Multiband Wigner-function formalism applied to the Zener band transition in a semiconductor

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The Wigner-function approach is used to describe the Zener transition between the conduction and the valence band in a semiconductor. In the Weyl quantization framework a diagonalization procedure is applied to the multiband $k\cdot p$ Hamiltonian and a new set of Wigner multiband functions is defined. An approximate closed-form solution is obtained by an iterative procedure which exploits the different time scales on which the intraband and interband dynamical variables evolve. The single-band limit has been discussed and some quantum corrections to the single-band trajectory have been obtained.

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I. INTRODUCTION

The theoretical analysis of current-voltage characteristics in semiconductor devices requires the study of the electronic motion in a general spatially dependent electric and magnetic field. The usual single-band transport approximation or the classical phase-space description of the charge motion is not always accurate to model the highly integrated nanometric semiconductor devices. In particular, in recent years there has been a growing interest for interband devices where tunneling effects become the main transport phenomena. A theoretical study of these structures require multiband models able to account for tunneling mechanisms between different bands induced by the heterostructure design and the applied external bias.[1] Different approaches based on the density matrix, nonequilibrium Green's functions, and the Wigner function have been proposed to achieve a full quantum description of electron transport which includes the interaction among the different bands.[2]

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. A phase-space approach may appear more intuitive compared with the more abstract density matrix and Green's function formalism. A multiband transport model, based on the Wigner-function approach, was introduced in Ref. 3 where a suitable projection procedure in a Bloch basis was proposed. In Ref. 4 a multiband equation of motion was derived by using the generalized Kadanoff-Baym nonequilibrium Green's function formalism, but the model equations derived there were still too hard to solve numerically. An important approximation was then introduced in Ref. 5, where the multiband Kane matrix[6] and the Luttinger-Kohn matrix[7] were considered. A multiband envelope function (MEF) model, based on the $k\cdot p$ Hamiltonian and which describes the Zener effect in the Schrödinger function formalism, was formulated in Refs. 8 and 9 and then extended to the Wigner-function approach (W-MEF) in Ref. 10. The W-MEF model consists of a system of evolution equations for the components of the multiband Wigner function. This system describes the full quantum coupling between the conduction and the valence bands and involve both the fast dynamical processes arising from the interband transition phenomena (and whose frequency is of the order of the energy gap) and the slow dynamical processes arising from the intraband motion of the electrons. This two-time-scale behavior was exploited in Ref. 11 in order to devise an approximation scheme to obtain a closed-form asymptotic solution of the multiband Wigner-function model equations. The interband tunneling mechanism was treated as a scatteringlike process which takes place when the momentum of the particle vanishes. The approximation procedure was restricted to a semiconductor structure subject to a uniform-in-space external electric field. In this work, we extend the previous results to the more realistic situation of a spatially varying electric field. Our procedure reveals the existence of an interesting regime of the electric field where the multiband quantum coupling between the conduction and valence bands affects the motion of the particles at the zero order in $\hbar$ (i.e., at the semiclassical level). In this regime, the dynamics of the single-band projection of the Wigner multiband function is governed by a quantum-corrected Hamiltonian and the correction terms depend on the Kane momentum, which, in the $k\cdot p$ formalism, measures the strength of the coupling between the valence and the conduction bands.[6,12]

This paper is organized as follow: in Sec. II we summarize the standard approximations used to reproduce the electronic interband tunneling mediated by scattering. In Sec. III we present the multiband kinetic model W-MEF, obtained by a diagonalization procedure of the $k\cdot p$ Hamiltonian in the multiband Weyl-Wigner formulation. In Sec. IV, we discuss the single-band limit of the W-MEF system and propose an iterative procedure to obtain an approximate closed-form solution. This approach allows us to treat the interband Zener tunneling process in the same way as the other scattering processes that occur in the semiconductor.

II. MULTIBAND TRANSITIONS

An electron in a semiconductor structure can perform a band transition essentially by two different mechanisms: either absorbing (or releasing) a quantum of energy represented by a photon or phonon (collisional or incoherent transition) or by a tunneling process induced by an external field (Hamiltonian or coherent transition). In a collisional transi-

tion, the dynamics of the particle is usually described as a coherent intraband motion randomly interrupted by scattering phenomena which modify abruptly the Hamiltonian trajectory of the particle. The treatment of the scattering processes is thus essentially classical and quantum mechanics is only used to evaluate the kernel of the scattering operator. The free evolution of a quantum statistical system defined by a density matrix ρ is governed by the energy spectrum of the lattice Hamiltonian. We have

$$\rho_{ij}(k,k',t) = \langle \psi_k^{i\dagger}(t_0)\psi_{k'}^{j}(t_0)\rangle e^{i/\hbar(E_k^i - E_{k'}^j)(t-t_0)}, \tag{1}$$

where we denoted with $\psi_n^{k\dagger}$ (ψ_n^k) the operator that creates (annihilates) a Bloch state in the nth band with quasimomentum k and energy E_k^n. In the problems of our concern, Eq. (1) describes a statistical mixture of Bloch states in conduction and in valence band. Since the differences of energy within the same band are typically much smaller than the band gap E_g, the exponential phases in Eq. (1) with $i=j$ tend to cancel each other. Therefore, we expect that the ith component of the density function ρ_{ii} evolves smoothly in time, while the nondiagonal elements ρ_{ij} oscillate at the frequency $E_g/\hbar$.

A typical example is the time evolution of a conduction-valence electron system in presence of a classical time-dependent electromagnetic field. The electromagnetic interaction between light and electron in a semiconductor is described by the Bloch equations (see Refs. 2 and 13 for the details)

$$\frac{d\rho_{ii}}{dt} = \frac{2}{\hbar}\mathcal{E}e^{-i\omega_0 t}\Im\{\rho_{ij}\}; \quad i=c,v; \quad j\neq i,$$

$$\frac{d\rho_{cv}}{dt} = -\frac{i}{\hbar}(E_c - E_v)\rho_{cv} + \frac{i}{\hbar}\mathcal{E}e^{-i\omega_0 t}(\rho_{cc}-\rho_{vv}),$$

where $\mathcal{E}$ is the electric field with oscillation frequency ω_0, E_c (E_v) is the minimum (maximum) of the conduction (valence) energy band, $\Im$ denotes the imaginary part, and we have $\rho_{cv}=\overline{\rho_{vc}}$ (the overbar means complex conjugation). An approximate solution can be obtained by writing the previous system in integral form and applying the Markov approximation

$$\rho_{cv}(t) = \mathcal{P}\int_{-\infty}^{t} e^{i(E_g/\hbar-\omega_0)t'}(\rho_{cc}-\rho_{vv})dt'$$

$$\simeq 2\pi\delta\left(\frac{E_g}{\hbar}-\omega_0\right)(\rho_{cc}-\rho_{vv}), \tag{2}$$

where $E_g=E_c-E_v$ and $\mathcal{P}$ denotes the principal value. We assumed that the phase of the exponential function varies much more rapidly than the rest of the integrand and can then be factored out of the integral. If we now try to apply the above procedure in the presence of a uniform and *static* electric field ($\omega_0=0$) as is the case of the Zener transition, the approximation of Eq. (2) cannot be fulfilled since the gap energy is constant and the exponential does not have any stationary point. Nevertheless, if the assumption that the density functions ρ_{cc} and ρ_{vv} are a slowly varying functions of time is not satisfied, it is possible to express ρ_{cv} in the same form of Eq. (2). This is the case of the Zener effect where the electrons are strongly accelerated by a static electric field and the assumption of local equilibrium for the ρ_{ii} is clearly inadequate. This procedure is described into detail in Sec. IV.

III. TWO BAND W-MEF MODEL

In this paper we adopt the MEF described in Ref. 8. This model is derived within the $k\cdot p$ framework and is so far very general. In particular 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 2×2 Schrödinger-like set of equations

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{\mathcal{H}}\Psi, \tag{3}$$

where

$$\hat{\mathcal{H}} = \begin{bmatrix} E_c + U(x) - \dfrac{\hbar^2}{2m^*}\dfrac{\partial^2}{\partial x^2} & -\dfrac{\hbar}{m_0}\dfrac{P_K\mathcal{E}(x)}{E_g} \\ -\dfrac{\hbar}{m_0}\dfrac{P_K\mathcal{E}(x)}{E_g} & E_v + U(x) + \dfrac{\hbar^2}{2m^*}\dfrac{\partial^2}{\partial x^2} \end{bmatrix} \tag{4}$$

is the Hamiltonian, $\Psi=(\Psi_c,\Psi_v)$ with Ψ_c and Ψ_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 and m^* are the bare and the effective masses of the electron. U is the "external" potential, which takes into account different effects such as 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.

