Wigner-function approach to multiband transport in semiconductors

Lucio Demeio\textsuperscript{a,*,} Luigi Barlettib, Andrea Bertonic, Paolo Bordonec, Carlo Jacobonic

\textsuperscript{a} Dipartimento di Matematica “V. Volterra”, Università degli Studi di Ancona, Via Brecce Bianche 1, 60131 Ancona, Italy
\textsuperscript{b} Dipartimento di Matematica “U. Dini”, Università degli Studi di Firenze, Firenze, Italy
\textsuperscript{c} Dipartimento di Fisica, Università di Modena e Reggio Emilia, Modena, Italy

Abstract

In this work we present a one-dimensional, multi-band model for electron transport in semiconductors that makes use of the Wigner-function formalism and that allows for energy bands of any shape. A simplified two-band model is then derived from the general equations, by using the parabolic band approximation.

Keywords: Wigner function; Quantum transport; Multi-band transport models

1. Introduction

The Wigner function approach to electron transport in semiconductors is widely used to describe the properties of electronic devices such as the Resonant Tunneling Diode (RTD) and others [1]. All existing transport models based on the Wigner function, however, rely on the following two approximations: (1) that only 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, the evolution equation for the Wigner function reduces to the evolution equation for semiclassical particles with an effective mass. This allows the inclusion of any external field (barriers and bias) by means of the standard potential scattering integral (pseudodifferential [2]) operator [3].

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 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 an evolution equation which allows for energy bands of any shape. In absence of external fields,

\*Corresponding author. Fax: +39-071-2204870.
E-mail address: demeio@popcsi.unian.it (L. Demeio).

0921-4526/02/$-see front matter \copyright{} 2002 Elsevier Science B.V. All rights reserved.
PII: S0921-4526(01)01354-0
the evolution equations are a generalization of an earlier result for a single band by Markowich et al. [4].

2. The density matrix and the Wigner function

The Wigner function, describing a statistical ensemble of electrons in phase space, is defined by a Fourier transformation of the density matrix. If ρ is the single particle density operator and ρ(r,s) = ⟨r|ρ|s⟩ is the corresponding density matrix in space representation, the Wigner function [5] is given by

\[ f(x,p) = \int \mathrm{d}η \langle x + \frac{η}{2} | ρ | x - \frac{η}{2} \rangle e^{-iπη/h}. \]  

(1)

In general, an electron in the crystal will be found in a statistical superposition of Bloch states belonging to different energy bands. 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-state representation. As a result, the Wigner function can be written as a double sum of contributions from all energy bands, \( f(x,p) = \sum_{m' n'} f_{n'm'}(x,p) \), where

\[ f_{n'm'}(x,p) = \int_{B^2} \mathrm{d}k' \mathrm{d}k'' ρ_{n'm'}(k', k'') x \int \mathrm{d}η \langle x + \frac{η}{2} | m'k' | x - \frac{η}{2} \rangle e^{-iπη/h}. \]  

(2)

Here, \( \{ |mk⟩ \} \) are the Bloch states, with \( m \) the band index, \( k \) the crystal momentum, \( B \) the Brillouin zone and \( ρ_{n'm'}(k', k'') = ⟨ m'k' | ρ | m''k''⟩ \). The functions \( f_{n'm'} \) are the projections of \( f \) onto the band subspaces. Eq. (2) can be written in a more compact form, as the result of a projection operator \( P_{n'm'} \) acting on the Wigner function \( f \), \( f_{n'm'}(x,p) = \langle P_{n'm'}f \rangle(x,p) \). By introducing the coefficients \( Φ_{n'm'}(k', k'', x,p) = \int \mathrm{d}η \langle x + \frac{η}{2} | m'k' | x - \frac{η}{2} \rangle e^{-iπη/h} \) (analogous to those introduced in Refs. [6–8]), and the transfer function

\[ W_{n'm'}(x,p, x', p') = \int_{B^2} \mathrm{d}k' \mathrm{d}k'' Φ_{n'm'}(k', k'', x,p) \]

\[ \times Φ_{m'n'}(k', k'', x', p'), \]  

(3)

the band projection \( f_{n'm'} \) can be written as

\[ f_{n'm'}(x,p) = \frac{1}{2\pi} \int \int \mathrm{d}x' \mathrm{d}p' W_{n'm'}(x,p, x', p') f(x', p') \]

\[ \equiv (P_{n'm'}f)(x,p). \]  

(4)

The last equality defines the linear integral operator \( P_{n'm'} \), which yields the projections \( f_{n'm'} \) from the total Wigner function \( f \).

