Multiband Quantum Transport Models for Semiconductor Devices

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1 Introduction

The modeling of semiconductor devices, which is a very active and intense field of research, has to keep up with the speed at which the fabrication technology proceeds; the devices of the last generations become smaller and smaller and they have reached a size so small that quantum effects dominate their behaviour. Quantum effects such as resonant tunneling and other size-quantized effects cannot be described by classical or semiclassical theories and need a full quantum description [Fre90, JAC92, KKFR89, MRS90, RBJ91, RBJ92]. A very important feature, that has appeared in the devices of the last generation and which requires a full quantum treatment, is the presence of the interband current, that is a contribution to the total current which arises from transitions between the conduction and the valence band states. Resonant interband tunneling diodes (RITD) are examples of semiconductor devices which exploit this phenomenon; they are of big importance in nanotechnology for their applications to high-speed and miniaturized systems [YSDX91, SX89]. In the band diagram structure of these diodes there is a small region where the valence band edge lies above the conduction band edge (valence quantum well), making interband resonance possible.

So far, most part of the existing literature has been devoted to quantum transport models where only conduction band electrons contribute to the current flow and under the parabolic band approximation, with only a small region of the Brillouin zone near the minimum of the band being populated. In bipolar models, the contribution of the valence band (the current due to the holes) is also included at the macroscopic level. Quantum models which include the interband resonance process are called "multiband models", and have largely been formulated and analyzed only in the last five to ten years. Like other models for semiconductor devices, they can essentially be

divided in two classes: Schrödinger-based models and Wigner-function-based (or density-matrix-based) models. The former ones aim at the calculation of the wave function for the system or device under study, and contain no statistics. The latter ones involve electron statistics or transport theory concepts.

Hydrodynamic models have also been formulated and discussed [Gar94]; again, for the most part only single-band hydrodynamics has received attention. Only recently, multiband hydrodynamic models, based on the multiband kinetic models mentioned above, have appeared.

In this review paper, we describe the multiband models that have recently been formulated in both classes. Attention is given to the definitions of the relevant quantities which characterize each model and to the advantages and disadvantages of each model compared to others. The technical details of the derivations of the various models, as well as the rigorous proofs of consistency and existence of the solutions, are diverted directly to the papers where the models have been described.

This paper is organized as follows: in Section 2 we briefly recall the Bloch theory of electrons moving in a periodic potential; Section 3 is devoted to the envelope-function theory; in Section 4 we deal with the multiband models based on the Schrödinger equation; Section 5 contains the statistical kinetic models based on the Wigner-function approach and in Section 6 we give an outline of the hydrodynamic models.

2 The Schrödinger equation and the wave function in a periodic potential

The starting point of any theoretical description of a quantum system is the Schrödinger equation, which we now discuss for a periodic Hamiltonian [RS72, MRS90].

We consider an ensemble of electrons moving in a semiconductor crystal. The electrostatic potential generated by the crystal ions is represented by a periodic potential $V_{\mathcal{L}}(x)$, the periodicity being described as follows:

$$V_{\mathcal{L}}(x+a) = V_{\mathcal{L}}(x), \qquad \forall a \in \mathcal{L},$$

where $\mathcal{L}$ is the periodic lattice of the crystal. The quantum dynamics of a single electron is, therefore, generated by the Hamiltonian

$$H = H_0 + V(x), \tag{1}$$

where $H_0 = p^2/2m + V_{\mathcal{L}}(x)$ is the periodic part of the Hamiltonian, which contains the kinetic energy and the periodic potential. Also, $p = -i\hbar\nabla$ is the momentum operator, m is the electron mass, $\hbar$ is Planck's constant over 2π and $V(x)$ is the potential due to external fields, such as barriers or bias. The periodic Hamiltonian H_0 has a complete system of generalized eigenfunctions

$b_n(x,k)$, called *Bloch waves*, where the "pseudomomentum" or "crystal momentum" variable k runs over the so-called *Brillouin zone*. This is defined as the centered fundamental domain of the reciprocal lattice $\mathcal{L}^*$, i.e.

$$B = \left\{ k \in \mathbb{R}^3 \,\middle|\, k \text{ is closer to 0 than to any other point of } \mathcal{L}^* \right\}.$$

The Bloch waves satisfy the generalized eigenvalue equation

$$H_0 b_n(x,k) = \epsilon_n(k) b_n(x,k), \tag{2}$$

(or $H_0 \,|\, nk\rangle = \epsilon_n(k) \,|\, nk\rangle$ in Dirac's notation), where the generalized eigenfunctions $\epsilon_n(k)$ are the *energy bands* of the crystal. Accordingly, the integer n is called "band-index".

