A WKB approach to the quantum multiband electron dynamics in the kinetic formalism.

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Abstract

We derive a WKB-like asymptotic expansion of the multiband Wigner function. The model, derived in the envelope function theory, is designed to describe the dynamics in semiconductor devices when the interband conduction-valence transition cannot be neglected. We derive a hierarchy of equations that to lowest order consist of two Hamilton-Jacobi equations corresponding to the classical dynamics of point particles with positive and negative kinetic energy. Our methodology is based on the Van Vleck approach and a WKB-like asymptotic expansion procedure is used to reduce the numerical complexity of the Wigner multiband evolution system. An approximate closed-form solution is obtained by an iterative procedure that exploits the different time scales on which the intraband and interband dynamical variables evolve. The interband tunneling mechanism appearing to the first order of the expansion is expressed in a very simple mathematical form. By exploiting the highly oscillating behaviour of the multiband Wigner functions we derive an asymptotic expression of the interband transition probability. The resulting formulation reveals particularly close to the classical description of the particles motion and this formal analogy is useful to gain new physical insight and to profit of the numerical method developed for classical systems. The approximates evolution equations are used to simulate the evolution of the Wigner quasi-distribution function in a IRTD diode.

Keywords: WKB, multiband kinetic dynamic, Wigner formalism.

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1. Introduction

Recently much attention has been paid to quantum transport models. In particular, multiband transport is a topic of growing interest among physicists and applied mathematicians studying semiconductor devices of nanometric size. Indeed, quantum effects cannot be neglected when the size of the electronic device becomes comparable to the electron wavelength, as in new generation devices. For this reason, quantum modeling becomes a crucial aspect in nanoelectronics research from the perspective of analog and digital applications. In the past several decades an increasing effort has
been devoted in deriving new approach to the charge transport whose validity spans from the classical transport to the full quantum dynamics. Despite the progress obtained in this field, a general framework where quantum effects can be easily included in a mesoscopic structure where also classical transport play an important role, is far from being achieved. Different approaches based on the density matrix, non equilibrium Green’s functions, and the Wigner function have been proposed to achieve a quantum description of electron transport [1]. Among them, the Wigner-function formalism is the one that bears the closest similarities to the classical Boltzmann equation, which suggests the possibility of using this formalism in order to obtain quantum corrections to the classical phase-space motion. The phase-space formulation of quantum mechanics offers a framework in which quantum phenomena can be described in a classical language and the question of the quantum-classical correspondence can be directly investigated. In particular, the visual representation of the quantum motion by quantum-corrected phases-plane trajectories, is a valuable aid to a conceptual understanding of the complex quantum dynamics.

We are interested in study semiconductor devices characterized by tunneling effects between different bands, as the resonant interband tunneling diode (RITD) (see for instance [2]–[3]). Unlike the usual semiconductor devices where the bulk band structure is slightly modified by the presence to some “external” electric field (due for example to the electrostatic interaction of charges or to an applied source-drain voltage), and the electronic current flows in a single band, the remarkable feature of a RITD is the possibility to achieve a coupling between “conduction” and “valence” states, allowing an interband current. Hence, the description of electron transport in such quantum devices requires multiband models able to account for tunneling mechanisms between different bands induced by the heterostructure design and the applied external bias. In electronics, the most popular model capable to describe the interaction of two bands is based on the Kane Hamiltonian [4]. By means of a perturbative approach and an averaging procedure, the effect of the periodic lattice potential is taken into account by some phenomenological parameters, such as the energy-band gap and the coupling coefficient (Kane momentum) between the two bands. It is well know that a strong formal analogy is present between the description of the quantum non-relativistic motion of a particle in a semiconductor expressed in the kp envelope function framework and the relativistic Dirac equation. This analogy has been for example widely exploited in graphene where the Fermi level is found near the gapless intersection of two approximately linear branches of the graphene spectrum [5]. As demonstrated in transport measurements by Novoselov [6], and in spectroscopic mea-
measurements by Zhou [7], the electronic properties of graphene are described by the Dirac equation (where the speed of light is replaced by the Fermi velocity), even though the microscopic Hamiltonian of carbon atoms is non-relativistic. The standard multiband semiconductor framework open thus the interesting possibility to test some mathematical procedure originally derived in the contest of high energy physics in a framework, the solid state physics, where a broad set of experimental data are available and the most of the semiconductor parameters can be controlled.

In the present contribution we adapt the WKB procedure for relativistic particles to the kinetic framework and we derive approximated equations for the quantum evolution of a multiband system constituted of charged particles. Historically, the early extension of the WKB method to the Dirac equation is due to Pauli [8], who showed that the phase of a WKB spinor is given by a solution of the Hamilton-Jacobi equation for relativistic point particles. Although the Pauli approach has been successfully applied to non-relativistic quantum mechanics, where it leads to the so-called Einstein-Brillouin-Keller quantization [9], in general it is possible to determine the amplitude of the semiclassical spinor only in some special cases. As pointed out in Ref. [10] in the full quantum-relativistic contest, the Dirac-like coupling among the different bands strongly affects the dynamics inside every single band. In particular at the semiclassical level it is possible to derive an effective dynamics where the particles follow a quantum-corrected Hamiltonian flux and the single-band classical Hamiltonian is replaced by the eigenvalue of the Dirac operator.