In our study we highlight the role of the multiband effects in the electronic motion and we provide some multiband corrections to the trajectories in the phase-space plane. For this purpose we rescale the equations of motion by using the following dimensionless asymptotic parameter

$$\gamma = \frac{\mathcal{E}_0 P_K \tau_0}{E_g m_0}.$$

Here, $\tau_0(\mathcal{E}_0)$ are the typical time (electric field) that characterize the interband phenomena; γ measures the strength of the interference effect between two different bands and its physical meaning will be discussed in detail in Sec. IV B. If we rescale the spatial and time variables $x'=x\gamma$, $t'=t\gamma$, then Eq. (3) remains unchanged but with $\tilde{\hbar}=\hbar\gamma$ instead of $\hbar$, and Eq. (4) becomes

$$\hat{\mathcal{H}} = \begin{bmatrix} E_c + U(x) - \dfrac{\tilde{\hbar}^2}{2m^*}\dfrac{\partial^2}{\partial x^2} & P_R(x) \\ P_R(x) & E_v + U(x) + \dfrac{\tilde{\hbar}^2}{2m^*}\dfrac{\partial^2}{\partial x^2}, \end{bmatrix} \tag{5}$$

where we dropped the primes for a simpler notation and

$$P_R(x) = -\tilde{\hbar}\frac{\mathcal{E}(x)}{\tau_0 \mathcal{E}_0}. \tag{6}$$

According to Ref. 5, the multiband Wigner function is defined as

$$\mathbf{F}(x,p,t) = \begin{pmatrix} f_{cc} & f_{cv} \\ \bar{f}_{cv} & f_{vv} \end{pmatrix}, \tag{7}$$

$$f_{ij} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \bar{\Psi}_i\left(x+\frac{\eta}{2}\right)\Psi_j\left(x-\frac{\eta}{2}\right)e^{-i/\tilde{\hbar}\eta p}d\eta, \tag{8}$$

where $i,j=c,v$. This definition is a straightforward extension of the single-band Wigner function to a multiband system. In the absence of electric fields, the definition of the diagonal components of the multiband Wigner function, f_{cc} and f_{vv}, agrees with the definition of the single-band Wigner function of electrons in conduction and valence bands, respectively. However, in the presence of a very strong electric field, the identification of f_{cc} and f_{vv} is not straightforward because of the coupling between the electron wave functions in the conduction and in the valence bands.

The evolution equation for the multiband Wigner function up to the first order in $\tilde{\hbar}$ read as:[10]

$$\frac{\partial f_{cc}}{\partial t} = -\frac{p}{m^*}\frac{\partial f_{cc}}{\partial x} + \mathcal{E}(x)\frac{\partial f_{cc}}{\partial p} + \mathcal{F}^+,$$

$$\frac{\partial f_{vv}}{\partial t} = \frac{p}{m^*}\frac{\partial f_{vv}}{\partial x} + \mathcal{E}(x)\frac{\partial f_{vv}}{\partial p} - \mathcal{F}^-,$$

$$\frac{\partial f_{cv}^r}{\partial t} = -\frac{2}{\tilde{\hbar}}\Omega f_{cv}^i + \mathcal{E}(x)\frac{\partial f_{cv}^r}{\partial p} + \frac{\tilde{\hbar}}{\tau_0\mathcal{E}_0}\frac{d\mathcal{E}}{dx}\frac{\partial(f_{cc}+f_{vv})}{\partial p}, \tag{9}$$

$$\frac{\partial f_{cv}^i}{\partial t} = \frac{2}{\tilde{\hbar}}\Omega f_{cv}^r + \mathcal{E}(x)\frac{\partial f_{cv}^i}{\partial p} + \frac{\mathcal{E}(x)}{\tau_0\mathcal{E}_0}(f_{cc}-f_{vv}),$$

where $f_{cv}^i = 2\Im\{f_{cv}\}$, $f_{cv}^r = 2\Re\{f_{vc}\}$. $\Im(\Re)$ denotes the imaginary (real) part and

$$\mathcal{F}^{\pm} = \frac{2}{\tau_0\mathcal{E}_0}\left[-\mathcal{E}(x)f_{cv}^i \pm \tilde{\hbar}\frac{d\mathcal{E}}{dx}\frac{\partial f_{cv}^r}{\partial p}\right],$$

$$\Omega(p) = \frac{E_g}{2} + \frac{p^2}{2m^*}.$$

The multiband Wigner system (9) exhibits a very complex dynamics, which is the source of many difficulties in the numerical approach. To overcome this difficulty a different approach based on the Weyl quantization procedure is proposed. Given a differential operator $\hat{\mathcal{A}}$ acting on the x variable, the Weyl quantization procedure establishes a unique correspondence between $\hat{\mathcal{A}}$ and a function $\mathcal{A}(x,p)$, which is the symbol of the operator. Formally we can define the Weyl operator such as $\mathcal{W}[\mathcal{A}(x,p)]=\hat{\mathcal{A}}$. In particular, if h is a differentiable function we have

$$(\hat{\mathcal{A}}h)(x) = \mathcal{W}[\mathcal{A}(x,p)]h = \frac{1}{2\pi\tilde{\hbar}}\int \mathcal{A}\left(\frac{x+y}{2},p\right)h(y)e^{i/\tilde{\hbar}(x-y)p}dydp. \tag{10}$$

In the framework of the Weyl quantization procedure, a generical mixed state is defined by its density operator $\hat{\mathcal{S}}_\psi$

$$\hat{\mathcal{S}}_\psi[h] = \int \rho_\psi(x,x')h(x')dx'$$

whose kernel is the density matrix

$$\rho_\psi(x,x') = \sum_{i,j}\rho_{ij}\boldsymbol{\psi}_i(x)\boldsymbol{\psi}_j^t(x').$$

Here ρ_{ij} are given coefficients, $\boldsymbol{\psi}_i$ is an orthonormal set of basis functions, and the superscript t denotes the transposition. The Weyl symbol $\mathcal{S}_\psi=\mathcal{W}^{-1}[\hat{\mathcal{S}}_\psi]$ is obtained by applying the Wigner transformation to the function $\rho_\psi(x,x')$

$$\mathcal{S}_\psi(x,p) = f_\psi(x,p) = \frac{1}{2\pi}\int \rho_\psi\left(x+\frac{\eta}{2},x'-\frac{\eta}{2}\right)e^{-i/\tilde{\hbar}p\eta}d\eta.$$

The matrix Θ,

$$\Theta = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1+\sigma} & \sqrt{1-\sigma} \\ -\sqrt{1-\sigma} & \sqrt{1+\sigma} \end{pmatrix},$$

$$\sigma = \frac{\Omega}{\sqrt{P_R^2+\Omega^2}}, \tag{11}$$

diagonalizes the hamiltonian symbol

$$\mathcal{H} = \mathcal{W}^{-1}[\hat{\mathcal{H}}] = \begin{bmatrix} U(x)+\Omega(p) & P_R(x) \\ P_R(x) & U(x)-\Omega(p), \end{bmatrix} \tag{12}$$

where $\hat{\mathcal{H}}$ is defined in Eq. (5). We derive the multiband Wigner-MEF system related to the set of wave function $\boldsymbol{\varphi}=\hat{\Theta}\boldsymbol{\psi}$. $\boldsymbol{\varphi}$ can de interpreted as a new set of basis functions defined by the rotation operator $\hat{\Theta}$. In the "rotated frame" the density operator $\hat{\mathcal{S}}_\varphi$ is

$$\hat{\mathcal{S}}_\varphi = \hat{\Theta}\hat{\mathcal{S}}_\psi\hat{\Theta}^\dagger, \tag{13}$$

where $\hat{\Theta}^\dagger$ denotes the dual operator of Θ. By using the property

$$\mathcal{W}^{-1}[\hat{\mathcal{A}}\hat{\mathcal{B}}] = [\mathcal{W}^{-1}(\hat{\mathcal{A}})]\#[\mathcal{W}^{-1}(\hat{\mathcal{B}})]$$

we derive the relationship between f_φ (the symbol of $\hat{\mathcal{S}}_\varphi$) and f_ψ

$$f_\varphi = \Theta \# f_\psi \# \Theta^t, \tag{14}$$

where # denotes the Moyal product. The Heisenberg evolution equation for the density operator $\hat{\mathcal{S}}_\psi$ is

$$i\tilde{\hbar}\frac{\partial \hat{\mathcal{S}}_\psi}{\partial t} = [\hat{\mathcal{H}}, \hat{\mathcal{S}}_\psi], \tag{15}$$

where the square brackets denote commutation. Applying the Weyl operator to the previous equation we obtain the evolution equation for $f_\varphi(x,p)$. We have

$$i\tilde{\hbar}\frac{\partial f_\varphi}{\partial t} = [\mathcal{H}', f_\varphi]_\# + o(\tilde{\hbar}), \tag{16}$$

where $\mathcal{H}' = \Theta \# \mathcal{H} \# \Theta^t$ and we have used

$$\Theta \# f_\psi \# \widetilde{\Theta^{-1}} = \Theta \# f_\psi \# \Theta^t + o(\tilde{\hbar}) = f_\varphi + o(\tilde{\hbar}).$$

Here $\widetilde{\Theta^{-1}}$ denotes the symbol of $\hat{\Theta}^{-1}$. The previous equation can be verified by noting that

$$(\widetilde{\Theta^{-1}} - \Theta^t) \# \Theta = o(\tilde{\hbar})$$

and

$$\widetilde{\Theta^{-1}}(x,p) = \Theta^t(x,p) + o(\tilde{\hbar}), \tag{17}$$

which follow from the expansion of the Moyal product with respect to $\tilde{\hbar}$