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

\[ \int \int \mathrm{d}x \mathrm{d}p f(x,p) = \sum_{n} \int \int \mathrm{d}x \mathrm{d}p f_{nn}(x,p). \]

3. General evolution equations

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

\[ i\hbar \frac{\partial f}{\partial t}(x,p,t) = \sum_{n} i\hbar \frac{\partial f_{nn}}{\partial t}(x,p,t), \]

and it must follow from the time evolution of the density matrix, which is governed by the Liouville–von Neumann equation. By considering separately the contribution to the time evolution due to the periodic potential and the contribution due to the external potential \( V \), \( \partial f / \partial t = (\partial f / \partial t)_V + (\partial f / \partial t)_0 \), after some algebra we find that

\[ i\hbar \left( \frac{\partial f_{nn}}{\partial t} \right)_0 (x,p,t) = \sum_{\mu \in L} \left[ \hat{e}_\mu(t) f_{n'n'}(x + \frac{\mu}{2}, p, t) \right] e^{i\mu k_0}, \]

\[ - \hat{e}_\mu(t) f_{n'n'}(x - \frac{\mu}{2}, p, t) \]  

(5)
and
\[
\frac{i\hbar}{\partial t} \left( \frac{\partial f_{m' n'}}{\partial t} \right)_{V}(x, p, t) \\
= \int \int \int d\xi' d\eta' \delta V(\xi', \eta') \hat{W}_{m' n'}(x, p, x', -\eta') \\
\times \hat{f}(x', \eta, t),
\]
where \( \hat{w}_m \) are the Fourier coefficients of the energy band function, \( \mu \) are vectors of the direct lattice \( L \), \( \delta V(x, \eta) = V(x + \eta/2) - V(x - \eta/2) \) and \( \hat{W}_{m' n'} \) and \( \hat{f} \) are the Fourier transforms of the transfer function \( W_{m' n'} \) and of the Wigner function \( f \), respectively. Eq. (6) can also be written in the form
\[
\frac{i\hbar}{\partial t} \left( \frac{\partial f_{m' n'}}{\partial t} \right)_{V}(x, p, t) \\
= \frac{1}{2\pi \hbar} \int d\xi' \int dp' dp'' W_{m' n'}(x, p, x', p'') \\
\times v_w(x', p'' - p') f(x', p', t),
\]
where
\[
v_w(x, p) = \frac{1}{2\pi \hbar} \int d\eta \delta V(x, \eta)e^{-i\eta \eta / \hbar},
\]
is the potential transfer function. Eq. (5) for the band projections \( f_{m' n'} \) is the equation that govern the time evolution of the Wigner function for an ensemble of electrons moving in a semiconductor crystal in the absence of external fields 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. Eq. (5) is a generalization to the multi-band case of an earlier result obtained by Markowich et al. [4] for a single band. In the case of a single parabolic band and in the absence of external potentials the evolution equation for the Wigner function \( f \) reduces to the free streaming part of the usual transport equation. That is, for a band \( \epsilon(k) \) having a minimum at \( k = 0 \),
\[
\frac{\partial f}{\partial t} + \frac{p}{m_*} \frac{\partial f}{\partial x} = 0,
\]
where \( m_* \) is the effective mass. If the energy band attains its minimum at \( k = k_* \), the evolution equation is
\[
\frac{\partial f}{\partial t} + \frac{p - \hbar k_*}{m_*} \frac{\partial f}{\partial x} = 0.
\]
It can be shown that the property of the standard Wigner function, that its evolution equation reduces to the classical collisionless Boltzmann equation in the case of linear and quadratic potentials, also holds, in a generalized form, in the multiband case. In fact, for both linear and quadratic potentials, the symbol \( \delta V \) 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. It can be shown that
\[
\frac{i\hbar}{\partial t} \left( \frac{\partial f_{m' n'}}{\partial t} \right)_{V}(x, p, t) = i\hbar \mathcal{P}_{m' n'} \left( \frac{\partial f}{\partial p} \right)(x, p, t).
\]
In the case of a constant applied external field, \( E \), we have \( F(x) = E \) and Eq. (9) becomes
\[
\frac{\partial f_{m' n'}}{\partial t}(x, p, t) = E \mathcal{P}_{m' n'} \left( \frac{\partial f}{\partial p} \right)(x, p, t).
\]
The simplification introduced by the differential operator is very important for numerical calculations.