The main result of this work is to extend this approach in order to derive a WKB-like asymptotic expansion of the multiband Wigner function. The approximate evolution equations can be used to obtain the Wigner quasi-distribution function in a IRTD diode. The interband tunneling mechanism appearing to the first order of the expansion is expressed in a very simple mathematical form, in contrast with the highly complex formulation of the exact evolution equation. In particular, by exploiting the highly oscillating behaviour of the multiband Wigner functions that was already observed in Ref. [11], we derive a asymptotic expression of the interband transition kernel which is formally close to the usual generation-recombination terms. This achievement allow to describe the interband transition phenomena at the same level of the more common scattering effects present in a semiconductor material. We derive a hierarchy of equations that to lowest order consist of two Hamilton-Jacobi equations corresponding to the classical dynamics of point particles with positive and negative kinetic energy, and that represent the electron motion in conduction and in valence band respectively. The condition that arises in next-to-leading order can be reduced
to two differential equations for $2 \times 2$ matrices describing the transport of the band degrees of freedom along particle orbits. Our methodology is based on the Van Vleck approach where a semiclassical representation of the time evolution kernel of the Schrödinger wave function in terms of a WBK ansatz is provided. Such a representation, usually derived from a Feynman path integral, to which the method of stationary phase is applied [12], makes use of a representation of the kernel in terms of an oscillatory integral.

1.1. WKB procedure

In this paper we adopt the multiband envelope function model (MEF) described in Ref. [13]. This model is derived within the $k \cdot p$ framework and is so far very general. This approach allows the description of electron transport in devices where tunneling mechanisms between different bands are induced by an external applied bias $U$. We consider a physical model in which only the valence and the conduction band are taken into account. Under this hypothesis the MEF model is a $2 \times 2$ Schrödinger-like set of equations

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi,$$

where

$$\hat{H} = \begin{pmatrix}
E_c + U(x) - \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} & -\frac{\hbar}{m_0} \frac{P_K E(x)}{E_g} \\
-\frac{\hbar}{m_0} \frac{P_K E(x)}{E_g} & E_v + U(x) + \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2}
\end{pmatrix}$$

is the Hamiltonian, $\Psi = (\Psi_c, \Psi_v)$ with $\Psi_c$ and $\Psi_v$ the conduction and valence Wannier envelope functions. $E_c$ ($E_v$) is the minimum (maximum) of the conduction (valence) energy band, $P_K$ is the Kane momentum and $m_0, m^*$ are the bare and the effective mass of the electron. $U$ is the “external” potential, which takes into account different effects, like the bias voltage applied across the device, the contribution from the doping impurities and from the self-consistent field produced by the mobile electronic charge. According to Ref. [14], the multiband Wigner function is defined as:

$$f(x, p, t) \equiv \begin{pmatrix}
f_{cc} & f_{cv} \\
f_{vc} & f_{vv}
\end{pmatrix},$$

$$f_{ij} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \overline{\Psi}_i \left(x + \frac{\hbar \eta}{2}\right) \Psi_j \left(x - \frac{\hbar \eta}{2}\right) e^{-ip\eta} \, d\eta,$$
where $i, j = c, v$. This definition is a straightforward extension of the single-band Wigner function to a multiband system. By differentiating Eq. (3) with respect to time, and by using Eq. (1), we obtain the evolution equation for the multiband Wigner function (W-MEF system),

$$i\hbar \frac{\partial f}{\partial t} = [\mathcal{H}, f]_\#,$$

where $[\mathcal{H}, f]_\# = \mathcal{H}#f - f#\mathcal{H}$ denotes the Moyal commutator with respect to the Moyal product $\#$, and $\mathcal{H}(x, p)$ is the Hamiltonian symbol with respect to the Weyl quantization procedure. We recall that, given a differential operator $\hat{A}$ acting on the $x$ variable, the Weyl quantization procedure establishes a unique correspondence of $\hat{A}$ with a function $A(x, p)$, which is the symbol of the operator. The relationship between the operator $\hat{A}$ and its symbol $A$ is given by

$$\left(\hat{A}\Psi\right)(x) = \frac{1}{2\pi\hbar} \int A\left(\frac{x + y}{2}, p\right) \Psi(y) e^{i\frac{\hbar}{2}(x-y)p} \, dy \, dp.$$

The Moyal product can then be expanded with respect to $\hbar$ according to

$$A#B = \sum_{k=0}^{\infty} \frac{\hbar^k}{(2i)^k} \sum_{|\alpha|+|\beta|=k} \frac{(-1)^{|\alpha|}}{\alpha! \beta!} \left(\partial_x^\alpha \partial_p^\beta A\right) \left(\partial_p^\alpha \partial_x^\beta B\right).$$