Using Dirac's notation, we choose the following normalization of the Bloch functions:

$$\langle nk \,|\, n'k' \rangle = |B|\, \delta_{nn'}\, \delta(k-k'), \tag{3}$$

so that any wave function Ψ can be decomposed as follows

$$\Psi(x) = \sum_n \int_B \frac{dk}{|B|}\, \sigma_n(k)\, b_n(x,k), \tag{4}$$

where

$$\sigma_n(k) = \int_{\mathbb{R}^3} dx\, \overline{b}_n(x,k)\, \Psi(x). \tag{5}$$

It is well known that the Bloch waves can be written in the form

$$b_n(x,k) = \mathrm{e}^{ik\cdot x} u_n(x,k), \tag{6}$$

where $u_n(x,k)$, called *Bloch functions*, are $\mathcal{L}$-periodic in x and have the property that $\{u_n(\cdot,k) \,|\, n \in \mathbb{N}\}$ is an orthonormal basis of $L^2(C)$ for any fixed $k \in B$, where C denotes the fundamental cell of the direct lattice $\mathcal{L}$. In particular,

$$\int_C \overline{u}_n(x,k)\, u_{n'}(x,k)\, dx = \delta_{nn'}, \qquad k \in B. \tag{7}$$

The electron population of the semiconductor material is partitioned into the energy bands of the Hamiltonian. The highest occupied energy band usually contains only a small electron population and therefore it has many unoccupied states; this is the conduction band. The states of all other (lower energy) bands are instead fully occupied and form the valence bands. In the older devices, based on resonant tunneling, only the electrons of the conduction band contribute to the flow of the current across the device. In some of the devices of the last generation, instead, the resonant tunneling occurs between states belonging to different bands, so that also the carrier population of the valence band contributes to the flow of current. For the description of these last devices, multiband models must be used.

3 Envelope function theory

The wave function of an electron moving under the action of a periodic potential, which we have described in the previous Section, is a fast oscillating object (both in time and space) and is therefore not well suited for numerical computations. A widely used methodology is that of smoothing out these fast oscillations, thus leading to the "envelope function" approach. Envelope functions can be introduced in basically two different ways, one due to Wannier [Wan62] (called the Wannier-Slater envelope functions) and one due to Luttinger and Kohn [LK55] (called the Luttinger-Kohn envelope functions). The Luttinger-Kohn envelope functions are the building blocks of the Kane model, which will be described in the next Section. Here, we introduce the definitions and outline the most important properties of both kinds of envelope functions.

3.1 Wannier-Slater envelope functions

The Wannier-Slater (W-S) envelope functions [Wan62] are defined as follows:

$$f_n(x) = \frac{1}{(2\pi)^{3/2}} \int_B \sigma_n(k)\, \mathrm{e}^{ix\cdot k} dk, \tag{8}$$

where $\sigma_n(k)$ is given by (5). Note that the W-S envelope functions are inverse Fourier transforms to which fast oscillations due to the periodic potential have been removed. In other words, each envelope function f_n has the property that its Fourier transform is supported in the Brillouin zone B. The W-S envelope functions are easily expressed in terms of the wave function by introducing "continuous-index Wannier functions"

$$a_n(x, x') = \frac{1}{(2\pi)^{3/2}} \int_B b_n(x, k)\mathrm{e}^{-ix'\cdot k} dk. \tag{9}$$

Using (5), (8) and (9) we get

$$f_n(x) = \int_{\mathbb{R}^3} \overline{a}_n(x', x)\Psi(x')\, dx', \tag{10}$$

and, conversely,

$$\Psi(x) = \sum_n \frac{1}{|B|} \int_{\mathbb{R}^3} a_n(x, x') f_n(x')\, dx'. \tag{11}$$

To better understand the meaning of the W-S envelope functions, consider the (discrete-index) Wannier functions [Wan62], which are the Fourier components of the Bloch waves with respect to k:

$$a_n(x - \lambda) = \int_B \frac{dk}{|B|}\, b_n(x, k)\mathrm{e}^{-ik\cdot\lambda} = \int_B \frac{dk}{|B|}\, u_n(x, k)\mathrm{e}^{ik\cdot(x-\lambda)}, \tag{12}$$

where λ is a point of the periodic lattice $\mathcal{L}$. The most important property of the Wannier functions is that they are localized at the sites of the lattice, with an exponential decay away from those sites. The Bloch waves, on the contrary, are delocalized and maintain their highly oscillatory behaviour throughout $\mathbb{R}$. The Wannier functions, like the Bloch waves, form a complete, generalized, orthonormal basis and any wave function can be expanded as

$$\Psi(x) = \sum_n \sum_{\lambda \in \mathcal{L}} f_n(\lambda) a_n(x - \lambda),$$

where

$$f_n(\lambda) = \int_B \frac{dk}{|B|}\, \sigma_n(k) \mathrm{e}^{ik\cdot\lambda}.$$

If the length scale of the crystal lattice is small with respect to the macroscopic scale described by the variable x, the Brillouin zone becomes very large and the Fourier coefficients $f_n(\lambda)$ can be replaced by the continuous Fourier transform, yielding definition (8).