4. A two band model

A simplified two band transport model can be derived from the exact Eqs. (5) and (6) by using the parabolic band approximation. In the case of two parabolic bands, the evolution equations for \( f_{11} \) and \( f_{22} \) due to the periodic potential alone are given by (8):
\[
\left( \frac{\partial f_{11}}{\partial t} \right)_0 + \frac{p - \hbar k_1}{m_1} \frac{\partial f_{11}}{\partial x} = 0
\]
(11)
\[
\left( \frac{\partial f_{22}}{\partial t} \right)_0 + \frac{p - \hbar k_2}{m_2} \frac{\partial f_{22}}{\partial x} = 0,
\]
(12)
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 \( f_{21} = f_{12}^\dagger \) have instead a different structure. From Eq. (5) we have

\[
\text{ih} \left( \frac{\partial f_{12}}{\partial t} \right)_0 = \left\{ \left[ e_1(k_1) + \frac{(p - h k_1)^2}{2m_1} \right] - \left[ e_2(k_2) + \frac{(p - h k_2)^2}{2m_2} \right] \right\} f_{12}(x,p) \\
- \frac{\text{ih}}{2} \left[ \frac{p - h k_1}{m_1} + \frac{p - h k_2}{m_2} \right] \frac{\partial f_{12}}{\partial x} \\
- \frac{1}{8} \left( \frac{h^2}{m_1} - \frac{h^2}{m_2} \right) \frac{\partial^2 f_{12}}{\partial x^2},
\]

(13)

For the evolution equation due to the external potential (see Eq. (6)), we need explicit expressions for the Bloch states, since they appear explicitly in the transfer function \( W_{mn}^{m' n'} \). If we assume for simplicity that the Bloch functions for each band are plane waves, that is \( \langle x | m k \rangle = e^{ikx} \psi_m(k, x) \approx e^{ik_0 x} e^{i(k_0^* - k_0)x} \), with \( k_0^* \) the crystal momentum at which the \( m \)th band attains its minimum and \( a \) the lattice period, we find, after some algebra, that the band projection of the Wigner function is given by

\[
f_{mn}^{m'n'}(x,p) = \frac{4\pi}{a} H\left( \frac{\pi}{a} \frac{p}{\hbar} + k_S \right) \\
\times \left[ dx' \Delta(\frac{x - x'}{a}) f(x', p) \right. \\
\left. \times e^{-i(2\pi(n'-n')/a - k_0)(x-x')} \right],
\]

with \( H(x) \) the Heaviside function, \( \Delta(x) = \sin(2\pi x)/x \). Note that \( f_{mn}^{m'n'} = 0 \) outside of the Brillouin zone. The evolution equation is given by

\[
\text{ih} \left( \frac{\partial f_{mn}^{m'n'}}{\partial t} \right)(x,p,t) = \left( \hat{\Theta} f \right)(x,p,t).
\]

(14)

where \( \hat{\Theta} \) is an operator acting on the whole Wigner function \( f \) and is given by

\[
\left( \hat{\Theta} f \right)(x,p) = \frac{2\pi}{a} H\left( \frac{\pi}{a} \frac{p}{\hbar} + k_S \right) \\
\times \left[ dx' \Delta(\frac{x - x'}{a}) f(x', p) \right. \\
\left. \times e^{-i(2\pi(n'-n')/a - k_0)(x-x')} \right]
\]

(15)

For a constant applied external field \( E \), the operator \( \hat{\Theta} \) becomes

\[
\left( \hat{\Theta} f \right)(x,p) = \frac{2\pi i \hbar E}{a} H\left( \frac{\pi}{a} \frac{p}{\hbar} + k_S \right) \\
\times \left[ dx' \Delta(\frac{x - x'}{a}) f(x', p) \right. \\
\left. \times e^{-i(2\pi(n'-n')/a - k_0)(x-x')} \right].
\]

(16)

The equations of the two-band model with a constant applied external field are then obtained by adding up Eqs. (11)–(13) with (14) and with \( \hat{\Theta} \) given by Eq. (16).

A numerical application of this two band model, aimed at investigating Zener tunneling, is underway and will be presented in a future work.

References