To attack the quantum evolution problem by solving directly the system of Eq. (5) is a difficult task: a preliminary theoretical study of the multiband Wigner evolution system showed the occurrence of a very complex dynamics [15]. The numerical complexity of this system prevent its direct application to a real device even in the simple cases where the one dimension approximation of the motion can be considered sufficiently accurate to reproduce the statical and dynamical characteristics. Furthermore conceptual problems arise if we address to the practical question of coupling a multiband quantum system with a classical evolution system (that is of paramount importance in a real device where typically quantum effects take place in a very narrow region, the active region, and the remaining domain can be well described by a classical distribution). It is very important to provide an accurate modelization of the interplay between quantum effects and classical transport (describing for example scattering mechanisms, heat flux, injection of charge and external driving voltage effects) to reproduce the observed thermodynamical and transport properties of a device. Since in the Wigner framework the quantum kinetic transport operators are defined in term of Fourier transform, which is strongly non-local, constraint are imposed to a possible numerical algorithm, making practically
impossible for example the use non structured mesh grids or, more simply, the definition of variable spatial and momentum discretization mesh size. For these reason, we are interested in reducing the numerical complexity of the Wigner multiband evolution system by using a WKB-like asymptotic expansion procedure. Instead of deriving a $\hbar$ expansion directly on the multiband Wigner function defined in Eq. (5), it is more convenient to expand the time evolution kernel of the Schrödinger wave function $\Psi$ and to use that the Wigner quasi-distribution function is defined through a bilinear transformation of $\Psi$.

We write the solution of Eq. (1) with initial condition $\Psi_I$ as follow

$$\Psi(x, t) = \int \mathcal{K}(x, x', t) \Psi_I(x') \, dx'$$

where $\mathcal{K}$ denotes the kernel of the evolution operator of $\Psi$ and it solves

$$i\hbar \frac{\partial \mathcal{K}}{\partial t} = \hat{H}(x) \mathcal{K}$$

with initial condition

$$\mathcal{K}(x, x', t_0) = \delta(x - x') I_{2\times2} ,$$

$I_{2\times2}$ denotes the $2 \times 2$ identity matrix. According to Eq. (7) the Wigner function can be expressed as

$$f(x, p, t) = \int \mathcal{K}\left(x + \frac{\hbar \eta}{2}, \theta - \frac{\hbar \tau}{2}\right) f_I\left(\theta, p'\right) \mathcal{K}\dagger\left(x - \frac{\hbar \eta}{2}, \theta + \frac{\hbar \tau}{2}\right) e^{i(p\eta - p'\tau)} \, d\eta \, d\theta \, dp' ,$$

where $\dagger$ denotes hermitian conjugate and $f_I$ is the initial condition for $f_{ij}$.

Explicitly

$$f_I(\theta, p') = \frac{1}{2\pi} \int \Psi_I(\theta - \frac{\hbar \tau}{2}) \Psi_I^\dagger(\theta + \frac{\hbar \tau}{2}) e^{-i\tau p'} \, d\tau$$

We are interested in deriving a asymptotic approximation of the evolution kernel $\mathcal{K}$. For future references we consider the following result: given a two-band wave function in the WKB representation

$$\Psi(x, t) = a(x, t) e^{i S(x, t)} ,$$

we have

$$(\hat{H}\Psi)(x) = e^{i S(x, t)} \left\{ \mathcal{H}_0 \left(x, \frac{\partial S}{\partial x}\right) a + \frac{\hbar}{i} \left[ \frac{\partial \mathcal{H}_0}{\partial p} \left(x, \frac{\partial S}{\partial x}\right) \frac{\partial a}{\partial x} + \frac{1}{2} \left[ \frac{\partial}{\partial x} \frac{\partial \mathcal{H}_0}{\partial p} \left(x, \frac{\partial S}{\partial x}\right) a \right] + \mathcal{H}_1 \left(x, \frac{\partial S}{\partial x}\right) a \right] - \frac{\hbar^2}{2} \frac{\partial^2 \mathcal{H}_0}{\partial p^2} \left(x, \frac{\partial S}{\partial x}\right) \frac{\partial^2 a}{\partial x^2} \right\} ,$$

(11)
where we have considered the following $\hbar$ expansion of the symbol $\mathcal{H}$

$$\mathcal{H}(x, p) = \sum_n \hbar^n \mathcal{H}_n(x, p).$$

Given two orthonormal $x$-dependent column vectors $e^+(x)$, $e^-(x)$ (and whose specific values will be defined in the following) the $2 \times 2$ matrix $\mathcal{K}$ can be decomposed as follows

$$\mathcal{K} = \mathcal{K}^+ + \mathcal{K}^-$$
$$\mathcal{K}^\pm = e^\pm [e^\pm]^\dagger \mathcal{K}.$$

We derive a semiclassical-like expansion of the evolution kernel in the spirit of the Van Vleck formula. In the present context it is convenient to represent the time evolution kernel in terms of the following oscillatory integral

$$\mathcal{K}^\pm(x, x') = \int \mathcal{K}^\pm \left(x; \xi = \frac{\partial S^\pm}{\partial x}, t\right) e^{i \hbar \left[S^\pm(x, p', t) + x'p'\right]} \, dp'$$
$$\mathcal{K}^\pm(x, \xi, t) = e^\pm(x, \xi) \left[a^\pm\right]^\dagger(x, \xi, t).$$

This method was developed for the study of scalar wave equations in the context of microlocal analysis, and subsequently found application to the development of several trace formulae \[16\]–\[17\]. In the case of the Schrödinger equation it leads to the same result as Gutzwilser’s original derivation which employed a stationary phase approximation of a Feynman path integral \[12\]. This approach is similar to the usual WKB method and the possibility of the band transition is reflected in these equations through their matrix character.