The dynamics of the W-S envelope functions can be deduced from (10) and (11), and from the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = H\Psi(x,t),$$

where H is the Hamiltonian operator (1). This yields (see [Bar03b] for the details of the derivation):

$$i\hbar \frac{\partial}{\partial t} f_n(x,t) = \widetilde{\epsilon}_n\left(-i\nabla\right) f_n(x,t) + \sum_{n'} \int_{\mathbb{R}^3} V^{\mathrm{WS}}_{nn'}(x,x') f_{n'}(x',t)\, dx'. \qquad (13)$$

Here,

$$V^{\mathrm{WS}}_{nn'}(x,x') = \frac{1}{|B|} \int_{\mathbb{R}^3} \overline{a}_n(y,x)\, V(y)\, a_n(y,x')\, dy \qquad (14)$$

are matrix-elements of the external potential with respect to the continuous-index Wannier functions and $\widetilde{\epsilon}_n\left(-i\nabla\right)$ are pseudo-differential operators associated to the energy bands with a cut-off outside the Brillouin zone, namely

$$\widetilde{\epsilon}_n\left(-i\nabla\right) f_n(x,t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^6} \mathbb{1}_B(k)\, \epsilon_n(k)\, f_n(x')\, \mathrm{e}^{ik\cdot(x-x')} dx' dk.$$

where $\mathbb{1}_B$ is the characteristic function of the Brillouin zone B.

3.2 Luttinger-Kohn envelope functions

A general definition of envelope functions in the sense of Luttinger and Kohn [Bur92, LK55] may be given as follows. Let $\{v_n(x) \,|\, n \in \mathbb{N}\}$ be $\mathcal{L}$-periodic functions that form an orthonormal basis of $L^2(C)$. Then, the Luttinger-Kohn (L-K) envelope functions of a wave function Ψ, with respect to the basis $v_n(x)$ are functions $F_n(x)$ such that

(i) $\Psi(x) = \sum_n F_n(x)\, v_n(x)$;
(ii) the F_n are slowly varying with respect to the lattice periodicity, namely

$$\operatorname{supp}\big(\hat{F}_n\big) \subset B, \qquad n \in \mathbb{N}\,, \tag{15}$$

where $\hat{F}_n$ denotes the Fourier transform of F_n.

Usually the basis functions v_n are chosen to be the Bloch functions $u_n(x,k)$ evaluated at $k=0$, so that

$$\Psi(x) = \sum_n F_n(x)\, u_n(x,0),$$

but, of course, other choices are possible. It can be proved that the L-K envelope functions are uniquely determined by the two conditions (i) and (ii) and that the Parseval-like equality

$$\|\Psi\|^2 = \frac{1}{|C|} \sum_n \|F_n\|^2 \tag{16}$$

holds. It is not difficult to see that the L-K envelope functions are easily expressed in terms of the wave function as follows:

$$f_n(x) = \int_B \frac{dk}{|B|^{1/2}} \int_{\mathbb{R}^3} dy\, \overline{\mathcal{X}}_n(y,k)\, \mathrm{e}^{ik\cdot x}\, \Psi(y), \tag{17}$$

where

$$\mathcal{X}_n(y,k) = \frac{1}{|B|^{1/2}}\, v_n(y)\, \mathrm{e}^{ik\cdot y}, \quad y \in \mathbb{R}^3,\ k \in B,\ n \in \mathbb{N}. \tag{18}$$

is a (generalized) Luttinger-Kohn basis [LK55]. By using the above relations it is possible to deduce the dynamics of L-K envelope functions. In the case $v_n(x) = u_n(x,0)$ we have [Wen99]

$$i\hbar \frac{\partial}{\partial t} F_n(x,t) = \epsilon_n(0)\, F_n(x,t) - \frac{\hbar^2}{2m}\, \Delta\, F_n(x,t) - \frac{\hbar^2}{m} \sum_{n'} K_{nn'} \cdot \nabla F_{n'}(x,t) + \sum_{n'} \int_{\mathbb{R}^3} V^{\mathrm{LK}}_{mn'}(x,x')\, F_{n'}(x',t)\, dx'. \tag{19}$$

Here, $\epsilon_n(0)$ is the m-th energy band evaluated at $k=0$ and

$$K_{nn'} = \int_C u_n(x,0) \nabla u_{n'}(x,0)\, dx = -K_{n'n} \tag{20}$$

are the matrix elements of the gradient operator between Bloch functions (which, we recall, are real-valued). The matrix-elements of the external potential are given by

$$V^{\mathrm{LK}}_{nn'}(x,x') = \frac{1}{(2\pi)^3} \int_B dk \int_{\mathbb{R}^3} dy \int_B dk' \times \times \left\{ \mathrm{e}^{ik\cdot x}\, \overline{\mathcal{X}}_n(y,k)\, V(y)\, \mathcal{X}_{n'}(y,k')\, \mathrm{e}^{-ik'\cdot x'} \right\}, \tag{21}$$

where, of course, u_n has to be used in definition (18) in place of v_n .

4 Pure-state multiband models

The equations of envelope-function dynamics, eqs. (13) and (19), are still too complicated for modeling purposes and, therefore, they should be considered as starting points for building simpler models rather then models *per se*.

First of all we note that, if the external potential is slowly varying with respect to the lattice period, then the $\mathcal{L}$-periodic function $\overline{u_n}(y,0)\,u_{n'}(y,0)$ in (21) (see definition (18)) can be substituted by its average on a periodic cell. Hence, we can write

$$V^{\mathrm{LK}}_{nn'}(x,x') \approx \frac{1}{|B|\,|C|\,(2\pi)^3}\int_C \overline{u}_n(z)\,u_{n'}(z)\,dz \times \\ \times \int_B dk \int_{\mathbb{R}^3} dy \int_B dk' \left\{ \mathrm{e}^{ik'\cdot x}\mathrm{e}^{-iy\cdot(k-k')}\mathrm{e}^{-ik'\cdot x'}\,V(y)\right\}$$

and so, using (7), $|C|\,|B| = (2\pi)^3$, and $B \approx \mathbb{R}^3$,

$$V^{\mathrm{LK}}_{nn'}(x,x') \approx \delta_{nn'}\delta(x-x')V(x-x'). \tag{22}$$

In other words, if the potential V is smooth enough, the complicated potential term in eq. (19) can be approximated by the simple multiplication by $V(x)$ of each F_n. The same property holds for $V^{\mathrm{WS}}_{nn'}(x,x')$ (see definition (14)) and the proof is similar.