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

Up to the first order in $\tilde{\hbar}$, $\mathcal{H}'$ becomes

$$\mathcal{H}' = \begin{pmatrix} \mathcal{H}^+ & -i\tilde{\hbar}\xi \\ i\tilde{\hbar}\xi & \mathcal{H}^-, \end{pmatrix}$$

where

$$\xi(x,p) = \mathcal{E}\frac{P_R}{P_R^2 + \Omega^2}\frac{p}{m^*}, \tag{18}$$

$$\mathcal{H}^\pm = \pm\sqrt{P_R^2 + \Omega^2} + U(x), \tag{19}$$

and Eq. (16) gives

$$i\tilde{\hbar}\frac{\partial f_\varphi}{\partial t} = [\mathcal{H}', f_\varphi] + \frac{\tilde{\hbar}}{2i}\left\{\frac{\partial \mathcal{H}'}{\partial p}, \frac{\partial f_\varphi}{\partial x}\right\} - \frac{\tilde{\hbar}}{2i}\left\{\frac{\partial \mathcal{H}'}{\partial x}, \frac{\partial f_\varphi}{\partial p}\right\} + o(\tilde{\hbar}), \tag{20}$$

where the square and curly brackets denote, respectively, the standard commutation and the anticommutation operators. The previous equation gives explicitly

$$\frac{\partial h_c}{\partial t} = -\frac{\partial \mathcal{H}^+}{\partial p}\frac{\partial h_c}{\partial x} + \frac{\partial \mathcal{H}^+}{\partial x}\frac{\partial h_c}{\partial p} - 2\xi\Re(h_{cv}), \tag{21}$$

$$\frac{\partial h_v}{\partial t} = -\frac{\partial \mathcal{H}^-}{\partial p}\frac{\partial h_v}{\partial x} + \frac{\partial \mathcal{H}^-}{\partial x}\frac{\partial h_v}{\partial p} + 2\xi\Re(h_{cv}), \tag{22}$$

$$\frac{\partial h_{cv}}{\partial t} = -i\frac{2}{\tilde{\hbar}}\sqrt{P_R^2 + \Omega^2}h_{cv} + \mathcal{E}\frac{\partial h_{cv}}{\partial p} + \xi(h_c - h_v). \tag{23}$$

Here, to ease notation, we have defined $(h_c, h_v, h_{cv}) = (f_{\varphi_{cc}}, f_{\varphi_{vv}}, f_{\varphi_{cv}})$. Since the functions h_c and h_v (intraband distribution functions) are the diagonal components of the Wigner multiband function in the basis $\boldsymbol{\varphi}$, where the $k\cdot p$ Hamiltonian is diagonal (up to the first order in $\tilde{\hbar}$), they represent the effective distribution functions of particles in a regime of strong band-to-band coupling. The system of Eqs. (21)–(23) shows that up to zero order in $\tilde{\hbar}$, the Wigner functions h_c and h_v follow the Hamiltonian flux generated by $\mathcal{H}^\pm$. The eigenvalues of the Hamiltonian operator thus provide the multiband quantum correction to the classical single-band Hamiltonian $\mathcal{H}_{\rm sb} = U(x) + \frac{p^2}{2m^*}$. We remark that the diagonalization procedure of the Hamiltonian symbol $\mathcal{H}$ which characterizes our approach to the Multiband Wigner dynamics, strongly reduces the coupling among the interband and the intraband multiband functions compared with respect to the original formulation of Eq. (9). In fact in the presence of a strong electric field the coupling parameter ξ approaches the asymptotic value $\xi^\infty = \lim_{\mathcal{E}\to\infty} \xi < \infty$ whereas the coupling term $\mathcal{F}^\pm$ in Eq. (9) goes to infinity. Furthermore the diagonal term $i\sqrt{P_R^2+\Omega^2}$ in Eq. (23) induces a fast-in-time oscillation of h_{cv} (whose frequency is on the order of $E_g/\hbar$) which, up to zero order in $\tilde{\hbar}$, decouples h_{cv} from the slowly varying intraband functions h_c and h_v. As pointed out in the Sec. II, within the standard approximation of the rotating phases, no coupling between the fast and the slow rotating components of the solution is retained and the transition phenomena cannot be taken into account. A more accurate approximation is thus required to model the interband tunneling processes.

The procedure outlined in this section is quite general. The matrix $\Theta(x,p)$ diagonalizes (in the x-p space) the symbol of the multiband Hamiltonian operator and defines a rotation in the Hilbert space spanned by the band degree of freedom. The operator $\hat{\Theta} = \mathcal{W}[\Theta(x,p)]$ can be used to define a new set of Wigner functions. This set of multiband Wigner functions evolve according to a Liouville-type system of equation and each component follows the Hamiltonian flux generated by the eigenvalues of the original Hamiltonian.

In Appendix B we give an alternative derivation of the system of Eqs. (21)–(23) based on a direct diagonalization of the original system of Eq. (9).

IV. W-MEF SYSTEM

We present some numerical result obtained by solving the W-MEF system of Eqs. (21)–(23). The numerical code is based on the splitting scheme algorithm described in Ref. 10. As an application of the multiband Wigner model we consider a simple interband diode consisting of a homogeneous semiconductor where a uniform electric field $\bar{\mathcal{E}}$ is applied in the domain $[-w,w]$. As initial datum we choose a vanishing function, and for boundary condition the function

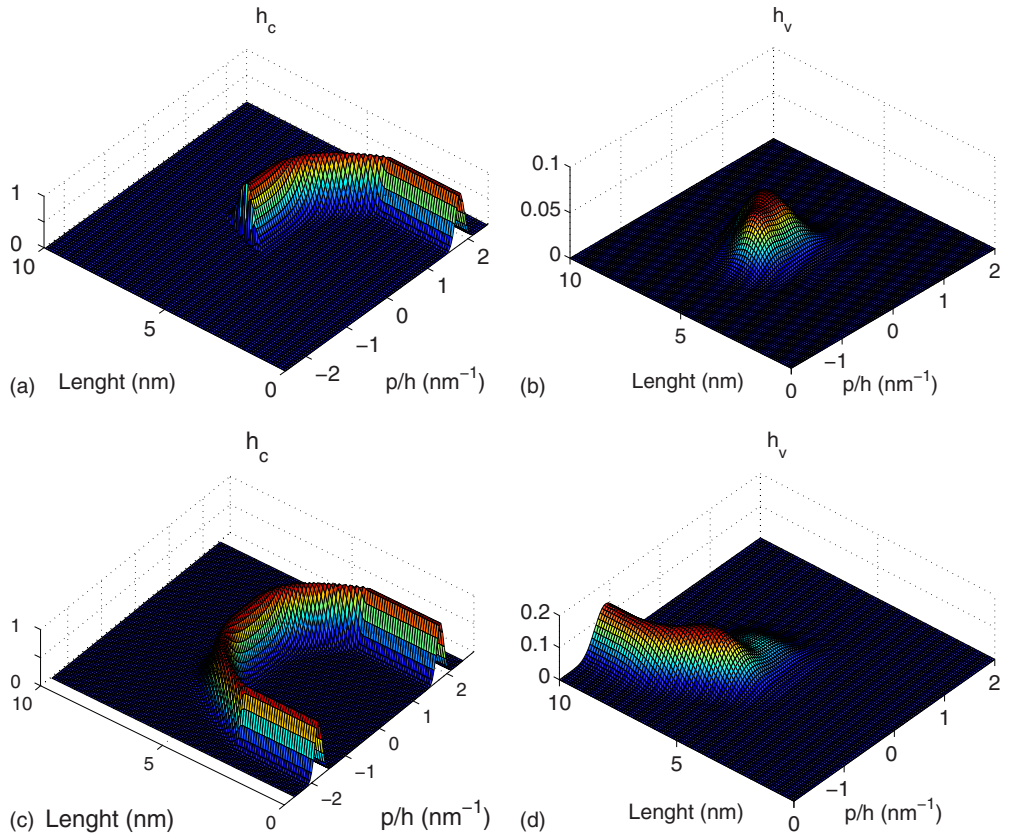

FIG. 1. (Color online) Snapshot of h_c and h_v functions for $t=50$ fs (up panel) and $t=100$ fs (down panel).

$$\begin{cases} h_c(p) = e^{-(p-p_0)^2/K_B T m^*} & \text{for } p > 0 \\ h_i(p) = 0 & \text{otherwise, } i = c,v,cv, \end{cases} \tag{24}$$

where K_B is the Boltzmann constant. Equation (24) describes a flux of conduction electrons injected into the diode with a positive mean momentum and Gaussian dispersion (see Fig. 1). In our simulation, we used the following parameters: $E_g=E_c-E_v=0.16$ eV, $m^*=0.023m_0$, $P_K/\hbar=5$ nm^{-1}, $p_0/\hbar=1.8$ nm^{-1}, $\bar{\mathcal{E}}=5\times10^{-3}$ eV nm^{-1}, $w=2$ nm, and $T=300$ K. The results of the simulation show that the conduction electron beam, described by the function h_c, is reflected back by the potential barrier. Besides, the gradient of the potential couples conduction and valence electrons, and the h_v component (representing the part of the electrons in valence band) grows giving rise to a nonvanishing flux of electrons traveling outside the diode. In Fig. 2 we show the contour plot of the same function of Fig. 1.

