WIGNER FUNCTION FOR MULTIBAND TRANSPORT IN SEMICONDUCTORS

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ABSTRACT

In this work we present a one-dimensional model of quantum electron transport in semiconductors that makes use of the Wigner function formalism and that takes into account the full band structure of the medium for energy bands of any shape. We introduce a multi-band Wigner function and derive the evolution equations for each component, with and without external fields, by using a Bloch states representation of the density matrix.

1 Introduction

The Wigner-function approach to quantum electron transport in semiconductors is widely used to describe the properties of electronic devices such as the

Resonant Tunneling Diode (RTD) and others [1, 2, 3]. By making use of phase space concepts, it presents a close analogy to the classical Boltzmann-equation approach; this has the advantage that many of the analytical and numerical techniques commonly used for the Boltzmann equation can be adapted to the Wigner function. In particular, the numerical complexity of other quantum statistical approaches to electron transport, such as the density-matrix approach [4, 5, 6] and the Green's-function approach [7, 8, 9], is significantly reduced in the kinetic models that make use of the Wigner function. Also, when dealing with space dependent problems in finite domains, it is always difficult to devise the correct boundary conditions to be imposed; because of the analogy with the classical Boltzmann equation, this difficulty is more easily overcome with the Wigner-function approach, since one can rely on imposing classical boundary conditions in a region sufficiently far from the quantum region, where classical effects dominate [3]. Also, adding collisions to the model equations that govern the evolution of the Wigner function is less complicated than including collisions into the other statistical models of quantum transport [2].

All existing transport models for semiconductors based on the Wigner function, however, rely on the following two approximations: 1) that only single-conduction-band electrons contribute to the current flow, and 2) that only a small region of the Brillouin zone near the minimum of the band is populated, leading to the parabolic band approximation. Under these conditions, conduction electrons can be considered as semiclassical particles having an effective mass related to the curvature of the energy band function near the minimum. The evolution equation for the Wigner function of the conduction electrons then becomes the evolution equation for free particles with an effective mass. This allows the inclusion of any fields (barriers or bias) by means of the standard pseudodifferential operator [1].

In the case of devices in which interband transitions or non-parabolicity

effects may occur, the single-band, effective mass approximation is not satisfactory. A correctly defined Wigner function for these phenomena should include the populations of all bands involved in the transport processes and the evolution equation that governs the time dependence of the Wigner function should take into account possible non-parabolicity effects. In this work, we remove the single-band approximation and the parabolic band approximation, by introducing a Wigner function which includes the populations of all energy bands and derive an evolution equation which allows for energy bands of any shape. The resulting equations provide an exact model for the description of collisionless electron transport in semiconductors without the single-band and the effective mass approximations. Collisions can be added to the model in standard ways. We also discuss the derivation of the effective mass approximation starting from the exact equations. Some of our results have already appeared in the literature for particular cases. In absence of external fields, the evolution equations are a generalization of an earlier result for a single band by Markowich, Mauser and Poupaud [10, 11]. A statistical description of multiband transport was formulated by Krieger and Iafrate [12, 13] by making use of accelerated Bloch states in a model based on the density matrix. A two band kinetic model without external fields was developed by Kuhn and Rossi [14] and by Hess and Kuhn [15] for the description of semiconductor lasers.

2 The density matrix and the Wigner function

In this work, we consider an ensemble of electrons moving in a semiconductor crystal, which is considered as an infinite homogeneous medium. The main quantity of a quantum statistical description of the electron ensemble in phase space is the Wigner function, which is defined by a suitable Fourier transformation of the density matrix. If ρ is the single particle density operator, the corresponding density matrix in the space representation is given by

$\rho(r,s) =< r|\rho|s >$, where Dirac's notation has been used. Then, the Wigner function [1] is derived from the density matrix by first considering a transformation from the variables r and s to the variables $x = (r+s)/2$ (center of mass variable) and $\eta = r - s$ (relative variable), and then taking Fourier transforms with respect to η:

$$f(x,p) = \int d\eta < x + \frac{\eta}{2}|\rho|x - \frac{\eta}{2} > e^{-ip\eta/\hbar}. \tag{1}$$

This relation can be inverted and the elements of the density matrix can be written in terms of the Wigner function:

$$< r|\rho|s >= \frac{1}{2\pi\hbar}\int dp f\left(\frac{r+s}{2}, p\right) e^{ip(r-s)/\hbar} \tag{2}$$

In general, an electron in the crystal will be found in a superposition of Bloch states belonging to different energy bands. If we wish to use the Wigner function approach in situations in which band to band transitions occur, the Wigner function has to contain the information about the electron populations of all energy bands and their dynamics. A suitable partition of the Wigner function among the energy bands is obtained by using the Bloch states and the matrix elements of the density operator in the Bloch states representation.