Another typical approximation is the effective-mass dynamics. This can be easily deduced from the Wannier-Slater equations (13) by simply substituting the energy-band function $\epsilon_n(k)$ with its parabolic approximation near a stationary point (that we assume to be always $k=0$ for the sake of simplicity). This, together with the approximation (22) yields a completely decoupled dynamics of the form

$$i\hbar\frac{\partial}{\partial t}\,f_n(x,t) = -\frac{\hbar^2}{2}\,\nabla\cdot\mathbb{M}_n^{-1}\nabla f_n(x,t) + V(x)\,f_n(x,t)$$

where $\mathbb{M}$ is the effective-mass tensor:

$$\mathbb{M}_n^{-1} = \nabla\otimes\nabla\,\epsilon_n(k)\,|_{k=0}.$$

The effective-mass model is widely used in semiconductor modeling and it has been rigorously studied, as an asymptotic dynamics, in Refs. [AP05], [BLP78] and [PR96]. However, if *interband effects* have to be included, then we have to go beyond the effective-mass approximation and to include at least two coupled bands.

4.1 The two-band Kane model

A simple multiband model was introduced by Kane [Kan56] in the early 60's in order to describe the electron transport with two allowed energy bands

separated by a forbidden region. The Kane model is a simple two-band model capable of including one conduction band and one valence band and it is formulated as two coupled Schrödinger-like equations for the conduction-band and valence-band envelope functions [BFZ03]. The coupling term is treated by the $k \cdot P$ perturbation method [Wen99], which gives the solutions of the single electron Schrödinger equation in the neighborhood of the bottom of the conduction band and the top of the valence bands, where the most part of electrons and holes, respectively, are concentrated. The Kane model is very important for the modeling of the RITD devices, and is widely used in literature [SX89, YSDX91].

From our point of view, the Kane model can be viewed as an approximate evolution equation for L-K envelope functions arising from eq. (19) when using the following approximations:

1. the external potential kernel (21) is substituted by the local and diagonal approximation (22);
2. only two bands (conduction and valence) are included;
3. the bottom of conduction band $E_c = \epsilon_c(0)$ and top of valence band $E_v = \epsilon_v(0)$ are viewed as functions of the position x (this allows to model band heterostructures).

Thus, using the indices c for conduction and v for valence, we have a two-term L-K envelope function expansion

$$\Psi(x) = \Psi_c(x)u_c(x) + \Psi_v(x)u_v(x),$$

of the wave function Ψ and the following evolution equations for Ψ_c and Ψ_v:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi_c(x,t) &= (E_c + V)(x)\,\Psi_c(x,t) - \frac{\hbar^2}{2m}\,\Delta\Psi_c(x,t) - \frac{\hbar^2}{m}K\cdot\nabla\Psi_v(x,t), \\ i\hbar\frac{\partial}{\partial t}\Psi_v(x,t) &= (E_v + V)(x)\,\Psi_v(x,t) - \frac{\hbar^2}{2m}\,\Delta\Psi_v(x,t) + \frac{\hbar^2}{m}K\cdot\nabla\Psi_c(x,t), \end{aligned} \tag{23}$$

which is the two-band Kane model. Note that the quantity K, called Kane momentum, is given by

$$K = K_{cv} = -K_{vc} = \int_C u_c(x)\,\nabla u_v(x)\,dx$$

(see (20) and recall that the Bloch functions u_c and u_v are real-valued). A word of caution has to be spent on the notation: Ψ_c and Ψ_v are not really band-projections (spectral projections) of the wave function, not only because of the envelope function approximation but also because the Hamiltonian operator defined by the right-hand side of eq. (23) is *not* diagonal, even in the absence of external potentials. The identification of Ψ_c and Ψ_v with spectral projections is only approximately true for $k \approx 0$.

The Kane model in the Schrödinger-like form (23) has been recently studied by J. Kefi, [Kef03], and in the Wigner-equation form by Borgioli, Frosali and Zweifel [BFZ03].

4.2 The Morandi-Modugno multiband model

In this section we briefly introduce the multiband envelope function model, introduced recently by Modugno and Morandi (M-M); for the complete derivation of the model we refer the reader to [MM05].