In this formula $\mathcal{K}$ is represented as the quantum-mechanical transition probability between $x$ and $x'$ averaged over all possible initial classical momenta $p'$. The explicit expressions of the vectors $e^\pm(x)$, the equations of motion of $a^\pm$ and of $S^\pm$, can be obtained by solving Eq. (8). In the spirit of the WKB approximation we consider a $\hbar$-expansion of Eq. (8) and we separate the zeroth order term from the higher order terms. In particular we will take advantage of the expansion of Eq. (11) and we fix the unknown $e^\pm(x)$ and of $S^\pm$ in order to satisfy the zeroth order equation. All the $\hbar$ corrections will be take into account by the vectors $a^\pm$. In this way we decompose the solution into simpler elements each of which has a specific interpretation: $S^\pm$ describe the classical interband motion of the particles in term of point-like trajectory, the vectors $e^\pm(x)$ define some local in space and momentum projectors in the conduction and valence band. This projection is similar to what we found in the usual effective mass approximation where the mixing
among different band branches, due to the presence of an external electric field, are discarded and the spectrum of the particle is defined only by the material in the surrounding of its classical position. Finally the vectors $a^\pm$ provide the quantum correction to the classical motion and are responsible of the band transition. The zeroth order of Eq. (8) gives

$$-\int \left\{ e^{i\phi} [S^+(x,p',t)+x'p']K^+ + e^{i\phi} [S^-(x,p',t)+x'p']K^- \right\} \frac{\partial S \pm}{\partial t} \, dp' =$$

$$\int \left\{ e^{i\phi} [S^+(x,p',t)+x'p']H_0 \left(x, \frac{\partial S^\pm}{\partial x}\right)K^+ + e^{i\phi} [S^-(x,p',t)+x'p']H_0 \left(x, \frac{\partial S^\pm}{\partial x}\right)K^- \right\} \, dp' .$$

This expression is satisfied if the vectors $e^\pm(p, x)$

$$e^\pm \equiv v^\pm \left(x, \frac{\partial S^\pm}{\partial x}\right)$$

are the eigenvector of the symbol $H_0(p, x)$ (see expansion of Eq. (12))

$$H_0(x, p)v^\pm(x, p) = \lambda^\pm(x, p)v^\pm(x, p)$$

and $S^\pm$ satisfy the Hamilton-Jacobi equations associated to the eigenvalues of the Hamiltonian

$$\frac{\partial S^\pm}{\partial t} + \lambda^\pm \left(x, \frac{\partial S^\pm}{\partial x}\right) = 0$$

$$S^\pm(t_0) = -xp' .$$

After some algebra it is possible to show that Eq. (8) is equivalent to the following system for the unknown $a^\pm$

$$\begin{align*}
\left(-\frac{1}{2} \frac{\partial}{\partial x} \frac{\partial \lambda^+}{\partial p} - e^+H_1v^+ - \frac{\partial \lambda^+}{\partial p} \frac{\partial}{\partial x} + \frac{\partial}{\partial t}\right) [a^+]^\dagger = &-e^\phi (S^- - S^+) \times \\
&\quad e^+ \left(\frac{\partial}{\partial t} - Q^+\right) e^- [a^-]^\dagger \quad (15)
\end{align*}$$

$$\begin{align*}
\left(-\frac{1}{2} \frac{\partial}{\partial x} \frac{\partial \lambda^-}{\partial p} - e^-H_1v^- - \frac{\partial \lambda^-}{\partial p} \frac{\partial}{\partial x} + \frac{\partial}{\partial t}\right) [a^-]^\dagger = &-e^\phi (S^+ - S^-) \times \\
&\quad e^- \left(\frac{\partial}{\partial t} - Q^-\right) e^+ [a^+]^\dagger \quad (16)
\end{align*}$$

where

$$Q^\pm = \frac{\partial H_0}{\partial p} \left(x, \frac{\partial S^\pm}{\partial x}\right) \left(\frac{\partial}{\partial x} + \frac{1}{2} \left[\frac{\partial}{\partial x} \frac{\partial H_0}{\partial p} \left(x, \frac{\partial S^\pm}{\partial x}\right)\right]\right)$$

$$+H_1 \left(x, \frac{\partial S^\pm}{\partial x}\right) - \frac{\hbar^2}{2} \frac{\partial^2 H_0}{\partial p^2} \left(x, \frac{\partial S^\pm}{\partial x}\right) \frac{\partial^2}{\partial x^2}$$
The initial condition of $\mathcal{K}$ given in Eq. (9) leads to the following initial condition for $a^\pm$