Let H_0 be the Hamiltonian containing only the kinetic energy and the periodic potential V_p, and given by $H_0 = p^2/2m + V_p$, and let $\Psi_m(x,k)$, $m \in \mathbf{N}$, $k \in B$, with B the Brillouin zone [10], be the eigenfunctions and $\epsilon_1(k)$, $\epsilon_2(k)$, $\ldots$, $\epsilon_{m-1}(k)$, $\epsilon_m(k)$, $\ldots$, the eigenvalues of H_0:

$$H_0\Psi_m(x,k) = \epsilon_m(k)\Psi_m(x,k),$$

or, using Dirac's notation,

$$H_0|m,k >= \epsilon_m(k)|m,k> . \tag{3}$$

The eigenfunctions are given by the Bloch functions

$$< x|mk >\equiv \Psi_m(x,k) = e^{ikx}u_{mk}(x) \tag{4}$$

and form a complete orthonormal set [16]. Here, $u_{mk}(x)$ is the periodic part of the Bloch function for the m-th band and the states $\{|mk>\}$, $m \in \mathbf{N}$, $k \in B$ are the Bloch states. If a is the period of the lattice, we have that $u_{mk}(x+a) = u_{mk}(x)$ and

$$e^{ik\mu} < x|mk> = < x+\mu|mk> \tag{5}$$

$\forall \mu \in L$, with L the direct lattice (therefore $\mu = \mu(l) = la$, $l \in \mathbf{Z}$). The functions $\epsilon_m(k)$ are the energy bands of the material and are periodic in the crystal momentum k with period $2\pi/a$. They can be expanded in a Fourier series,

$$\epsilon_m(k) = \sum_{\mu \in L} \widehat{\epsilon}_m(\mu) e^{ik\mu}, \tag{6}$$

where $\widehat{\epsilon}^*_m(\mu) = \widehat{\epsilon}_m(-\mu)$, since the $\epsilon_m(k)$ are real functions of k. By using the completeness of the Bloch states $\{|mk>\}$ in equation (1), the Wigner function can be written as a double sum of contributions from all energy bands:

$$f(x,p) = \sum_{m'm''} f_{m'm''}(x,p) \tag{7}$$

where

$$\begin{aligned} f_{m'm''}(x,p) &= \int_{B^2} dk'dk'' \rho_{m'm''}(k',k'') \times \\ &\quad \times \int d\eta < x + \frac{\eta}{2}|m'k' >< m''k''|x - \frac{\eta}{2} > e^{-ip\eta/\hbar} \end{aligned} \tag{8}$$

and

$$\rho_{m'm''}(k',k'') = < m'k'|\rho|m''k'' > \tag{9}$$

are the elements of the density operator in the Bloch states representation. Equation (8) can be written in a more compact form, by introducing a projection operator $\mathcal{P}_{m'm''}$ such that, $(\mathcal{P}_{m'm''} f)(x,p) = f_{m'm''}(x,p)$. Let us first define the coefficients

$$\Phi_{m'm''}(k',k'',x,p) = \int d\eta < x + \frac{\eta}{2}|m'k' >< m''k''|x - \frac{\eta}{2} > e^{-ip\eta/\hbar}. \tag{10}$$

These integrals have the property that

$$\frac{1}{2\pi\hbar}\int\int dxdp\,\Phi_{m'm''}(k',k'',x,p)=\delta_{m'm''}\delta(k'-k''), \tag{11}$$

which can be easily derived from the orthogonality of the Bloch states. After substituting into (8) we have:

$$f_{m'm''}(x,p)=\int_{B^2}dk'dk''\rho_{m'm''}(k',k'')\Phi_{m'm''}(k',k'',x,p). \tag{12}$$

The coefficients $\rho_{m'm''}(k',k'')$ of the density matrix can be written in terms of the Wigner function by using (2). After some algebra, we have:

$$\begin{aligned}
&\rho_{m'm''}(k',k'')=<m'k'|\rho|m''k''>=\\
&=\int\int drds<m'k'|r><r|\rho|s><s|m''k''>=\\
&=\frac{1}{2\pi\hbar}\int\int dxdpf\,(x,p)\int d\eta<m'k'|x+\frac{\eta}{2}><x-\frac{\eta}{2}|m''k''>e^{ip\eta/\hbar}=\\
&=\frac{1}{2\pi\hbar}\int dx\int dp\Phi^{*}_{m'm''}(k',k'',x,p)f\,(x,p)\,.
\end{aligned}$$

Finally, by introducing the transfer function

$$W_{m'm''}(x,p,x',p')=\int_{B^2}dk'dk''\Phi_{m'm''}(k',k'',x,p)\Phi^{*}_{m'm''}(k',k'',x',p'), \tag{13}$$

the band projection $f_{m'm''}$ can be written as

$$f_{m'm''}(x,p)=\frac{1}{2\pi\hbar}\int\int dx'dp'W_{m'm''}(x,p,x',p')f\,(x',p')\equiv(\mathcal{P}_{m'm''}f)(x,p). \tag{14}$$

The last equality defines the linear integral operator $\mathcal{P}_{m'm''}$, which yields the projections $f_{m'm''}$ from the total Wigner function f. It is easy to see that $\mathcal{P}_{m'm''}$ is a projection operator. The functions $f_{m'm''}$, which are the projections of f onto the band subspaces, and the coefficients $\rho_{m'm''}(k',k'')$ are similar to the ones introduced in [17, 18, 19].