A. Single-band limit

We explore the single-band limit of Eqs. (21)–(23). If the electric field (band gap) goes to zero (infinity), the nondiagonal terms of the Hamiltonian of Eq. (4) vanish and the dynamics of the electrons in the conduction band is decoupled from those of the valence band. We define the parameter $\Upsilon=\frac{P_R}{\Omega}$ which is vanishing in the single-band limits $(\mathcal{E},1/E_g)\to0$ and we determine the correction to the single-band Wigner dynamics. By expanding Eq. (14) with respect to Υ we obtain

$$h_c = f_{cc}[1+\Upsilon^2] + \Im\{f_{cv}\}\Upsilon + f_{vv}\Upsilon^2 + o(\Upsilon^2), \tag{25}$$

$$h_v = f_{vv}[1+\Upsilon^2] - \Im\{f_{cv}\}\Upsilon + f_{cc}\Upsilon^2 + o(\Upsilon^2), \tag{26}$$

$$h_{cv} = f_{cv}[1-\Upsilon^2] + o(\Upsilon^2). \tag{27}$$

In the single-band limit, the new multiband Wigner function $\mathbf{H}=\begin{pmatrix} h_c & h_{cv} \\ \bar{h}_{cv} & h_v \end{pmatrix}$ agrees with the original variables $\mathbf{F}$ defined in Eq. (7), as expected. This limit defines the correct initial and boundary conditions for the system of Eqs. (21)–(23). In fact, to model semiconductor structures, it is convenient to prescribe nonvanishing initial conditions only in the regions where the electric field is negligible (and where $\mathbf{H}\simeq\mathbf{F}$). Consistently with the Wigner formalism, here the Wigner distribution function can be approximated with the classical distribution function (these initial conditions are used when the initial quantum correlation of the particles can be neglected[14]). For h_{cv} the classical limit $\hbar\to0$ gives

$$\lim_{\hbar\to0} h_{cv} = 0.$$

This limit is consistent with the assumption that h_{vc} represents the quantum correlation between the conduction and the valence eigenspaces, which has not a classical counterpart.

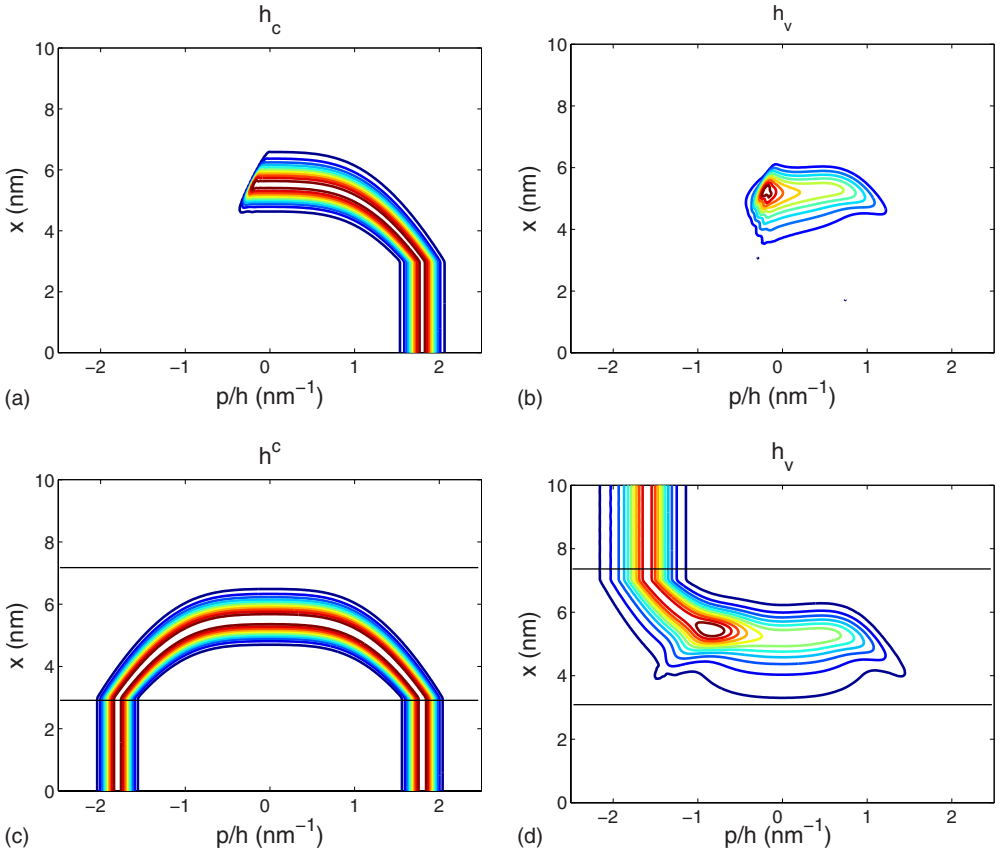

FIG. 2. (Color online) Contour plot of the h_c and h_v functions. The region with nonvanishing electric field is bounded by the horizontal lines.

B. Multiband correction to the classical single-band motion

Usually, the classical limit of a single-particle quantum system is obtained by expanding the Wigner equation of motion with respect to $\hbar$.[15] The evolution equation of the Wigner function (to all orders in $\hbar$) in presence of the single-band Hamiltonian $\mathcal{H}_{\mathrm{sb}}=U(x)-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}$ is

$$\frac{\partial f}{\partial t}=-\frac{p}{m^*}\frac{\partial f}{\partial x}+\theta[f], \tag{28}$$

$$\theta[f]=\frac{i}{2\pi\hbar m^*}\int \delta U(x,\eta)e^{i(p-\bar{p})\eta/m^*}f(x,\bar{p})d\eta d\bar{p}, \tag{29}$$

where $\delta U(x,\eta)=U(x+\frac{\hbar}{2m^*}\eta)-U(x-\frac{\hbar}{2m^*}\eta)$. Here the Wigner function f is defined in same way as in Eq. (8) with $i=j$ and with $\hbar$ instead of $\tilde{\hbar}$. The θ operator admits the following $\hbar$ expansion

$$\theta[f]=\sum_{\lambda}\frac{1}{(2\lambda+1)!}\left(\frac{\hbar}{2i}\right)^{2\lambda}\frac{d^{2\lambda+1}U}{dx^{2\lambda+1}}\frac{\partial^{2\lambda+1}f}{\partial p^{2\lambda+1}}. \tag{30}$$

In the classical regime only the term $\lambda=0$ is retained and θ reduces to the force operator $\mathcal{E}(x)\frac{\partial}{\partial p}$. From Eq. (30) it is evident that the motion becomes classical when the derivatives of the electric field are small. We remark that in presence of a uniform electric field $\mathcal{E}(x)=\bar{\mathcal{E}}$, the Wigner equation reduces exactly to the classical Liouville equation independently of the strength of the field. This consideration suggest us that it is possible to approximate the electronic motion by the classical evolution equation whenever the electric field can be considered approximatively constant in a given spatial domain $\mathfrak{D}$. Attention has to be payed to the fact that the θ operator is a highly nonlocal-in-space operator [as is evident from Eq. (29)] and a strong gradient of the electric field located well faraway to $\mathfrak{D}$ can affect the motion of the particles inside $\mathfrak{D}$ (see, for example, Refs. 16 and 17 where the higher-order terms are retained in the description of the Wigner equation of motion in the presence of an electromagnetic field). In Fig. 3 we compare the solution of the quantum Wigner equation with respect the classical counterpart for increasing electric fields. The profile of the electric field is plotted in Fig. 3(e). In Figs. 3(a)–3(d) we show the contour plot of the stationary state of Eq. (28) in the domain $[0,L]$. At the interfaces we model an incoming thermal distribution of particles in $x=0$ by using the following boundary conditions:

$$f(x=0,p>0)=\frac{m_{\parallel}^* K_B T}{\pi\hbar^2}\ln[1+e^{-1/K_B T(p^2/2m^*+E_c-\mu)}],$$

$$f(x=L,p<0)=0,$$

where K_B is the Boltzmann constant and T is the temperature of the particles.