$$a^\pm(x, \xi, t_0) = e^\pm(x, \xi).$$

The system of Eq. (15) takes into account the band transition process. In a rather general framework in Ref. [11]-[18] was showed that the band transition is a complex coherent phenomena where the interference effects between the conduction and the valence components of the distribution generate a highly oscillating-in-time solution. Furthermore the usual $\hbar$ expansion of the solution which is a characteristic features of the WKB approach fail to give a good convergence. In fact high order terms play a important role in the band transition phenomena when the external potential becomes strong enough to give a relevant contribution to the current flux. In the practical application of a band-to-band model to semiconductor devices we are usually interested in the long time behaviour of the solution, and the main goal is to obtain a accurate estimation of the transition probability. In this contest, in the same spirit of the Markovian approximation where the memory effects are integrated out by defining a two-time temporal scale (the fast time scale including memory effect and the microscopical detail of the scattering processes, and the long time scale which describing the evolution of the mean quantities), the fast processes which take place on the femtosecond scale and describe all the interference effects of the wave function are considered of minor importance. Due to the presence of high oscillating terms (whose frequency is proportional to the differences of the energy between the two band, evaluate along the pseudo-classical path) we introduce the following hierarchy of approximated solutions (fixed-point like expansion)

$$a^\pm = \lim_{n \to \infty} a^\pm_n$$

with

$$-e^\pm \left( S^\mp - S^\pm \right) e^\mp \left( \frac{\partial}{\partial t} - Q^\mp \right) e^\mp \left[ a^\mp_n \right]^\dagger =$$

This ansatz is equivalent to the asymptotic procedure in term of the “Dyson like” expansion derived in Ref. [11]. Noting that $|\frac{\partial S^\pm}{\partial t} - \frac{\partial S^\mp}{\partial t}| > E_g$, in the case of in a wide gap semiconductor, the exponential term which appears in Eq. (15) is a fast oscillating function and gives a relevant contribution to the motion only in the neighborhood of the minimum of the oscillation frequency. Corresponding, the solution can be estimated by means of a
stationary phase procedure. This iterative procedure is very similar to the Dyson formalism, which is used to describe electron scattering phenomena in semiconductors. This analogy is useful in order to describe the tunneling process in which a particle “disappears” from to a given band and it “appears” in a different branch of the band diagram in a similar way as the generation of an electron-hole pair by the absorption of a photon.

To obtain a suitable approximated analytic solution of Eq. (15) in the general case is a difficult task even in the stationary phases approximation. A simple approximation can be obtained if we limit ourselves to the simplified case of a uniform static electric field. In this case Eq. (13) gives

\[ S^\pm = -x(p' + \mathcal{E}t) \pm \int_{t_0}^{t} \left( \frac{(p' + \mathcal{E}\tau)^2}{2} + \frac{E_g}{2} \right) \, d\tau \]

and the system of Eq. (15) becomes

(19)

\[
\begin{cases}
\left( (p' + \mathcal{E}t) \frac{\partial}{\partial x} + \frac{\partial}{\partial t} \right) [a^+]^\dagger = -i \frac{P_K \mathcal{E}}{E_g m_0} e^{-\frac{i}{\hbar} \varphi(t)} [a^-]^\dagger \\
\left( -(p' + \mathcal{E}t) \frac{\partial}{\partial x} + \frac{\partial}{\partial t} \right) [a^-]^\dagger = -i \frac{P_K \mathcal{E}}{E_g m_0} e^{\frac{i}{\hbar} \varphi(t)} [a^+]^\dagger
\end{cases}
\]

where

\[ \varphi = \int_{t_0}^{t} \left( (p' + \mathcal{E}\tau)^2 + E_g \right) \, d\tau , \]

with initial conditions

\[ a^+ (t_0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad a^- (t_0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \]

We denote with \( \alpha_i, \beta_i \), the components of \( a^+ \) and \( a^- \) respectively e. i. \( a^+ = (\alpha_1, \alpha_2)^\dagger \); \( a^- = (\beta_1, \beta_2)^\dagger \). It is easy to show that the quantity \( |\alpha_n|^2 + |\beta_n|^2 \) with \( n = 1, 2 \) is conserved. In fact

(20)

\[ \frac{\partial (|\alpha_n|^2 + |\beta_n|^2)}{\partial t} = 2 \frac{P_K \mathcal{E}}{E_g} \left( \Re \left\{ e^{-\frac{i}{\hbar} \varphi(t)} \beta_n \alpha_n \right\} - \Re \left\{ e^{\frac{i}{\hbar} \varphi(t)} \alpha_n \beta_n \right\} \right) = 0 \]

Since both the initial datum and the eigenvector of \( \mathcal{H}_0 \) does not depend on \( x \), we can obtain a simple expression for the solution. Eq. (19) becomes

\[
\begin{aligned}
\frac{\partial \alpha_n}{\partial t} &= -i \frac{P_K \mathcal{E}}{E_g m_0} e^{-\frac{i}{\hbar} \varphi(t)} \beta_n \\
\frac{\partial \beta_n}{\partial t} &= -i \frac{P_K \mathcal{E}}{E_g m_0} e^{\frac{i}{\hbar} \varphi(t)} \alpha_n \\
\end{aligned}
\]