The starting point is the W-S envelope function dynamics (13). When the potential V is smooth enough, we can approximate the matrix-elements $V^{\mathrm{WS}}_{nn'}$ in the same way as we deduced eq. (22), obtaining

$$V^{\mathrm{WS}}_{nn'}(x,x') \approx \frac{1}{|B|\,(2\pi)^{3/2}} \int_{\mathbb{R}^3} dk \int_{\mathbb{R}^3} dk' \left\{ \mathrm{e}^{ik\cdot x} B_{nn'}(k,k')\, \hat{V}(k-k')\, \mathrm{e}^{-ik'\cdot x'} \right\} \tag{24}$$

where

$$B_{nn'}(k,k') = \frac{1}{|C|} \int_C \overline{u}_n(z,k)\, u_{n'}(z,k')\, dz. \tag{25}$$

By using the eigenvalue equation (2) one obtains

$$B_{nn'}(k,k') = \frac{1}{|C|} \frac{\hbar}{m} (k-k') \frac{P_{nn'}(k,k')}{\Delta E_{nn'}(k,k')}, \quad \text{for } n \neq n',$$

where

$$P_{nn'}(k,k') = \int_C \overline{u}_n(x,k)(-i\hbar\nabla) u_{n'}(x,k')\, dx \tag{26}$$

and

$$\Delta E_{nn'}(k,k') = \epsilon_n(k) - \epsilon_{n'}(k') - \frac{\hbar^2}{2m}(k^2 - k'^2).$$

Moreover, as can be deduced from eq. (3), the diagonal terms are simply given by

$$B_{nn}(k,k') = \frac{|B|}{(2\pi)^3} = \frac{1}{|C|}. \tag{27}$$

Using (24), (25) and (27) in eq. (13) (and recalling that $B \approx \mathbb{R}^3$) we get

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} f_n(x,t) &= \epsilon_n(-i\nabla)\, f_n(x,t) + V(x)\, f_n(x,t) \\ &+ \frac{\hbar}{m} \sum_{n' \neq n} \int_{\mathbb{R}^3} dk \int_{\mathbb{R}^3} dk' \, \frac{\mathrm{e}^{ik\cdot x}}{(2\pi)^3} \frac{P_{nn'}(k,k')}{\Delta E_{nn'}(k,k')}\, \hat{V}(k-k')\, \hat{f}_{n'}(k',t) \end{aligned}$$

where a diagonal part and a non-diagonal part of the dynamics can be clearly distinguished. Assuming, for the sake of simplicity, that the stationary point of each band is $k = 0$ and that the crystal momentum k remains small during the whole evolution, we can expand the term $P_{nn'}/\Delta E_{nn'}$, which characterizes the interband coupling, to first order in k and k'. After some manipulations by means of standard perturbation techniques, we get the multiband equation

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t} f_n(x,t) &= \epsilon_n\left(-i\nabla\right) f_n(x,t) + V(x)\, f_n(x,t) \\
&- \frac{i\hbar}{m}\nabla V(x)\cdot\sum_{n'\neq n}\frac{P_{nn'}}{\Delta E_{nn'}} f_{n'}(x,t) - \frac{\hbar}{m}\nabla V(x)\cdot\sum_{n'\neq n}\frac{M^*_{nn'}}{\Delta E_{nn'}}\nabla f_{n'}(x,t) \\
&- \frac{\hbar}{m}\sum_{n'\neq n}\frac{M_{nn'}}{\Delta E_{nn'}}\left[\nabla^2 V(x) f_{n'}(x,t) + \nabla V(x)\cdot\nabla f_{n'}(x,t)\right]. \qquad (28)
\end{aligned}
$$

where we put $P_{nn'} \equiv P_{nn'}(0,0)$, $\Delta E_{nn'} \equiv \Delta E_{nn'}(0,0)$ and

$$
M_{nn'} = \frac{\hbar}{m}\sum_{n''\neq n'}\frac{P_{nn''}P_{n''n'}}{E_n - E_{n''}}, \quad M^*_{n'n} = \frac{\hbar}{m}\sum_{n''\neq n'}\frac{P_{nn''}P_{n''n'}}{E_{n'} - E_{n''}}
$$

are effective-mass terms. A simple two-band model can be built using the following assumptions:

1. only two bands (c and v) are included;
2. the energy band operator $\epsilon_n\left(-i\nabla\right)$ is substituted by its parabolic approximation (effective-mass energy band);
3. the interband terms of order greater than 2 in k are neglected (this amounts to neglecting terms proportional to the matrices $M_{nn'}$);
4. the bottom of the conduction band and the top of the valence band are functions of the position x (as in the two-band Kane model).

This yields

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\Phi_c(x,t) &= (E_c + V)(x)\,\Phi_c(x,t) - \frac{\hbar^2}{2}\nabla\cdot\mathbb{M}_c^{-1}\nabla\Phi_c(x,t) \\
&\quad - \frac{i\hbar}{mE_g(x)}\nabla V(x)\cdot P\,\Phi_v(x,t), \\
i\hbar\frac{\partial}{\partial t}\Phi_v(x,t) &= (E_v + V)(x)\,\Phi_v(x,t) - \frac{\hbar^2}{2}\nabla\cdot\mathbb{M}_v^{-1}\nabla\Phi_v(x,t) \\
&\quad - \frac{i\hbar}{mE_g(x)}\nabla V(x)\cdot P\,\Phi_c(x,t),
\end{aligned} \qquad (29)
$$

where $E_g(x) = E_c(x) - E_v(x)$ is the band-gap. Contrarily to the Kane model (23), in the the M-M model (29) the envelope functions Φ_c and Φ_v are true band-functions, to the extent that in the absence of external potentials ($V = 0$) the dynamics is diagonal.