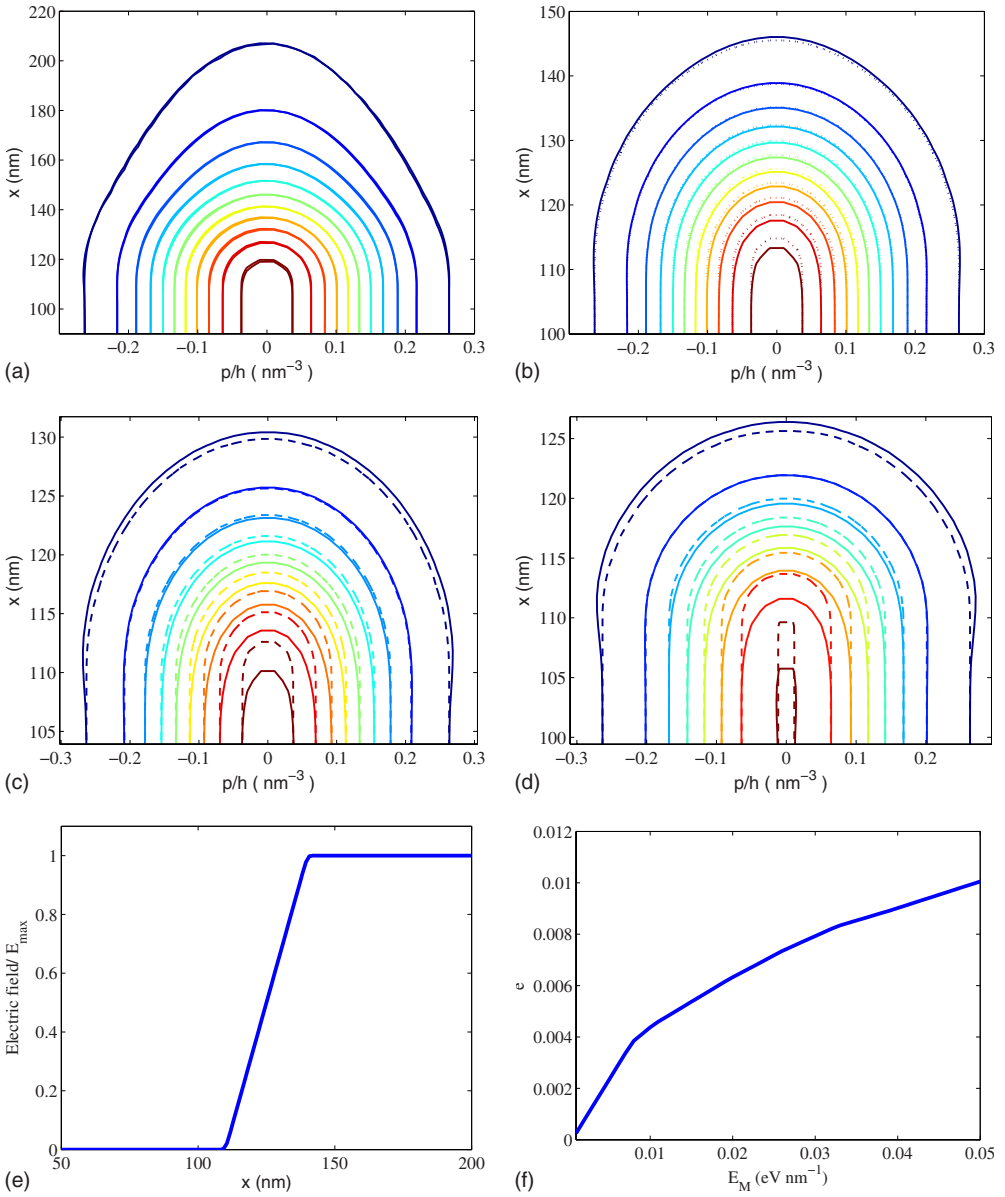

FIG. 3. (Color online) (a)–(d): Contour plots of the solution of Eq. (28) (solid line) compared with the classical solution (dashed line) for different values of the maximum of the electric field $\mathcal{E}_M$: (a) $\mathcal{E}_M=10^{-3}$ eV nm^{-1}, (b) $\mathcal{E}_M=5\times10^{-3}$ eV nm^{-1}, (c) $\mathcal{E}_M=10^{-2}$ eV nm^{-1}, and (d) $\mathcal{E}_M=5\times10^{-2}$ eV nm^{-1}. (e) Electric field used in the simulation normalized with respect the maximum $\mathcal{E}_M$. (f) Plot of the error parameter $\mathfrak{e}$ with respect to $\mathcal{E}_M$.

In Fig. 3(f) we plot the quantity

$$\mathfrak{e} = \sqrt{\frac{\int_0^L \int_{-\infty}^{\infty} |f - f_{\rm cl}|^2 dpdx}{\int_0^L \int_{-\infty}^{\infty} |f|^2 dpdx}},$$

where $f_{\rm cl}$ is the solution of the classical evolution equation, as a function of the maximum value of the eternal electric field $\mathcal{E}_M$. $\mathfrak{e}$ is the error done if we approximate the single-band quantum system by its classical limit. Our simulations show that for an electric field on the order of 5×10^{-3} eV nm^{-1} (which is, for example, the typical electric field attained in a usual semiconductor device as a metal-oxide semiconductor) the two solutions are practically identical. Now we consider the corrections to the motion arising from the multiband Hamiltonian of Eq. (5). It is immediate to verify that in the single-band limit the coupling coefficient ξ vanishes and the system (21)–(23) decouples. Thus the evolution is described by two Liouville equation (one for each band) with Hamiltonian

$$\mathcal{H}^{\pm} = \pm\sqrt{P_R^2 + \Omega^2} + U(x) = \pm\frac{p^2}{2m^*} + U(x) \pm \frac{E_g}{2}\left(1 + \frac{\Omega}{E_g}\Upsilon^2\right) + o(\Upsilon^2). \quad (31)$$

TABLE I. Numerical value of the parameters used in the single-band limits. Here $\mathcal{E}_M=5\times10^{-3}$ eV nm^{-1}.

	GaAs	Ge	GaSb	InAs	InSb
$\frac{\Omega\Upsilon^2}{E_g}\|_{p=0}$	8×10^{-5}	7.5×10^{-4}	1.1×10^{-3}	1.4×10^{-2}	2.2×10^{-1}

The zero order is the classical single-band Hamiltonian. In our procedure Υ is the parameter which measures the strength of the band-to-band coupling: in Table I we report the value of $\frac{\Omega\Upsilon^2}{E_g}|_{p=0}=\frac{\hbar P_K\mathcal{E}}{E_g^2 m_0}$ for various semiconductors. We see that for an electric field $\mathcal{E}$ on the order of 5×10^{-3} eV nm^{-1} [where according to Fig. 3(f) the single-band dynamics is essentially local-in-space] the last term in Eq. (31) gives some non-negligible corrections to the single-band Hamiltonian in materials such as InSb or InAs. We conclude that it is possible to have multiband quantum correction to the single-band trajectories even if the electric field is so small that the nonlocal quantum effect can be considered negligible. From a mathematical point of view, our expansion procedure is defined with respect to the asymptotical parameter $\tilde{\hbar}=\gamma\hbar$, and the range of its application is in the limit $\hbar\to0$ and $\gamma\to\infty$ while $\tilde{\hbar}$ is kept fixed. The Hamiltonian flux of $\mathcal{H}^+$ (similar results can be obtained with $\mathcal{H}^-$) is

$$\dot{x}=\frac{\partial\mathcal{H}^+}{\partial p}=\frac{1}{\sqrt{1+\left(\frac{P_R}{\Omega}\right)^2}}\frac{p}{m^*}$$
$$\dot{p}=-\frac{\partial\mathcal{H}^+}{\partial x}=-\mathcal{E}-\frac{1}{\sqrt{1+\left(\frac{\Omega}{P_R}\right)^2}}\frac{\hbar P_K}{m_0E_g}\frac{d\mathcal{E}}{dx}. \tag{32}$$

In Fig. 4 we compare the single-band trajectory with the quantum-corrected trajectory for InAs by using the same parameter of Fig. 3(a). It is worth noting that the multiband trajectory shows a small penetration in the region with the repulsive potential with respect to the single-band case. This is mainly due to the term $\sqrt{1+(\frac{P_R}{\Omega})^2}$ in Eq. (32) which multiplies the effective mass of the particle. The particle thus moves with a larger effective mass, i.e., a function of the classical position and momentum. This effect partially compensates the reduction in the mass in semiconductors with a small band gap like InAs or InSb.

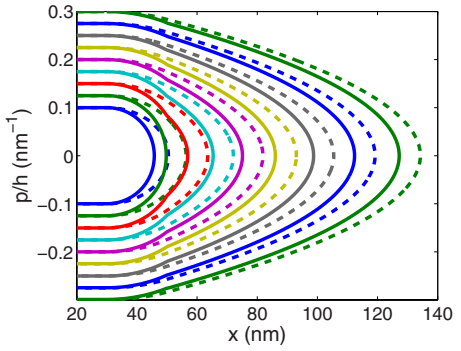

FIG. 4. (Color online) Pseudocharacteristic (continuous lines) compared with the classical characteristic (dashed lines).

Comparing Eq. (28) with the first-order differential Eqs. (21)–(23), we see that the first-order W-MEF hierarchy discards the quantum interference effects between the particles inside each band. These intraband interference effects are expressed by the higher order terms of the $\hbar$ expansion of θ and give rise to the typical oscillations of the Wigner function. According to the discussion of Sec. II, we preserve only the band-to-band higher frequencies interference effects (which are on the order of $E_g/\hbar$). This strong quantum oscillation regime is used in Sec. IV C to efficiently decouple the interband dynamics represented by h_{cv} with respect to the smooth-in-time intraband dynamics represented by h_c and h_v.