The macroscopic quantities such as particle density, current and energy, are likewise expressed as a sum of band terms. It can be shown that only the diagonal terms contribute to the total number of particles, that is

$$\int\int dxdpf(x,p)=\sum_{m}\int\int dxdpf_{mm}(x,p).$$

This follows from the fact that $\int\int dxdpf_{m'm''}(x,p) = 0$ for $m' \neq m''$, as results from equation (11).

3 General evolution equations

The time evolution of the Wigner fuction is given by the sum of the time evolutions of the band projections,

$$i\hbar\frac{\partial f}{\partial t}(x,p,t) = \sum_{m'm''} i\hbar\frac{\partial f_{m'm''}}{\partial t}(x,p,t),$$

and it must follow from the time evolution of the density matrix, which is governed by the Liouville-von Neumann equation

$$i\hbar\frac{\partial \rho}{\partial t} = [H,\rho]. \tag{15}$$

We shall analyze separately the contribution to the time evolution due to the periodic potential, and determined by the Hamiltonian H_0, and the contribution due to the external potential V. We shall write explicitely

$$\frac{\partial \rho}{\partial t} = \left(\frac{\partial \rho}{\partial t}\right)_0 + \left(\frac{\partial \rho}{\partial t}\right)_V, \tag{16}$$

where $i\hbar(\partial\rho/\partial t)_0 = [H_0,\rho]$ and $i\hbar(\partial\rho/\partial t)_V = [V,\rho]$. Similarly, we shall write

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_0 + \left(\frac{\partial f}{\partial t}\right)_V \tag{17}$$

for the Wigner function.

We begin by considering the time evolution of the Wigner function due to the periodic potential. From equation (12) we have:

$$i\hbar\left(\frac{\partial f_{m'm''}}{\partial t}\right)_0(x,p,t) = \int_{B^2} dk'dk''i\hbar\left(\frac{\partial \rho_{m'm''}}{\partial t}\right)_0(k',k'',t)\Phi_{m'm''}(k',k'',x,p) \tag{18}$$

and, by using equations (3) and (15),

$$\begin{aligned} i\hbar\left(\frac{\partial \rho_{m'm''}}{\partial t}\right)_0(k',k'',t) &= < m'k'|[H_0,\rho]|m''k'' > = \\ &= [\epsilon_{m'}(k') - \epsilon_{m''}(k'')]\rho_{m'm''}(k',k'',t). \end{aligned}$$

By using the Fourier expansion (6) for the energy bands, we then have:

$$
\begin{aligned}
& i\hbar \left(\frac{\partial f_{m'm''}}{\partial t} \right)_0 (x,p,t) = \\
& \int_{B^2} dk'dk''[\epsilon_{m'}(k') - \epsilon_{m''}(k'')]\rho_{m'm''}(k',k'',t)\Phi_{m'm''}(k',k'',x,p) = \\
& = \int_{B^2} dk'dk'' \sum_{\mu \in L} [\widehat{\epsilon}_{m'}(\mu)e^{ik'\mu} - \widehat{\epsilon}_{m''}(\mu)e^{ik''\mu}] \times \\
& \times \rho_{m'm''}(k',k'',t)\Phi_{m'm''}(k',k'',x,p). \qquad (19)
\end{aligned}
$$

In order to obtain a closed system of equations for the $f_{m'm''}$'s, the right hand side of equation (19) must be rewritten in terms of the $f_{m'm''}$'s themselves. By using (5) and following [11], we have that $e^{ik\mu} < x + \eta/2|mk >=< x + \mu + \eta/2|mk >$ and $e^{ik\mu} < mk|x - \eta/2 >=< mk|x - \mu - \eta/2 >$ and, after substituting in (19) and using the explicit expression for the coefficients (10), we have:

$$
\begin{aligned}
& i\hbar \left(\frac{\partial f_{m'm''}}{\partial t} \right)_0 (x,p,t) = \sum_{\mu \in L} \int_{B^2} dk'dk''\rho_{m'm''}(k',k'',t) \times \\
& \times \left[\widehat{\epsilon}_{m'}(\mu)\Phi_{m'm''}(k',k'',x + \frac{\mu}{2},p) - \widehat{\epsilon}_{m''}(\mu)\Phi_{m'm''}(k',k'',x - \frac{\mu}{2},p) \right] e^{ip\mu/\hbar}.
\end{aligned}
$$