5 Statistical multiband models: density matrix and Wigner function

We now turn our attention to the multiband models that make use of statistical concepts, mainly of the Wigner-function approach [Wig32, MRS90,

BJ99, JBBB01, Bar03a]. A multiband model involving the density matrix was already introduced by Krieger and Iafrate [KI87, IK86] by taking matrix elements of the density operator between Bloch states. Subsequently, a number of multiband models based on Wigner-function approach were developed. In [Bar03b, Bar04a, BD02] envelope functions were used to construct the multiband Wigner function; in [BFZ03] a Wigner version of the Kane model was introduced; in [DBBBJ02, DBBJ02, DBJ03a, DBJ03b] the multiband Wigner function was obtained by using the Bloch-state representation of the density matrix.

We recall that statistical states in quantum mechanics are described either in terms of the density operator ρ or the Wigner function $f(x,p)$, [Fey72]. The density operator is usually defined by a statistical mixture of states, say $\{\Psi_j \,|\, j \in \mathbb{N}\}$, where $\Psi_j(x)$ are the wave functions that characterize each state of the mixture. If $\lambda_j \geq 0$ is the probability distribution of the states, then $\sum_j \lambda_j = 1$ and the density operator is given by

$$\rho = \sum_j \lambda_j \,|\, \Psi_j \rangle\langle \Psi_j \,| \tag{30}$$

in Dirac's notation, and the density matrix in the space representation is given by

$$\rho(x,x') = \sum_j \lambda_j \, \Psi_j(x)\overline{\Psi}_j(x') = \sum_j \lambda_j \, \langle x \,|\, \Psi_j\rangle\langle \Psi_j \,|\, x'\rangle. \tag{31}$$

The Wigner function $f(x,p)$ is defined by the Wigner-Weyl transform of the density operator, that is

$$f(x,p) = \int \frac{d\eta}{(2\pi\hbar)^3} \, \rho\left(x + \frac{\eta}{2}, x - \frac{\eta}{2}\right) \mathrm{e}^{-ip\eta/\hbar}. \tag{32}$$

In the theoretical models based on the solution of the Schrödinger equation (pure states), the calculation of the current across the device, $j(x)$, follows the standard quantum-mechanical definition

$$J(x) = -\frac{\hbar}{m} \, \mathrm{Im} \, \left(\Psi(x)\nabla\overline{\Psi}(x)\right). \tag{33}$$

In the statistical models, instead, the current is expressed in terms of the density matrix or in terms of the Wigner function. In the first case the current is

$$J(x) = -\frac{i\hbar}{2m} \left(\nabla_x - \nabla_{x'}\right) \rho(x,x')|_{x=x'}, \tag{34}$$

and, in the Wigner picture, by

$$J(x) = \frac{1}{m} \int p f(x,p) \, dp, \tag{35}$$

an expression which is, remarkably, identical to the classical expression for the current in statistical systems. It can be easily shown that, in the case of pure states, these two expressions coincide with (33).

5.1 Wigner-function based statistical models

A suitable partition of the Wigner function among the energy bands can be obtained by using the completeness of the Bloch states in equation (32). We adopt hereafter Dirac's notation and consider, for the sake of simplicity, the one-dimensional case only. By defining the coefficients Φ_{mn} and the integral kernel W_{mn},

$$\Phi_{mn}(k,k',x,p) = \int\int \frac{d\eta}{2\pi\hbar} \left\langle x+\frac{\eta}{2} \,\middle|\, nk \right\rangle \left\langle nk' \,\middle|\, x-\frac{\eta}{2} \right\rangle \mathrm{e}^{-ip\eta/\hbar} \quad (36)$$

$$W_{mn}(x,p,x',p') = \int_{B^2} dkdk' \Phi_{mn}(k,k',x,p)\Phi^*_{mn}(k,k',x',p'), \quad (37)$$

the Wigner function can be written as a sum of projections over the Floquet subspaces of the energy bands (see [DBBJ02] for details):

$$f(x,p) = \sum_{mn} f_{mn}(x,p), \quad (38)$$

where

$$f_{mn}(x,p) = \int_{B^2} dkdk' \rho_{mn}(k,k')\Phi_{mn}(k,k',x,p). \quad (39)$$

By expressing ρ as a function of f, we can write $f_{mn} = \mathcal{P}_{mn} f$, where $\mathcal{P}_{mn}$ is the linear integral operator

$$\left(\mathcal{P}_{mn} f\right)(x,p) \equiv \frac{1}{2\pi\hbar} \int\int dx'dp' W_{mn}(x,p,x',p') f\left(x',p'\right) .$$

Here, $\rho_{mn}(k,k') = \langle mk \,|\, \rho \,|\, nk' \rangle$ are the matrix elements of the density operator in the Bloch-state representation and the linear integral operator $\mathcal{P}_{mn}$ is a projection operator and yields the Wigner projections f_{mn} from the total Wigner function f.