C. Interband transition

Because of the coupling among the intraband functions h_c and h_v and the real part of h_{cv} [see Eqs. (21) and (22)], interband transition can occur. In this section we will describe the transition processes where the electrons are scattered from the conduction band to the valence band. The same considerations apply for the inverse transition. For the sake of simplicity we assume that for $t=t_0$ only the conduction band is populated, so that we have the following initial condition for the multiband Wigner function

$$h_i=\begin{cases}h_c^I(x,p) & i=c\\ 0 & i=v,cv.\end{cases}$$

The integral solutions of the intraband evolution Eqs. (21) and (22) and of the interband evolution Eq. (23) are formally given by

$$h_{cv}(x,p,t')=\int_{t_0}^{t'}\xi[x,\tilde{p}(t'-t'')]h_-[x,\tilde{p}(t'-t''),t'']\times e^{i\int_{t''}^{t'}\mathcal{H}_{cv}[x,\tilde{p}(t'-\tau)]d\tau}dt'', \tag{33}$$

$$h_c(x',p',t)=h_c^I(x',p')-2\Re\left\{\int_{t_0}^{t}\xi[\tilde{x}_c(t'),\tilde{p}_c(t')]\times h_{cv}[\tilde{x}_c(t'),\tilde{p}_c(t'),t']dt'\right\}, \tag{34}$$

where ξ is given by Eq. (18) and

$$\mathcal{H}_{cv}(x,p)=\frac{2}{\tilde{\hbar}}\sqrt{P_R^2(x)+\Omega^2(p)},$$

$$h_-=h_c-h_v,$$

$$\tilde{p}(\tau)=\tilde{p}(x,p,\tau)=p+\mathcal{E}(x)\tau.$$

Equation (33) can be derived introducing the auxiliary function $g(x,p,t)=h_{cv}(x,p-\mathcal{E}t,t)$ in Eq. (23). We obtain

$$\frac{\partial g}{\partial t}=-i\mathcal{H}_{cv}(x,p-\mathcal{E}t)g+\xi(x,p-\mathcal{E}t)h_-.$$

In Eq. (34) we have defined the following Hamiltonian flux $(\tilde{x}_c,\tilde{p}_c)$

$$\frac{\partial \tilde{x}_c}{\partial t} = \frac{\partial \mathcal{H}^+}{\partial p}(\tilde{x}_c,\tilde{p}_c); \quad \tilde{x}_c(t_0) = x'$$

$$\frac{\partial \tilde{p}_c}{\partial t} = -\frac{\partial \mathcal{H}^+}{\partial x}(\tilde{x}_c,\tilde{p}_c); \quad \tilde{p}_c(t_0) = p'.$$

Inserting Eq. (33) in Eq. (34) we obtain

$$h_c(x',p',t) = h_c^I(x',p') - \Re\left\{\int_{\mathcal{D}_{T,\eta}} \mathcal{F}(T+\eta,T-\eta) \times e^{i\Phi(T+\eta,T-\eta)} dT d\eta\right\}, \tag{35}$$

where the integration domain $\mathcal{D}_{T,\eta}$ is

$$\mathcal{D}_{T,\eta} = \begin{cases} T \le t; & \eta > 0 \\ T > t; & \eta > T - t \end{cases}$$

and

$$\Phi(t',t'') = \int_{t''}^{t'} \mathcal{H}_{cv}[\tilde{x}_c(t'),\tilde{p}_i(t',\tau)] d\tau,$$

$$\tilde{p}_i(t_1,t_2) = \tilde{p}[\tilde{x}_c(t_1),\tilde{p}_c(t_1),t_2],$$

$$\mathcal{F}(t',t'') = 2\xi[\tilde{x}_c(t'),\tilde{p}_c(t')]\xi[\tilde{x}_c(t'),\tilde{p}_i(t',t'')] \times h_-[\tilde{x}_c(t'),\tilde{p}_i(t',t''),t''].$$

Due to the presence of the highly oscillating function $e^{i\Phi}$ we can apply the stationary phases approximation to evaluate the integral of Eq. (35). The stationary points are defined by

$$\frac{\partial \Phi}{\partial T} = \frac{\partial \Phi}{\partial \eta} = 0. \tag{36}$$

To solve Eq. (36), we approximate the profile of the electric field with a constant field $\bar{\mathcal{E}} = \mathcal{E}(x_0)$ in the neighborhood of the coordinate x_0 where the transition takes place. Since $\frac{\partial \Phi}{\partial \eta} > E_g$, Eq. (36) cannot be satisfied and the stationary point is reached when[18]

$$\frac{\partial \Phi}{\partial T} = \mathcal{H}_{cv}(p_1) - \mathcal{H}_{cv}(p_2) = 0,$$

$$\frac{\partial^2 \Phi}{\partial \eta^2} = \bar{\mathcal{E}}\left(\left.\frac{\partial \mathcal{H}_{cv}}{\partial p}\right|_{p=p_2} - \left.\frac{\partial \mathcal{H}_{cv}}{\partial p}\right|_{p=p_1} \right) = 0$$

with $p_1 = p' - \bar{\mathcal{E}}(T+\eta-t_0)$ and $p_2 = p' - \bar{\mathcal{E}}(T-\eta-t_0)$. The solutions are

$$T = t_0 + \frac{p'}{\bar{\mathcal{E}}},$$

$$\eta = 0.$$

The stationary point thus coincides with the turning point of the x characteristic (that is its intersection with the axis $p=0$). More generally, for an x dependent electric field, the exponential term gives a nonvanishing contribution to the integral of Eq. (35) only when $\tilde{p}_c(T)=0$ and the particle is at rest. To estimate the integral of Eq. (35) we neglect the temporal evolution of h_-, and we obtain the following Markov-type approximation of the interband tunneling processes

$$h_c(x',p',t) \simeq h_c^I(x',p') - h_-[\tilde{x}_c(x',p',t^*),\tilde{p}_c(x',p',t^*),t^*]\mathcal{T}^\infty(t), \tag{37}$$

where for $t=t^*$ we have $\tilde{p}_c(x',p',t^*)=0$ and

$$\mathcal{T}^\infty(t) = \Re\int_{\mathcal{D}_{T,\eta}} \tilde{\mathcal{F}}(T+\eta,T-\eta) e^{i\Phi(T+\eta,T-\eta)} dT d\eta,$$

$$\tilde{\mathcal{F}}(t_1,t_2) = 2\xi[\tilde{x}_c(t_1),\tilde{p}_c(t_1)]\xi[\tilde{x}_c(t_1),\tilde{p}_i(t_1,t_2)].$$

$\mathcal{T}^\infty$ represents the interband probability transition and depends only from the electric field $\mathcal{E}(x)$. $\mathcal{T}^\infty$ can be approximated by (the detail of the calculations are given in Appendix A)

$$\mathcal{T}^\infty(t) \simeq \theta_H[\tilde{p}_c(x',p',t)]\mathcal{T}_{cv}(x),$$

where θ_H is the step function and $\mathcal{T}_{cv}$ is given by

$$\mathcal{T}_{cv} = \xi_1^2 \frac{\pi^2}{2\sqrt[3]{D^2}} \mathrm{Ai}^2\left(\frac{C-H_1}{\sqrt[3]{D}}\right). \tag{38}$$

The effective equation of motion for the Wigner functions h_c, h_v can be obtained by differentiating with respect to the time Eq. (37) and coming back to the (x,p) variables by inverting the system

$$\begin{cases} \tilde{x}_c(x',p',t) = x \\ \tilde{p}_c(x',p',t) = p. \end{cases} \tag{39}$$

The final result is

$$\frac{\partial h_c}{\partial t} = -\frac{\partial \mathcal{H}^+}{\partial p}\frac{\partial h_c}{\partial x} + \frac{\partial \mathcal{H}^+}{\partial x}\frac{\partial h_c}{\partial p} - (h_c - h_v)\delta(p)\mathcal{E}(x)\mathcal{T}_{cv}(x).$$

Applying the same procedure to the h_v function we obtain the final Zener Boltzmann-type system

$$\begin{aligned} \frac{\partial h_c}{\partial t} &= -\frac{\partial \mathcal{H}^+}{\partial p}\frac{\partial h_c}{\partial x} + \frac{\partial \mathcal{H}^+}{\partial x}\frac{\partial h_c}{\partial p} + \left.\frac{\partial h_c}{\partial t}\right|_Z \\ \frac{\partial h_v}{\partial t} &= \frac{\partial \mathcal{H}^-}{\partial p}\frac{\partial h_v}{\partial x} + \frac{\partial \mathcal{H}^-}{\partial x}\frac{\partial h^-}{\partial p} + \left.\frac{\partial h_v}{\partial t}\right|_Z, \end{aligned} \tag{40}$$

where

$$\left.\frac{\partial h_v}{\partial t}\right|_Z = -\left.\frac{\partial h_c}{\partial t}\right|_Z = \int \mathcal{W}(p,p')[h_c(p') - h_v(p')]dp',$$

$$\mathcal{W}(p,p') = \mathcal{T}_{cv}\mathcal{E}(x)\delta(p)\delta(p').$$

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.