After rearranging terms we finally obtain:

$$
\begin{aligned}
& i\hbar \left(\frac{\partial f_{m'm''}}{\partial t} \right)_0 (x,p,t) = \\
& = \sum_{\mu \in L} \left[\widehat{\epsilon}_{m'}(\mu) f_{m'm''}(x + \frac{\mu}{2},p,t) - \widehat{\epsilon}_{m''}(\mu) f_{m'm''}(x - \frac{\mu}{2},p,t) \right] e^{ip\mu/\hbar} \qquad (20)
\end{aligned}
$$

Equations (20) for the band projections $f_{m'm''}$ are the equations that govern the time evolution of the Wigner function of an ensemble of electrons moving in a semiconductor crystal in the absence of external fields and of collisions, and that allows for energy bands of any shape. Note that, as was to be expected, the populations of the bands do not interact and each contribution to the Wigner function evolves independently in the absence of external fields. Equation (20) is a generalization to the multi-band case of an earlier result obtained by Markowich, Mauser and Poupaud [11] for a single band. In the

next Section, we shall relate these equations to the better known equations of the effective mass approximation.

Next, we consider the time evolution of the Wigner function due to the external potentials:

$$i\hbar \left(\frac{\partial f}{\partial t}\right)_V (x,p,t) = \int d\eta < x + \frac{\eta}{2}|[V,\rho]|x - \frac{\eta}{2} > e^{-ip\eta/\hbar}. \qquad (21)$$

We recall that the right hand side of equation (21), can be cast in the form [1]

$$\int d\eta < x + \frac{\eta}{2}|[V,\rho]|x - \frac{\eta}{2} > e^{-ip\eta/\hbar} = (\Theta(\delta V)f)(x,p,t) \qquad (22)$$

where $\Theta(\delta V)$ is the pseudodifferential operator with symbol $\delta V(x,\eta) = V(x+\eta/2) - V(x-\eta/2)$,

$$(\Theta(\delta V)f)(x,p,t) = \int d\eta \delta V(x,\eta)\hat{f}(x,\eta,t)e^{-ip\eta/\hbar},$$

and

$$\hat{f}(x,\eta,t) = \frac{1}{2\pi\hbar}\int dp f(x,p,t)e^{ip\eta/\hbar}$$

is the Fourier transform of the Wigner function with respect to the momentum variable. Expressions (21)-(22) remain valid also in the multiband case, with f the total Wigner function. We are however interested in the time evolution of the single components $f_{m'm''}$, which can be obtained by acting on both sides of equation (21) with the operator $\mathcal{P}_{m'm''}$. From equation (22) we have:

$$\begin{aligned}
&\mathcal{P}_{m'm''}(\Theta(\delta V)f)(x,p,t) = \\
&= \frac{1}{2\pi\hbar}\int\int dx'dp' W_{m'm''}(x,p,x',p')(\Theta(\delta V)f)(x',p',t) = \\
&= \frac{1}{2\pi\hbar}\int\int dx'dp' W_{m'm''}(x,p,x',p')\int d\eta \delta V(x',\eta)\hat{f}(x',\eta,t)e^{-ip'\eta/\hbar} = \\
&= \frac{1}{2\pi\hbar}\int dx'\int dp' W_{m'm''}(x,p,x',p')e^{-ip'\eta/\hbar}\int d\eta \delta V(x',\eta)\hat{f}(x',\eta,t) = \\
&= \int\int dx'd\eta \widehat{W}_{m'm''}(x,p,x',-\eta)\delta V(x',\eta)\hat{f}(x',\eta,t),
\end{aligned}$$

where

$$\widehat{W}_{m'm''}(x,p,x',\eta) = \frac{1}{2\pi\hbar}\int dp' W_{m'm''}(x,p,x',p')e^{ip'\eta/\hbar}$$

is the Fourier transform of $W_{m'm''}$ with respect to the last variable, and finally

$$i\hbar \left(\frac{\partial f_{m'm''}}{\partial t} \right)_V (x,p,t) = \int\int dx' d\eta \widehat{W}_{m'm''}(x,p,x',-\eta) \delta V(x',\eta) \hat{f}(x',\eta,t). \tag{23}$$

The full time evolution of the band projection $f_{m'm''}$ of the Wigner function, due to both the periodic potential of the crystal lattice and the external potential, is obtained by adding the two contributions of equation (20) and equation (23):

$$\begin{aligned} i\hbar \frac{\partial f_{m'm''}}{\partial t} = \\ = \sum_{\mu \in L} \left[\widehat{\epsilon}_{m'}(\mu) f_{m'm''}(x + \frac{\mu}{2}, p, t) - \widehat{\epsilon}_{m''}(\mu) f_{m'm''}(x - \frac{\mu}{2}, p, t) \right] e^{ip\mu/\hbar} + \\ + \int\int dx' d\eta \widehat{W}_{m'm''}(x,p,x',-\eta) \delta V(x',\eta) \hat{f}(x',\eta,t). \end{aligned} \tag{24}$$

Equation (24) gives the full time evolution of each component of the Wigner function, in presence of an external field and in the absence of collisions.