; \( n = 1, 2. \)
If we take the substitution $P_K \rightarrow -P_K$ it is immediate to verify that $\beta_2 = \alpha_1$ and $\alpha_2 = \beta_1$. By approximating $\alpha_1$ up to the second order of the fixed point expansion of Eq. (17) we obtain

$$\alpha_1 = \alpha_1(t_0) - \left( \frac{P_K \mathcal{E}}{E_g m_0} \right)^2 \int_{t_0}^{t} \int_{t_0}^{t'} e^{-i \frac{\phi(t') - \phi(t''')}{\hbar}} \alpha_1(t'') \, dt'' \, dt' \simeq 1 - \left( \frac{P_K \mathcal{E}}{E_g m_0} \right)^2 \int_{t_0}^{t} \int_{t_0}^{t'} e^{-i \frac{\phi(t') - \phi(t'')}{\hbar}} \, dt'' \, dt' \simeq 1 - 2\pi^2 \left( \frac{P_K \mathcal{E}}{E_g m_0} \right)^2 \mathrm{Ai}^2 \left( \frac{E_g \sqrt{\mathcal{E}}}{\hbar} \right) \theta \left( t + \frac{p'}{E} \right).$$

In Appendix 4 we give the detail of the calculation. We note the strong similarity of this result with the transition integral obtained in Ref. [11] and Ref. [18] where a different approach is considered. In particular in Ref. [18] a numerical study showed that these formulae provide a good estimation of the exact interband transition probability for a realistic set of the semiconductor parameters.

1.2. Stationary phases approximation

The explicit form of the coefficients defining $K$ can be used to obtain the expression of the Wigner function. In particular Eq. (10) gives

$$f = \sum_{i,j=\pm} f^{ij}$$

$$f^{ij}(x,p,t) = \int \mathbf{K}^i \left( x + \frac{h\eta}{2}, P - \frac{r}{2} \right) f_I (\theta, -P) \mathbf{K}^j \left( x - \frac{h\eta}{2}, P + \frac{r}{2} \right) \left[ e^{i \left[ S^i \left( x + \frac{h\eta}{2}, P - \frac{r}{2}, \theta \right) - S^i \left( x - \frac{h\eta}{2}, P + \frac{r}{2}, \theta + \hbar \eta \right) \right]} \right] \, d\eta \, d\theta \, dP \, dr.$$

In this representation we have that $K^+ f_I K^{+\dagger}$ describes both the intraband conduction dynamics and the interband transition from the valence band to the conduction band, while $K^- f_I K^{-\dagger}$ describes the valence dynamics including the transition from conduction to the valence band. Finally the mixed terms $K^+ f_I K^{-\dagger}$, $K^- f_I K^{+\dagger}$ represent the non diagonal correlation that in the original formulation was mainly represented by the terms $f_{cv}$ and $f_{vc}$. To obtain a manageable expression for the diagonal terms of the quasi-distribution function $f^{ij}$ (representing the interesting quantities for a physical point of view), we apply the stationary phases approximation to
Eq. (22). In particular Eq. (22) for \( i = j = \pm \) is of the form

\[
f^{ij}(x, p, t) = \int \mathcal{G}(x, \eta, r, \vartheta, P) e^{i \frac{\hbar}{\pi} [S^i(x + \frac{\eta}{2}, \vartheta) - S^j(x - \frac{\eta}{2}, \vartheta) - \frac{\vartheta}{r} + \frac{\hbar \eta}{r}]} \, d\vartheta \, dP \, d\eta \, dr,
\]

where \( \mathcal{G} \) is assumed sufficiently smooth. To apply the stationary approximation we expand the generating functions \( S^i \) with respect to \( \eta \) and \( r \) and we discard the \( (\eta, r) \) dependence of the function \( \mathcal{G} \). We obtain

\[
f^{ii}(x, p, t) \simeq \int \mathcal{G}(x, \vartheta, P) \Phi(x, \vartheta, P) \, d\vartheta \, dP
\]

\[
\Phi = \int e^{i \frac{\hbar}{\pi} \left[ \left( \frac{\partial S^i}{\partial x} \right)_{(x, P)} + p \right] \eta + \left( \frac{\partial S^i}{\partial P} \right)_{(x, P)} \vartheta} \, d\eta \, dr
\]

\[
= 4\pi^2 \hbar \delta \left( \frac{\partial S^i}{\partial x} \right)_{(x, P)} + p \delta \left( \frac{\partial S^i}{\partial P} \right)_{(x, P)} + \vartheta
\]

Since the functions \( S^\pm \) solve the Hamilton-Jacobi Equation (13), \( S^\pm \) are generating functions for canonical transformations

\[
(x' = \frac{x_0}{\partial S^j}, p_0 = P) \rightarrow (x, \frac{\partial S^i}{\partial x}).
\]