V. CONCLUSION

In this paper we have developed a model for the description of the Zener transition in a semiconductor by using the Wigner-function approach. We demonstrate the existence of physical regimes where the main quantum corrections to the classical motion are the deformation of the characteristics and the interband tunneling. These results are derived in a full quantum contest and the expansion procedure is intended to preserve the classical description of the motion. A suitable diagonalization procedure in the Weyl quantization framework is proposed and a new set of Wigner multiband functions are defined. We have introduced an approximate solution in closed form based on an iterative expansion which allows for a clear and intuitive physical picture of the interband transition process, leading to an analogy with electron scattering processes in semiconductors. We discussed the range of applicability of the expansion procedure which is at the basis of the evolution system of Eqs. (21)–(23), and its relationship with the usual single-band expansion, based on the Planck constant $\hbar$. The single-band limit has been discussed and some quantum correction to the single-band trajectory has been obtained. We showed that the solution is characterized by the presence of two different regimes: the fast processes arising form band-to-band oscillation (intraband motion), and whose frequency is the order of the band gap; and the slow dynamical processes that determine the intraband motion of the particle in term of the Hamiltonian characteristic flux of the particles. The coupling between the intraband and the interband components of the solution only occurs when the particle crosses the $p=0$ axis. One of the main advantages of our diagonalization procedure is the possibility to separate the fast evolving components of the solution from the slow dynamics, which were mixed in the original formulation.

ACKNOWLEDGMENT

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APPENDIX A: THE TRANSITION RATE $\mathcal{T}^{\infty}(t)$

In this section we will evaluate the integral

$$\mathcal{T}^{\infty}(t) = \lim_{t\to\infty} \mathcal{T}(-\infty, t),$$

$$\mathcal{T}(t_0,t) = \Re\left\{\int_{t_0}^{t} g(t')\int_{t_0}^{t'} f(t'')dt''dt'\right\}, \tag{A1}$$

with

$$\bar{f} = g = \xi(t)e^{i\int_{t^*}^{t}\lambda(\tau)d\tau}, \tag{A2}$$

where

$$\lambda(\tau) = \frac{2}{\tilde{\hbar}}\sqrt{P_R^2(x_0) + \Omega^2[\tilde{p}(\tau)]} \tag{A3}$$

with $\frac{d\lambda}{dt}(t^*)=0$ and ξ is given in Eq. (18). By using the standard properties of the Fourier transform we have

$$\mathcal{T}^{\infty} = 2\pi^2\left|\sum_{n=-N}^{N}\tilde{\xi}_n \exp i\left(\int_{t^*}^{t}\lambda(\tau)d\tau + H_n t\right)\right|^2, \tag{A4}$$

where we have expanded ξ in Fourier series in a convenient interval $[-J_0, J_0]$

$$\xi(t) = \sum_{n=-N}^{N}\tilde{\xi}_n e^{iH_n t}; \quad H_n = n\frac{\pi}{J_0}.$$

To get an analytical approximation of the previous formula it is convenient to approximate

$$\int_{t^*}^{t}\lambda(\tau)d\tau \simeq Ct + D\frac{t^3}{3}, \tag{A5}$$

where the coefficients in the right-hand side can be obtained by a least-square fitting approximation

$$D = \frac{45}{8(t^*+t_0)^5}\int_{t^*-t_0}^{t^*+t_0}\left(\lambda\tau^2 - \frac{(t^*+t_0)^2}{3}\lambda\right)d\tau, \tag{A6}$$

$$C = \frac{1}{2(t^*+t_0)}\int_{t^*-t_0}^{t^*+t_0}\lambda d\tau - \frac{(t^*+t_0)^2}{3}D. \tag{A7}$$

To estimate t_0 we note that when $\int_{t^*}^{t''}\lambda(\tau)d\tau$ grows, the exponential in Eq. (A1) gives a vanishing contribution the integral. Expanding λ around its minimum $\lambda(t^*)$ we obtain

$$\lambda(t) \simeq \lambda(t^*) + \ddot{\lambda}(t^*)\frac{(t-t^*)^2}{2}.$$

We define a fitting parameter $\varsigma > 1$ such as for $t=t^*+t_0$ we have

$$\frac{\lambda(t^*+t_0)}{\lambda(t^*)} = \varsigma$$

and we obtain t_0

$$t_0 = t^* + \varsigma\frac{(4P_R^2 + E_g^2)m^*}{4\mathcal{E}^3 E_g}.$$

Equation (A4) becomes

$$\mathcal{T}^{\infty} = 2\pi^2\left|\sum_{n=-N}^{N}\tilde{\xi}_n\frac{1}{\sqrt[3]{D}}\mathrm{Ai}\left(\frac{C+H_n}{\sqrt[3]{D}}\right)\right|^2 \tag{A8}$$

where Ai is the Airy function

$$\frac{2\pi}{\sqrt[3]{\mathcal{B}}}\mathrm{Ai}\left(\frac{\mathcal{A}}{\sqrt[3]{\mathcal{B}}}\right) = \int_{-\infty}^{\infty} e^{i(\mathcal{A}t+\mathcal{B}/3t^3)}dt. \tag{A9}$$

Finally, if we approximate ξ with a single oscillating function we obtain

$$\xi(t) = \frac{\mathcal{E}^2}{m^*}\frac{P_R}{P_R^2 + \Omega^2[\mathcal{E}^2(t-t^*)]}(t-t^*)$$

$$\simeq \tilde{\xi} = \xi_1 \sin[H_1(t-t^*)]e^{i(\mathcal{A}t+\mathcal{B}/3t^3)}dt, \tag{A10}$$

where

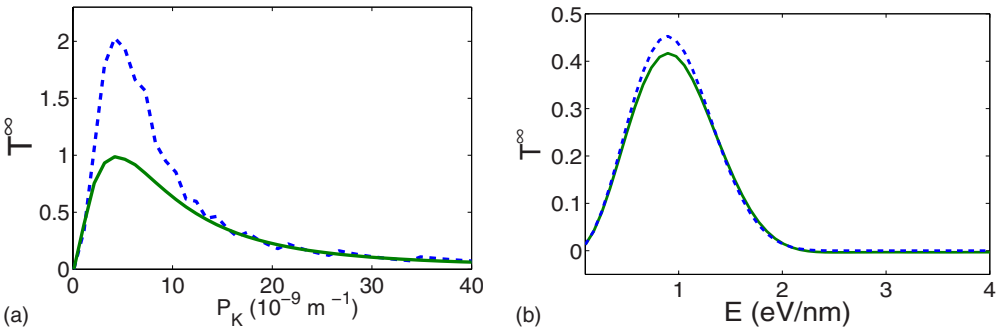

FIG. 5. (Color online) Estimation of the error in the approximation of $\mathcal{T}^\infty$. Left panel: exact (dashed blue line) and approximated (continuous green line) values of $\mathcal{T}^\infty$ for different values of P_K. Right panel: exact (dashed blue line) and approximated (continuous green line) values of $\mathcal{T}^\infty$ for different values of the electric field $\mathcal{E}$.

$$\dot{\xi}(J_0/2) = \dddot{\xi}(J_0/2) = 0$$

$$\frac{\pi}{J_0} = H_1 = 2\pi\sqrt{\frac{E_g}{2m^*}}\frac{\mathcal{E}}{P_R^2 + \left(\frac{E_g}{2}\right)^2}$$

$$\xi_1 = \xi(J_0/2).$$

In Fig. 5 we compare the exact values of $\mathcal{T}^\infty$ obtained by direct numerical integration of Eq. (A1), with the single harmonic approximation of Eq. (38), for different values of the Kane parameter P_K and the electric field $\mathcal{E}$.

APPENDIX B: DERIVATION OF THE W-MEF SYSTEM

In Sec. III we presented a diagonalization procedure which transform the system of Eq. (9) into the system of Eqs. (21)–(23) and we defined the new set of multiband functions h_c, h_v, and h_{cv}. The derivation was based on the Weyl quantization framework and we exploited the properties of the Moyal product to obtain the Wigner multiband evolution equation in a rather simple way, avoiding cumbersome calculations. In this appendix we derive the same results by using an alternative approach based on the operator mechanics framework.

We write Eq. (9) in the compact form

$$\frac{\partial \mathbf{f}}{\partial t} = \left(\mathbf{A}_0 + \tilde{\hbar}\mathbf{A}_x\frac{\partial}{\partial x} + \tilde{\hbar}\mathbf{A}_p\frac{\partial}{\partial p}\right)\mathbf{f}, \tag{B1}$$

where $\mathbf{f}=(f_{cc}+f_{vv};f_{cc}-f_{vv};f_{cv}^i;f_{cv}^r)^t$ and

$$\mathbf{A}_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -P_R & 0 \\ 0 & P_R & 0 & \Omega \\ 0 & 0 & -\Omega & 0 \end{pmatrix}; \quad \mathbf{A}_p = \begin{pmatrix} \mathcal{E} & 0 & 0 & \frac{dP_R}{dx} \\ 0 & \mathcal{E} & 0 & 0 \\ 0 & 0 & \mathcal{E} & 0 \\ \frac{dP_R}{dx} & 0 & 0 & \mathcal{E} \end{pmatrix};$$

$$[\mathbf{A}_x]_{i,j} = -\frac{p}{m^*}(\delta_{i,1}\delta_{j,2} + \delta_{j,1}\delta_{i,2}),$$

We search for a new set of pseudodistribution functions, for which the zeroth-order dynamics is diagonal. In order to illustrate our diagonalization procedure, we consider the oversimplified case where the electric field vanishes and thus the $\mathbf{A}_p$ operator is identically zero. The Eq. (B1) simplifies

$$\frac{\partial \mathbf{f}}{\partial t} = \left(\mathbf{A}_0 + \tilde{\hbar}\mathbf{A}_x\frac{\partial}{\partial x}\right)\mathbf{f}.$$