3.1 Quantum effects for linear and quadratic potentials

It is well known that in the case of linear and quadratic potentials the pseudodifferential operator of the transport equation for the standard Wigner function reduces to the classical differential operator of the Boltzmann equation. We now show that this property holds in the multiband case with a slight modification.

In the case of linear and quadratic potentials, the symbol δV of the pseudodifferential operator factors in the form

$$\delta V(x,\eta) = V(x + \eta/2) - V(x - \eta/2) = -F(x)\eta$$

where $F(x)$ is the force. For a linear potential, $V(x) = -Ex$ and we have $F(x) = E$; for a quadratic potential, $V(x) = \alpha x^2/2$ and we have $F(x) = -\alpha x$.

In either case, the standard pseudodifferential operator with the potential becomes the differential operator in p-space of the classical Boltzmann equation:

$$\begin{aligned}\Theta(\delta V)f &= \int d\eta \delta V(x,\eta)\hat{f}(x,\eta)e^{-ip\eta/\hbar} = \\ &= -F(x)\int d\eta\eta\hat{f}(x,\eta)e^{-ip\eta/\hbar} = i\hbar F(x)\frac{\partial f}{\partial p}.\end{aligned}$$

In the multiband case, a more general result is obtained and we have for equation (23):

$$i\hbar\left(\frac{\partial f_{m'm''}}{\partial t}\right)_V(x,p,t) = \mathcal{P}_{m'm''}(\Theta(\delta V)f)(x,p,t) = i\hbar\mathcal{P}_{m'm''}\left(F\frac{\partial f}{\partial p}\right)(x,p,t). \tag{25}$$

In the case of a constant applied external field, E, we have $F(x) = E$ and equation (25) becomes

$$\left(\frac{\partial f_{m'm''}}{\partial t}\right)_V(x,p,t) = E\mathcal{P}_{m'm''}\left(\frac{\partial f}{\partial p}\right)(x,p,t). \tag{26}$$

The simplification introduced by the differential operator is very important for numerical calculations.

4 The parabolic band approximation and the effective mass

The single band model with the parabolic band approximation is used to describe the electron population near the minimum of the conduction band. In electronic devices such as the RTD, this approximation is justified since these electrons are responsible for most part of the flow of current. In the parabolic band approximation, the evolution equation for the Wigner function simplifies considerably. Moreover, in the absence of external fields the evolution equations in the parabolic band approximation can be written out without the explicit knowledge of the eigenfunctions of the Hamiltonian (the Bloch states), and they reduce to the standard free-streaming part of the Wigner equation.

In the presence of external fields, instead, little progress can be made without the knowledge of the Bloch states for the material under study. For this reason, we shall analyze the field-free case only, leaving the case with the field for a separate work [20].

In the single band model, the total Wigner function f coincides with the projection onto the conduction band and the sum over m' and m'' in equation (7) collapses to a single term, say $m' = m'' = 1$. Equation (20) with $m' = m'' = 1$ then gives the time evolution of the Wigner function of the conduction band for a band of arbitrary shape in the absence of external fields.

For a band $\epsilon(k)$ having a minimum at $k = 0$, in the parabolic band approximation and in the absence of external potentials, the evolution equation for the Wigner function f is given by

$$\frac{\partial f}{\partial t} + \frac{p}{m_*}\frac{\partial f}{\partial x} = 0,$$

with

$$m_* = \hbar^2 \left(\frac{\partial^2 \epsilon}{\partial k^2} \right)^{-1}_{k=0}$$

the effective mass. If the energy band attains its minimum at $k = k_*$,

$$\epsilon(k) = \epsilon(k_*) + \frac{\hbar^2 (k - k_*)^2}{2m_*}, \tag{27}$$

with the effective mass defined by

$$m_* = \hbar^2 \left(\frac{\partial^2 \epsilon}{\partial k^2} \right)^{-1}_{k=k_*}, \tag{28}$$

the evolution equation is

$$\frac{\partial f}{\partial t} + \frac{p - \hbar k_*}{m_*}\frac{\partial f}{\partial x} = 0 \tag{29}$$

In this section, we shall discuss the parabolic band approximation from the exact equation (20) for a single band and illustrate its range of validity. Throughout this Section, we shall omit the band index from the band energy function

