal{O}(\varepsilon),
$$

with $\underline{a} = \frac{\underline{v}(k)}{v_N(k)}$. Thanks to our hypothesis $(H2)$, $\underline{a}$ is rationally independent, and thus $T_{\underline{a}}$ is ergodic, for almost every k in B. Birkhoff's ergodic theorem yields:

$$
\frac{\gamma}{t_0 n} \sum_0^n F(T_{\underline{a}}^j(\underline{y}), y_N) \to \frac{\gamma}{t_0} \int_{[0,1]^{N-1}} \int_0^{t_0} \sigma((\underline{y}, y_N) + v(k)t)\, dt\, d\underline{y}.
$$

Moreover, using the periodicity of $\sigma(y, k, k')$ with respect to y, we have:

$$\begin{aligned}
\frac{\gamma}{t_0} \int_{[0,1]^{N-1}} & \int_0^{t_0} \sigma((\underline{y}, y_N) + v(k)t)\, dt\, d\underline{y} \\
& = \frac{\gamma}{t_0} \int_{[0,1]^{N-1}} \int_0^{t_0} \sigma(\underline{y} + \underline{v}(k)t, y_n + t/t_0)\, dt\, d\underline{y} \\
& = \frac{\gamma}{t_0} \int \int_{[0,1]^{N-1}} \int_0^{t_0} \sigma(\underline{y}, y_n + t/t_0)\, dt\, d\underline{y} \\
& = \gamma \int \int_{[0,1]^{N-1}} \int_0^{1} \sigma(\underline{y}, y_n + t)\, dt\, d\underline{y} \\
& = \gamma \overline{\sigma}(k, k'),
\end{aligned}$$

which gives (17).

Next , we note that:

$$\int_\alpha^\beta \sigma(x/\varepsilon + v(k)t/\varepsilon)\, dt = \int_0^\gamma \sigma((x + v(k)\alpha)/\varepsilon + v(k)t/\varepsilon)\, dt.$$

We denote

$$G_\varepsilon(y) = \int_0^\gamma \sigma(y + v(k)t/\varepsilon)\, dt,$$

and $y_\varepsilon = (x + v(k)\alpha)/\varepsilon$. Since y_ε lies in a torus, up to a subsequence, it converges to y_0, and we can write

$$G_\varepsilon((x + v(k)\alpha)/\varepsilon) = (G_\varepsilon(y_\varepsilon) - G_\varepsilon(y_0)) + G_\varepsilon(y_0).$$

The first part converges to 0 thanks to the equicontinuity of G_ε, and by (17) we already know that $G_\varepsilon(y_0)$ converges to $\gamma\overline{\sigma}$. Finally, since the limit is independent on the subsequence and G_ε is bounded, the whole sequence converges. The proof of Lemma 3.1 is now complete.

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