We apply the Fourier transform with respect the x variable and we obtain

$$\frac{\partial \hat{\mathbf{f}}}{\partial t} = (\mathbf{A}_0 + i\tilde{\hbar}\mu\mathbf{A}_x)\hat{\mathbf{f}}, \tag{B2}$$

where $\hat{\mathbf{f}}(\mu)$ is the Fourier transform of $\mathbf{f}(x)$. We denote with $\mathbf{\Theta}(\mu,p)$ the matrix which diagonalize $\mathbf{A}_0+i\tilde{\hbar}\mu\mathbf{A}_x$

$$\mathbf{\Theta}^{-1}(\mathbf{A}_0 + i\tilde{\hbar}\mu\mathbf{A}_x)\mathbf{\Theta} = \mathbf{\Lambda}(\mu,p). \tag{B3}$$

In term of the new variable $\hat{\mathbf{h}}=\mathbf{\Theta}^{-1}\hat{\mathbf{f}}$ the Eq. (B2) becomes

$$\frac{\partial \hat{\mathbf{h}}}{\partial t} = \mathbf{\Lambda}(\mu,p)\hat{\mathbf{h}}. \tag{B4}$$

By Fourier antitransforming we recover the equation of motion in the spatial variable x. In particular, to each term of the μ expansion of the matrix $\mathbf{\Lambda}(\mu,p)$ corresponds a differential operator in the x space of the same order. Furthermore, from the definition of $\mathbf{\Lambda}(\mu,p)$ in Eq. (B3), it is evident that $\mathbf{\Lambda}$ depends on μ via $\tilde{\hbar}\mu$ and thus an expansion of $\mathbf{\Lambda}$ with respect to μ is equivalent to an expansion with respect $\tilde{\hbar}$. Semiclassical approximations of the Wigner-MEF system arise when the transport equation for $\mathbf{h}$ has the same structure of the Liouville equation, which is a first-order differential equation with respect to the kinetic variables x and p. It is thus sufficient to expand $\mathbf{\Lambda}(\mu,p)$ up to the first order with respect to $\tilde{\hbar}$ in Eq. (B4) and Fourier transform to obtain the evolution equation in the x space

$$\frac{\partial \mathbf{h}}{\partial t} = \left[\mathbf{\Lambda}(0,p) + \left.\frac{\partial \mathbf{\Lambda}}{\partial \mu}\right|_{\mu=0}\frac{\partial}{\partial x} + o(\tilde{\hbar})\right]\mathbf{h}(x).$$

The relationship between $\mathbf{h}$ and the original variable $\mathbf{f}$ is obtained by expanding the $\mathbf{\Theta}$ operator up to the first order in

μ. This procedure can be extended to the general case of a x-dependent electric field $\mathcal{E}(x)$ in following way: we generalize Eq. (B3) defining the following operator acting on $\mathbf{f}$

$$\mathbf{\Theta f} = \left[\Theta^0 + \tilde{\hbar}\left(\Theta^1 + \Theta_x \frac{\partial}{\partial x} + \Theta_p \frac{\partial}{\partial p} \right) \right] \mathbf{f} = \mathbf{h}, \tag{B5}$$

where the Θ operators defined in the previous formula are 4×4 matrices on the x and p variables. We choose $\mathbf{\Theta}$ such as

$$\mathbf{\Theta}^{-1}\left(\mathbf{A}_0 + \tilde{\hbar}\mathbf{A}_x \frac{\partial}{\partial x} + \tilde{\hbar}\mathbf{A}_p \frac{\partial}{\partial p} \right) \mathbf{\Theta} = \mathbf{\Lambda} + \tilde{\hbar}\mathbf{T}. \tag{B6}$$

$\mathbf{T}$ is a matrix representing the first-order contribution to the transition, which will be evaluated in the following: $\mathbf{\Lambda}(x, \tilde{\hbar}\frac{\partial}{\partial x})$ is a diagonal matrix of pseudodifferential operators (i.e., each element of $\mathbf{\Lambda}$ is a differential operator acting on $\mathbf{h}$ and admitting a $\tilde{\hbar}$ expansion). Thus

$$\begin{aligned}
&\mathbf{\Lambda}_{i,j}\left(x, p, \tilde{\hbar}\frac{\partial}{\partial x}, \tilde{\hbar}\frac{\partial}{\partial p} \right) \\
&= \delta_{ij} \lambda^i \left(x, p, \tilde{\hbar}\frac{\partial}{\partial x}, \tilde{\hbar}\frac{\partial}{\partial p} \right) \\
&= \delta_{ij} \sum_{n=0;|m|\le n}^{\infty} \tilde{\hbar}^n \left(\eta^i_{n,x^m}(x,p) \frac{\partial^m}{\partial x^m} + \eta^i_{n,p^m}(x,p) \frac{\partial^m}{\partial p^m} \right) \\
&= \delta_{ij} \left[\lambda^i_0 + \tilde{\hbar}\left(\eta^i_0(x) + \eta^i_x \frac{\partial}{\partial x} + \eta^i_p \frac{\partial}{\partial p} \right) \right] + o(\tilde{\hbar}),
\end{aligned} \tag{B7}$$

where for simplicity $\lambda^i_0(x,p) = \eta^i_{0,0}$ and we suppressed the n index in the other terms. We evaluate the matrix $\mathbf{\Theta}$, in order to satisfy Eq. (B6) up to the first order in $\tilde{\hbar}$. We define by $\mathbf{u}^k$ the column vector operator equal to the kth column of $\mathbf{\Theta}$ (i.e., $\mathbf{u}^k_i = \mathbf{\Theta}_{i,k}$, where the i index denotes the ith component of the vector $\mathbf{u}^k$) and we multiply Eq. (B6) with $\mathbf{\Theta}$ from the left. We obtain

$$\left[\mathbf{A}_0(x) + \tilde{\hbar}\mathbf{A}_x \frac{\partial}{\partial x} + \tilde{\hbar}\mathbf{A}_p \frac{\partial}{\partial p} \right] \mathbf{u}^k = \mathbf{u}^k \lambda^k + \tilde{\hbar} \sum_j \mathbf{u}^j T_{j,k}, \tag{B8}$$

where, according to the $\tilde{\hbar}$ expansion of Θ, $\mathbf{u}^k$ is given by

$$\begin{aligned}
\mathbf{u}^k\left(x, p, \frac{\partial}{\partial x}, \frac{\partial}{\partial p} \right) &= \mathbf{u}^k_0(x,p) + \tilde{\hbar}\left[\mathbf{v}^k_0(x,p) \right. \\
&\left. + \mathbf{v}^k_x(x,p)\frac{\partial}{\partial x} + \mathbf{v}^k_p(x,p)\frac{\partial}{\partial p} \right]
\end{aligned}$$

The zeroth order of Eq. (B8) is

$$\mathbf{A}_0(x,p)\mathbf{u}^k_0 = \lambda^k_0 \mathbf{u}^k_0$$

and the $\mathbf{u}^k_0$ are the eigenvectors of the zeroth-order operator $\mathbf{A}_0$. Here the x and p variables act just like a parameter. We calculate the first order of Eq. (B8) and we multiply from the left by $\mathbf{u}^{r\dagger}_0$, where $\dagger$ denotes the algebraic conjugation. We obtain

$$(\bar{\lambda}^r_0 - \lambda^k_0)(\mathbf{u}^r_0, \mathbf{v}^k_\gamma) = \delta_{r,k}\eta^k_\gamma - \mathbf{u}^{r\dagger}_0 \mathbf{A}_\gamma \mathbf{u}^k_0 \quad \gamma = x,p \tag{B9}$$

$$\begin{aligned}
(\bar{\lambda}^r_0 - \lambda^k_0)(\mathbf{u}^r_0, \mathbf{v}^k_0) = \delta_{r,k}\eta^k_0 - \mathbf{u}^{r\dagger}_0 \left(\mathbf{A}_x \frac{\partial \mathbf{u}^k_0}{\partial x} - \mathbf{v}^k_x \frac{\partial \lambda^k_0}{\partial x} \right. \\
\left. + \mathbf{A}_p \frac{\partial \mathbf{u}^k_0}{\partial p} - \mathbf{v}^k_p \frac{\partial \lambda^k_0}{\partial p} \right) + T_{r,k},
\end{aligned} \tag{B10}$$

where $(,)$ denotes the ordinary scalar product $(\mathbf{a},\mathbf{b}) = \mathbf{a}^\dagger \mathbf{b}$. Finally to determine the unknown $\mathbf{u}^k$ up to the first order, we expand $\mathbf{v}^k$ on the $\mathbf{u}^k_0$ basis

$$\mathbf{v}^k_\gamma = \sum_k (\mathbf{u}^n_0, \mathbf{v}^k_\gamma)\mathbf{u}^k_0; \quad \gamma = 0, x, p$$

and the expansion coefficients can be found from Eqs. (B9). After some algebra, we obtain the equation of motion for $\mathbf{h} = \mathbf{\Theta f}$ [see Eq. (B6)], which agrees with the Wigner-MEF system given in Eqs. (21)–(23).

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