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

$$i\hbar \frac{\partial f}{\partial t}(x,p,t) = \sum_{mn} i\hbar \frac{\partial f_{mn}}{\partial t}(x,p,t),$$

given by [DBBJ02]

$$i\hbar \frac{\partial f_{mn}}{\partial t} = \sum_{\mu\in\mathcal{L}} \left[\widehat{\epsilon}_m(\mu) f_{mn}(x+\frac{\mu}{2},p,t) - \widehat{\epsilon}_n(\mu) f_{mn}(x-\frac{\mu}{2},p,t)\right] \mathrm{e}^{ip\mu/\hbar} + \int\int dx'd\eta \widehat{W}_{mn}(x,p,x',-\eta)\delta V(x',\eta)\widehat{f}(x',\eta,t), \quad (40)$$

where $\widehat{W}_{mn}$ is the Fourier transform of W_{mn} with respect to the momentum variable:

$$\widehat{W}_{mn}(x,p,x',\eta) = \frac{1}{2\pi\hbar}\int dp' W_{mn}(x,p,x',p')\mathrm{e}^{ip'\eta/\hbar}. \tag{41}$$

Equation (40) is the equation that governs the time evolution of the Floquet projections f_{mn} of the Wigner function for an ensemble of electrons moving in a semiconductor crystal in the presence of external fields and allowing for energy bands of arbitrary shape. The first term, containing the sum over the lattice vectors, refers to the action of the periodic potential of the crystal lattice, while the last term, written in the form of an integral operator, refers to the action of the external or self-consistent fields acting on the electrons. The first term, as shown in [DBBJ02], reduces to the usual free-streaming operator in the case of a single parabolic band; for this reason we shall refer to this term as to the streaming term, while the second term will be called the force term, in analogy with the corresponding force term of the Boltzmann equation. These equations show that, in the absence of external fields, different bands remain dynamically uncoupled and each contribution to the Wigner function evolves independently. In the case $V(x) \equiv 0$, these equations were already written by Markowich, Mauser and Poupaud [MRS90, MMP94] for a single band. It can be shown that, in the case of a single parabolic band, eq. (40) reduces to the usual Wigner equation in the effective mass approximation

$$\frac{\partial f}{\partial t} + \frac{p}{m^*}\frac{\partial f}{\partial x} + \frac{i}{\hbar}\Theta[\delta V]f = 0,$$

where m^* is the (one-dimensional) electron effective mass in the selected band and

$$\left(\Theta[\delta V]f\right)(x,p) = \frac{1}{2\pi\hbar}\int_{\mathbb{R}^2} \mathrm{e}^{-i(p-p')\xi/\hbar}\,\delta V(x,\xi)\,f(x,p')\,d\xi\,dp' \tag{42}$$

is a pseudo-differential operator with symbol

$$\delta V(x,\xi) = V\left(x+\frac{\xi}{2}\right) - V\left(x-\frac{\xi}{2}\right). \tag{43}$$

A multiband model for electron transport in semiconductors, based on the density-matrix approach, was introduced by Krieger and Iafrate in [KI87, IK86]. They considered a statistical ensemble of electrons moving under the action of an external time-dependent electric field. Here, we briefly summarize this model in a simplified form. Their model is obtained by expanding the density matrix elements in Bloch functions:

$$\rho(y,z) = \sum_{mn}\int_{B^2} dk dk' \rho_{mn}(k,k') b_m(k,y)\bar{b}_n(k',z), \tag{44}$$

where $\rho_{mn}(k,k') = \langle mk\,|\,\rho\,|\,nk'\rangle$ are the already-introduced matrix elements between Bloch functions, whose evolution is given by

$$i\hbar\frac{\partial\rho_{mn}(k,k')}{\partial t} = \left[\epsilon_m(k) - \epsilon_n(k')\right]\rho_{mn}(k,k') + \sum_l \int_B dk''\left[V_{ml}(k,k'')\rho_{ln}(k'',k') - V_{ln}(k'',k')\rho_{ml}(k,k'')\right]. \quad (45)$$

Here, $V_{mn}(k,k') = \langle mk \,|\, V \,|\, nk'\rangle$ are the matrix elements of the external potential in the Bloch representation. The main source of difficulty with this approach lies exactly in these matrix elements, which are ill-defined for most potentials of practical interest.

The Wigner-function formalism has also been used by Buot and Jensen [Buo74, Buo76, Buo86, BJ90] to formulate multiband models within the framework of the Lattice-Weyl transform, in which a non-canonical definition of the Wigner function, based on a discrete Fourier Transform, was introduced. This definition of the Wigner function makes use of the Wannier functions introduced by (12). Let $\{\,|\,m\lambda\rangle, m \in \mathbb{N},\ \lambda \in \mathcal{L}\}$ be the states corresponding to the Wannier functions (see eq. (12)); here, $\mathcal{L}$ is the direct lattice and the vectors λ are elements of the direct lattice. We can consider matrix elements of the density operator ρ in the Wannier representation,

$$\rho_{mn}(\lambda,\mu) = \langle m\lambda \,|\, \rho \,|\, n\mu\rangle$$

with $\lambda, \mu \in \mathcal{L}$. A Wigner function is then introduced by

$$f_{mn}(k,\lambda) = \mathcal{N}\sum_{v\in\mathcal{L}} \rho_{mn}(\lambda+v, \lambda-v)\mathrm{e}^{2ikv}, \quad (46)$$

where $\mathcal{N}$ is a normalization factor, $\lambda \in \mathcal{L}$ is a lattice vector and $k \in B$. This definition of the Wigner function is sometimes called discrete Wigner-Weyl transform, and has a similar structure of the definition given in (32); there are however some important differences: the Wigner function is only defined on the lattice points; it is defined by a Fourier series, rather that the Fourier transform; it is a function of the crystal momentum, which has not been integrated over. According to (35), the current density is then given by

$$J(\lambda) = \sum_{mn}\int_B \frac{dk}{|B|}\,\frac{p}{m} f_{mn}(k,\lambda), \qquad (p = \hbar k)$$

and is also defined on the lattice points.