($\epsilon(k)$ instead of $\epsilon_m(k)$) and from the band projection (f instead of $f_{m'm''}$) of the Wigner function. We shall also write $\partial f/\partial t$ for $(\partial f/\partial t)_0$ throughout this and the next Section. Equation (20) for a single band of arbitrary shape is

$$i\hbar\frac{\partial f}{\partial t}(x,p,t) = \sum_{\mu\in L}\widehat{\epsilon}(\mu)\left[f(x+\frac{\mu}{2},p,t) - f(x-\frac{\mu}{2},p,t)\right]e^{ip\mu/\hbar}. \qquad (30)$$

By expanding the nonlocal terms in the square brackets in a Taylor series about $\mu = 0$, we obtain:

$$\begin{aligned} i\hbar\frac{\partial f}{\partial t}(x,p,t) &= \sum_{\mu\in L}\widehat{\epsilon}(\mu)\left[\sum_{n=0}^{\infty}2\left(\frac{\mu}{2}\right)^{2n+1}\frac{1}{(2n+1)!}\frac{\partial^{2n+1}f}{\partial x^{2n+1}}\right]e^{i\mu p/\hbar} = \\ &= \sum_{n=0}^{\infty}\frac{2^{-2n}}{(2n+1)!}\frac{\partial^{2n+1}f}{\partial x^{2n+1}}\sum_{\mu\in L}\widehat{\epsilon}(\mu)\mu^{2n+1}e^{i\mu p/\hbar} = \\ &= -i\sum_{n=0}^{\infty}\frac{2^{-2n}(-1)^n}{(2n+1)!}\left[\frac{\partial^{2n+1}\epsilon}{\partial k^{2n+1}}\right]_{p/\hbar}\frac{\partial^{2n+1}f}{\partial x^{2n+1}} = \\ &= -i\left[\frac{\partial\epsilon}{\partial k}\right]_{p/\hbar}\frac{\partial f}{\partial x} + i\frac{1}{4!}\left[\frac{\partial^3\epsilon}{\partial k^3}\right]_{p/\hbar}\frac{\partial^3 f}{\partial x^3} + \ldots. \end{aligned}$$

For the parabolic band given in (27) the third derivatives of the energy band vanish exactly and we obtain the evolution equation (29) for the Wigner function. Notice that the first non-parabolicity correction is proportional to the third derivative of the energy band at the minimum and it involves the third partial derivative of the Wigner function with respect to the space variable. The non-parabolicity correction to the free-streaming equation dosn't appear as a small term in some parameter, but it is of the same order of magnitude as the free-streaming terms. This fact needs further understanding, particularly since the parabolic band approximation is known to work well when only states near the minimum of the band contribute to the density matrix (and thus to the Wigner function).

It is also interesting to compare the exact solution of equation (30) with the solution of the corresponding free-streaming equation obtained in the effective mass approximation.

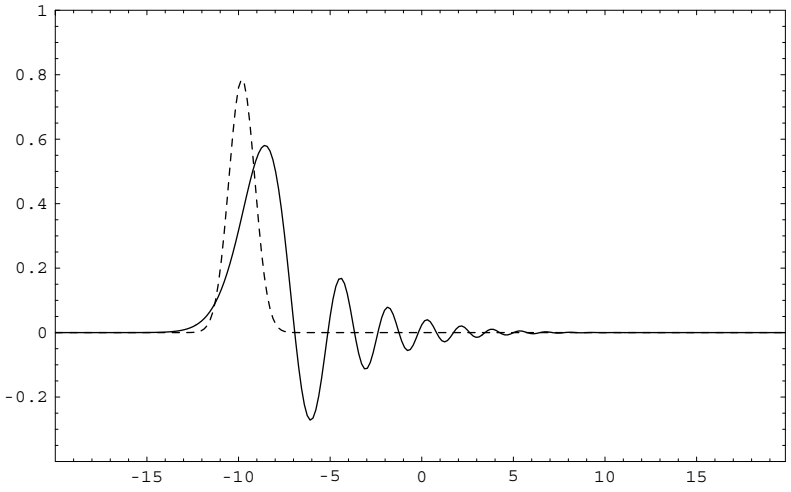

Figure 1: $f(x,p)$ as a function of x, $0 \leq x \leq 20$ for $p \approx 0.5$, and for $t = 20$; exact solution from (31) (solid line), free-streaming approximation from equation (29) (dashed line). Dimensionless variables as defined in the text.