More specifically the spatial derivative \( \frac{\partial S^\pm}{\partial x} \equiv p_0^\pm(t) \) is the momentum of a particle traveling along the trajectory connecting the initial point of coordinate \((x', P)\) for \( t = t_0 \), with the final point \((x, \frac{\partial S^j}{\partial x})\). In the case of a uniform electric field we thus obtain that the zeroth order diagonal Wigner functions \( f^{++}, f^{--} \), follow the trajectory

\[
\begin{align*}
p(t) &= P + \mathcal{E} t \\
x(t) &= \vartheta + \int_{t_0}^{t} p(\tau) \, d\tau
\end{align*}
\]

and (similar formula for \( f^{--} \))

\[
f^{++} \simeq 4\pi^2 \hbar \left( \begin{array}{cc}
\alpha_1 & \alpha_2 \\
0 & 0
\end{array} \right) f_I \left( x - \int_{t_0}^{t} (P + \mathcal{E} \tau) \, d\tau, \mathcal{E} (t-t_0) + p \right) \left( \begin{array}{c}
\varpi_1 \\
\varpi_2
\end{array} \right).
\]

We choose the following physical based initial condition for \( f_{ij} \)

\[
f_I = \left( \begin{array}{cc}
f_{0cc} & 0 \\
0 & f_{0vv}
\end{array} \right)
\]
which represents a initial distribution of particles in conduction and in valence band where the interference effects are discarded. It is immediate to verify that with the previous initial conditions, the component of the multiband Wigner function $f^{++} (f^{--})$ is a matrix with a single non-vanishing value $f^{++}_{11} (f^{--}_{22})$ that we will denote with $f^{+} (f^{-})$. In same way the mixed term $f^{+-} (f^{-+})$ has a single out-of-diagonal component. Since we are interested to obtain the equation of motion of the diagonal components we limit ourselves to the function $f^{+}$ and $f^{-}$. We differentiate the integral equation with respect to the time and we obtain the approximated effective evolution system for the diagonal components of the multiband Wigner function

\[
\begin{cases}
\frac{\partial f^{+}}{\partial t} = \frac{p}{m^*} \frac{\partial f^{+}}{\partial x} + E \frac{\partial f^{+}}{\partial p} + N(p,t) (f^{-} - f^{+}) \\
\frac{\partial f^{-}}{\partial t} = -\frac{p}{m^*} \frac{\partial f^{-}}{\partial x} + E \frac{\partial f^{-}}{\partial p} + N(p,t) (f^{+} - f^{-})
\end{cases}
\]

with initial conditions $f^{+}(t_0) = f^{0cc}$, $f^{-}(t_0) = f^{0vv}$. We defined

\[N(p,t) = \frac{\partial |\alpha_1|^2}{\partial t} \simeq 4\pi^2 \left( \frac{P_K \sqrt{E}}{E_g m_0} \right)^2 A_1^2 \left( \frac{E_g}{\sqrt{E^2}} \right) \delta(p),\]

and we have used Eq. (20). This formulation reveals that the effect of the interband transition is taken into account as an effective scattering process that occurs when the particle is at rest.

2. Numerical Application

We use the system of Eq. (24) to simulate the steady state of a simple IRDT diode. In particular we are interested to obtain the correction to the stationary current due to the interband tunneling. The diode consist of two homogeneous regions separated by a region of constant electric field and realizing a barrier in $x = 0$ (corresponding to the source contact) for conduction electron and in $x = L$ (corresponding to the drain contact) for holes in the valence band. At the boundary of the simulation domain we assume that the semiconductor is connected with metallic contacts, which at the microscopical level are described by a flux of electrons injected into the diode with a Fermi dispersion (see figure 1). We fix the potential of the source contact (corresponding to $x = 0$) equal to zero and the drain potential equal to $V_b + V_{ex}$ where $V_b$ is the built-in potential and $V_{ex}$ is the external potential. The resulting electric potential in the domain $[0, L]$ is thus equal to $(V_b + V_{ex})/L$. In our simulation, we used the following parameters: $E_g = 0.02$ eV, $P_K = 5 \times 10^9$ m$^{-1}$, $L = 10$ nm, the lattice temperature
is $T = 100$ K, the doping concentration in the drain (source) contact is $N_D = 10^{19}$ cm$^{-3}$ ($N_A = 10^{19}$ cm$^{-3}$) and $V_b = 0.05$ eV.

The results of the simulation can be interpreted as follows. $f^+$ ($f^-$) describes the motion of the electron ensemble in the conduction (valence) band. It shows that the conduction electron and valence beam is (mainly) reflected back by the potential barrier. Besides, the gradient of the potential couples conduction electrons with valence ones. Due to the tunneling a flux of electrons can travel from the source to the drain contact. Electrons tunnel through the junction barrier because filled electron states in the conduction band on the side become aligned with empty valence band hole states. As voltage increases, the diode begins to operate as a normal diode, where electrons travel by diffusion across the junction.

In figure 1 we plot stationary values of the electron conduction distribution $f^+$ and the valence hole distribution $1 - f^-$ for an external applied potential $V_{ext} = 0.01$ eV. The figure show that the electrons cumulate near
the source contact and the holes near the drain contact. In figure 2 we show the effects of the inclusion of the interband transition to the usual non interactive two band motion. Since to each value of the the external potential $V_{ex}$ corresponds a flux of electron inside the device, by varying $V_{ex}$ we obtain the Current-Voltage characteristic of the diode. We plot the results obtained if we discard the interband transitions (dotted blue line) (that is with $N \equiv 0$ in Eq. (24)) and if we include the multiband corrections (continuous green line). Since we are considering a highly doped diode the intraband diffusion process of electron inhibit the formation of a negative differential resistance in the diagram, nevertheless, even in this case the simulation show that the tunneling processes cannot be discarded.