For the comparison, which is only qualitative, we have used dimensionless variables: the space variable x is measured in units of a, the momentum p in units of $\hbar/a$, time t in units of $ma^2/\hbar$ and the crystal momentum k in units of $1/a$. In the dimensionless variables, the free-streaming equation becomes

$$\frac{\partial f}{\partial t} + p\frac{\partial f}{\partial x} = 0.$$

Also, we have chosen $\epsilon(k) = 1 - \cos k$, $-\pi \leq k \leq \pi$, for the band profile (thus $k_* = 0$) and $0 \leq x \leq 20$. Note that, with these dimensionless quantities, the phase-space momentum p and the crystal momentum k, though different variables, are measured in the same units. We have followed the time evolution of an initial Gaussian shaped Wigner function in phase space, according to the exact equation and according to the free-streaming approximation. Equation (30) can be solved explicitely by using Fourier Transforms in space. If $\hat{f}_k$ is the $k-$th Fourier component of f with respect to x, it is easy to see that

$$\hat{f}_k(p,t) = \hat{f}_k(p,0)e^{i\alpha_k(p)t} \tag{31}$$

where

$$\alpha_k(p) = 2i\sum_\mu \widehat{\epsilon}(\mu)\sin\frac{k\mu}{2}e^{ip\mu/\hbar}.$$

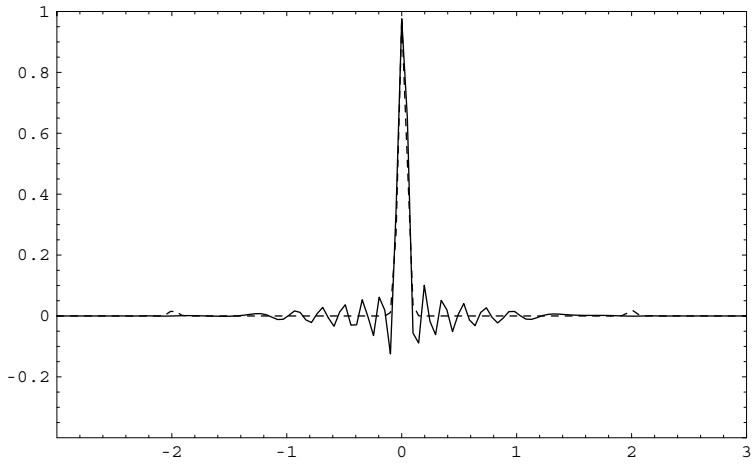

Figure 2: $f(x,p)$ as a function of p, $-\pi \leq p \leq \pi$ for $x = 0$, and for $t = 20$; exact solution from (31) (solid line), free-streaming approximation from equation (29) (dashed line). Dimensionless variables as defined in the text.

The main features of the comparison are shown in Figures 1, 2 and 3. Figure 1 shows $f(x,p)$ as a function of x for a fixed value of p, $p \approx 0.5$, and a fixed value of t. Figure 2 shows $f(x,p)$ as a function of p for a fixed value of x, $x = 0$, and the same fixed value of t. This value of t is such that the range of phase space momenta where the bulk of the Wigner function lies, when interpreted in terms of the crystal momentum variable, still corresponds to the parabolicity region of the band. Figure 3 shows the average position

$$< x > (p,t) = \frac{\int x f(x,p,t) dx}{\int f(x,p,t) dx} \tag{32}$$

as a function of time for $0 \leq t \leq 30$ and for $p \approx 0.5$. The solid lines represent the exact solution and the dashed lines represent the free-streaming approximation.

From these figures, it is clear that the free-streaming approximation cannot describe the oscillatory behaviour of the Wigner function in phase space. The oscillations, however, contribute little to the moments and the results for the average quantities shows a better agreement (see Figure 3). This example underlines the conceptual and practical difference between the Wigner variable

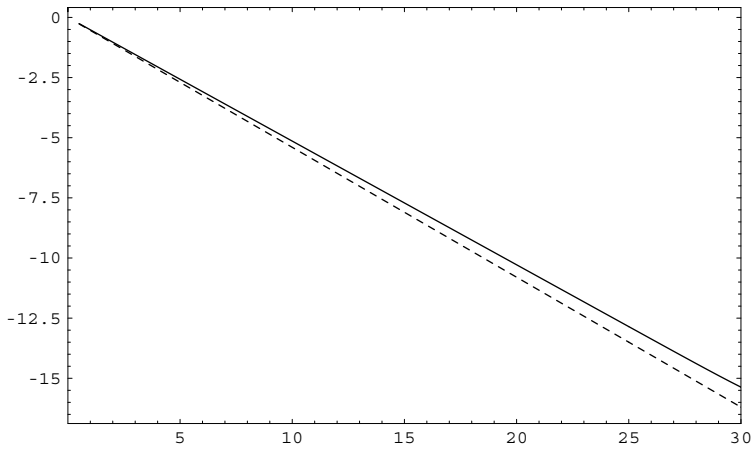

Figure 3: Average position $< x >$ from equation (32) as a function of t, $0 \leq t \leq 30$ for $p \approx 0.5$; exact solution (solid line), free-streaming approximation (dashed line). Dimensionless variables as defined in the text.

p and the crystal momentum k of the Bloch functions. It has to be remarked that other effects, such as external fields and collisions, will alter this picture significantly; in particular, collisions may help the particles stay near the band minimum, while external fields will tend to move them farther away. We shall examine these details in a separate work.

4.1 A two-band model with no external fields

It is interesting to exemplify our concepts with a simple two-band model which, for now, does not include external fields. In a two-band model the Wigner function and its evolution equation are given by equations (7) and (20) where now $m' = 1, 2$ and $m'' = 1, 2$. The Wigner function is then given by the sum of four contributions, f_{11}, f_{12}, f_{21} and f_{22}. It can be seen easily from equation (8) that $f_{12} = f_{21}^*$, while f_{11} and f_{22} are real. Each of the four contributions evolves according to equation (20). In the parabolic band approximation, the differential equations for f_{11} and f_{22} are identical to (29):

$$\frac{\partial f_{11}}{\partial t} + \frac{p - \hbar k_1}{m_1} \frac{\partial f_{11}}{\partial x} = 0 \tag{33}$$

$$\frac{\partial f_{22}}{\partial t} + \frac{p-\hbar k_2}{m_2}\frac{\partial f_{22}}{\partial x} = 0, \tag{34}$$

where m_1 and m_2 are the effective masses for band 1 and band 2 respectively and k_1 and k_2 are the values of the crystal momentum at which band 1 and band 2 attain their minimum. The evolution equations for f_{12} and $f_{21} = f_{12}^*$ have instead a different structure. From equation (20), after a simple calculation, we have

$$i\hbar\frac{\partial f_{12}}{\partial t} = \left\{\left[\epsilon_1(k_1) + \frac{(p-\hbar k_1)^2}{2m_1}\right] - \left[\epsilon_2(k_2) + \frac{(p-\hbar k_2)^2}{2m_2}\right]\right\} f_{12}(x,p) + \\ - \frac{i\hbar}{2}\left(\frac{p-\hbar k_1}{m_1} + \frac{p-\hbar k_2}{m_2}\right)\frac{\partial f_{12}}{\partial x} - \frac{1}{8}\left(\frac{\hbar^2}{m_1} - \frac{\hbar^2}{m_2}\right)\frac{\partial^2 f_{12}}{\partial x^2},$$

which, by introducing $\omega_{12} = (\epsilon_1(k_1) - \epsilon_2(k_2))/\hbar$, $\Omega_{12}(p) = \omega_{12} + (p-\hbar k_1)^2/(2m_1\hbar) - (p-\hbar k_2)^2/(2m_2\hbar)$ and

$$g_{12}(x,p) = f_{12}(x,p)e^{i\Omega_{12}(p)t},$$

can be cast in the more elegant form

$$\frac{\partial g_{12}}{\partial t} + \frac{1}{2}\left(\frac{p-\hbar k_1}{m_1} + \frac{p-\hbar k_2}{m_2}\right)\frac{\partial g_{12}}{\partial x} - \frac{i\hbar}{8}\left(\frac{1}{m_1} - \frac{1}{m_2}\right)\frac{\partial^2 g_{12}}{\partial x^2} = 0. \tag{35}$$

Note that in the definition of the Wigner function (7) f_{12} and f_{21} appear only in the combination $f_{12} + f_{21}$, consistently with the Wigner function's being real. The time evolution of the real and imaginary parts is given by the system obtained by taking real and imaginary parts of (35).

Equation (35) shows that the time evolution of f_{12} is the composition of an oscillatory term, a free streaming term and a diffusive term. The frequency of the oscillatory term, Ω_{12}, is proportional to the difference in the total energy of the particle in the two bands; the velocity of the free streaming term is an average of the velocities of the particle in the two bands and the diffusion coefficient in the diffusive term depends, in magnitude and sign, on the relative magnitude of the effective masses.

Equations (33), (34) and (35) completely describe the time evolution of all the components of the Wigner function in the two band model with the parabolic band approximation and in the absence of external fields. Note these evolution equations are uncoupled.

5 Conclusions

In this work we have developed a model describing the multiband transport of electrons in a semiconductor crystal by using the Wigner function approach. An infinite homogeneous medium, with space-independent band profiles, has been assumed throughout. We have defined the components of the Wigner function on each band subspace by introducing a projection operator that acts on the total Wigner function and gives the band projection as a result. We have derived exact evolution equations for each Wigner projection, with and without external fields. In absence of fields the equations are uncoupled, as expected. This confirms that band transitions can occur only in presence of external fields or collisions. The numerical approach to the model equations is underway.

Finally, we have discussed the effective mass approximation in the absence of external fields and compared the exact time evolution with the free-streaming evolution that governs the Wigner function in the effective mass approximation.

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