3. Conclusion

In this contribution we present a WKB-like asymptotic expansion of the multiband Wigner function designed to describe the dynamics in semiconductor devices in presence of the interband conduction-valence tunneling. The interband tunneling mechanism appearing to the first order of the expansion is expressed in a very simple mathematical form. We derive a hierarchy of equations that to lowest order consist of two Hamilton-Jacobi equations corresponding to the classical dynamics of point particles with positive and negative kinetic energy. We obtain the equation of motion for the multiband Wigner functions in term of the (pseudo)classical trajectories in the conduction and valence phase plane, related to the Hamilton-Jacobi functions $S^+$ e $S^-$. The resulting formulation reveals particularly close to the classical description of the particles motion and the approximate evolution equations are used to simulate the evolution of the Wigner quasi-distribution function in a IRTD diode. Our finding pave the way to explore the WKB approximation in the Wigner framework in order to obtain quantum-corrected equation of motion which are more tractable for a numerical point of view with respect to the full quantum formulation and that can find application in the solid state field. The simulations show that for a highly doped $n-p$ junction where of a strong electric field is present, our model predict a non-negligible correction to the total current of the device.

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4. Appendix

In this Appendix we give some detail of the approximation of Eq. (21). For sake of simplicity we assume as initial time \( t_0 = -\infty \) and we consider

\[
\mathcal{T}(t) = \int_{-\infty}^{t} \int_{-\infty}^{t'} f(t') g(t'') \, dt'' \, dt'
\]

(25)

\[
f(t) = \overline{g} = e^{-\frac{i}{\hbar} \varphi(t)}
\]

(26)

\[
\varphi = \int_{t}^{t*} \left( (p' + \mathcal{E} \tau)^2 + E_g \right) \, d\tau
\]

(27)

It is immediate to verify that \( \mathcal{T} \) does not depend of the time \( t^* \). For our purpose it is convenient to fix \( t^* = -\frac{p'}{\mathcal{E}} \) which is the stationary point corresponding to \( \frac{\partial^2 \varphi}{\partial t^2} = 0 \). By using the following property of the Fourier transform

\[
\int_{-\infty}^{t} g(t'') \, dt'' = \int_{-\infty}^{\infty} \frac{\hat{g}(k)}{i k} e^{i k t} \, dk + \frac{\hat{g}(0)}{2}
\]

(28)

where \( \hat{g}(k) \) denotes the Fourier transform, \( \mathcal{T} \) becomes

\[
\mathcal{T}(t) = \int_{-\infty}^{\infty} \frac{\hat{g}(k)}{i k} \int_{-\infty}^{t} f(t') e^{i k t'} \, dk \, dt' + \frac{\hat{g}(0)}{2} \int_{-\infty}^{t} f(t') \, dt'
\]

(29)

In Ref. [18] some numerical test showed that in presence of a highly oscillating function such as \( f(t) \), a very good estimate of the transition probability \( \mathcal{T} \) which avoid time oscillation and preserves the limit \( t \to \infty \) can be obtained with the simple approximation

\[
\int_{-\infty}^{t} f(t') e^{i k t'} \, dt' \simeq \theta(t - t^*) \int_{-\infty}^{\infty} f(t') e^{i k t'} \, dt'
\]

(30)

where \( \theta \) is the step function. This formula express that the transition process take place around the stationary point \( t^* \), corresponding to the minimum oscillation frequency of \( \varphi(t') \). We obtain

\[
\mathcal{T}(t) \simeq \theta \left( t + \frac{p'}{\mathcal{E}} \right) \left[ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\hat{g}(k) \hat{f}(-k)}{i k} \, dk \, dt' + \frac{1}{2} \int_{-\infty}^{\infty} g(t') \, dt' \int_{-\infty}^{\infty} f(t') \, dt' \right]
\]

from the definition of \( f \) and \( g \) given in Eq. (26) we have that \( \hat{g}, \hat{f} \) are real functions and \( \hat{g}(k) = \hat{f}(-k) \). The first integral vanish and we obtain

\[
\mathcal{T}(t) = \frac{1}{2} \theta \left( t + \frac{p'}{\mathcal{E}} \right) \left[ \int_{-\infty}^{\infty} f(t') \, dt' \right]^2 = \theta \left( t + \frac{p'}{\mathcal{E}} \right) \frac{2 \pi^2 \sqrt{\mathcal{E}^2}}{\mathcal{E}^2} \text{Ai}^2 \left( \frac{E_g}{\sqrt{\mathcal{E}^2}} \right)
\]

where \( \text{Ai} \) denotes the Airy function \( \text{Ai}(x) \equiv \frac{1}{2\pi} \int \exp \left[ i \left( xy + \frac{y^3}{3} \right) \right] \, dy \).
REFERENCES