5.2 Reduced Wigner-Bloch-Floquet models

Equations (40) are the most general time evolution equations that can be written for the Floquet projections of the multiband Wigner function in presence of external fields and in absence of collisions. The action of the periodic potential is described by the first term, which contains the Fourier coefficients of the energy bands, and which reduces to the usual free-streaming operator

in the parabolic-band approximation. The second term describes the action of the external potential. We note that, while the first term requires only the knowledge of the energy band functions, the second term requires the knowledge of the Bloch eigenfunctions of the material of interest. Therefore, the model equations (40) are very hard to solve in full generality in practical applications, and the derivation of a set of simplified models is needed. In the following subsections, we outline some of the reduced models which have been derived within the Bloch-Floquet approach.

Two-band model in the parabolic band approximation without external fields

It is interesting to consider a simple two-band model in the parabolic band approximation and without external fields, in order to study the off-diagonal Floquet projections of the Wigner function, which arise in this case. In a two-band model, the Wigner function and its evolution equation are given by equations (38) and (40) without external fields, and with $m = 0, 1$ and $n = 0, 1$. The Wigner function is given by the sum of four contributions, f_{00}, f_{01}, f_{10} and f_{11}. It can be seen easily from equations (36), (39) and (37) that $f_{01} = \overline{f}_{10}$, while f_{00} and f_{11} are real. Each of the four contributions evolves according to equations (40). In the parabolic band approximation, the differential equations for f_{00} and f_{11} are:

$$\begin{aligned} \frac{\partial f_{00}}{\partial t} + \frac{p - \hbar k_0}{m_0} \frac{\partial f_{00}}{\partial x} &= 0 \\ \frac{\partial f_{11}}{\partial t} + \frac{p - \hbar k_1}{m_1} \frac{\partial f_{11}}{\partial x} &= 0, \end{aligned} \tag{47}$$

where m_0 and m_1 are the effective masses for band 0 and band 1 respectively and k_0 and k_1 are the values of the crystal momentum at which band 0 and band 1 attain their minimum. The evolution equations for f_{01} and $f_{10} = \overline{f}_{01}$ have instead a different structure. A simple calculation shows that:

$$\begin{aligned} i\hbar \frac{\partial f_{01}}{\partial t} = &\left\{ \left[\epsilon_0(k_0) + \frac{(p - \hbar k_0)^2}{2m_0} \right] - \left[\epsilon_1(k_1) + \frac{(p - \hbar k_1)^2}{2m_1} \right] \right\} f_{01}(x, p) + \\ &- \frac{i\hbar}{2} \left(\frac{p - \hbar k_0}{m_0} + \frac{p - \hbar k_1}{m_1} \right) \frac{\partial f_{01}}{\partial x} - \frac{1}{8} \left(\frac{\hbar^2}{m_0} - \frac{\hbar^2}{m_1} \right) \frac{\partial^2 f_{01}}{\partial x^2}. \end{aligned} \tag{48}$$

which follows from equation (40) after expanding $f_{mn}(x \pm \eta/2, p, t)$ in Taylor series about $\mu = 0$ and using parabolic profiles for the two bands. By introducing the frequencies

$$\begin{aligned} &\omega_{01} = (\epsilon_0(k_0) - \epsilon_1(k_1))/\hbar \\ &\Omega_{01}(p) = \omega_{01} + (p - \hbar k_0)^2/(2m_0\hbar) - (p - \hbar k_1)^2/(2m_1\hbar) \end{aligned}$$

and the new function

$$g_{01}(x,p,t) = f_{01}(x,p,t)\mathrm{e}^{i\Omega_{01}(p)t},$$

equation (48) can be cast in the more elegant form

$$\frac{\partial g_{01}}{\partial t} + \frac{1}{2}\left(\frac{p-\hbar k_0}{m_0} + \frac{p-\hbar k_1}{m_1}\right)\frac{\partial g_{01}}{\partial x} - \frac{i\hbar}{8}\left(\frac{1}{m_0} - \frac{1}{m_1}\right)\frac{\partial^2 g_{01}}{\partial x^2} = 0. \quad (49)$$

Note that in the definition of the Wigner function (38) f_{01} and f_{10} appear only in the combination $f_{01}+f_{10}$, consistently with the Wigner function being real. Equation (48) shows that the time evolution of f_{01} is given by three contributions: an oscillatory term, a free streaming term and a diffusive term with imaginary diffusion coefficient (Schrödinger-like term). The frequency of the oscillatory term, Ω_{01}, is proportional to the difference of the total energies of the particles of the two bands; the velocity of the free streaming term is an average of the relative velocities of the particle with respect to the two minima and the imaginary diffusion coefficient vanishes when the two effective masses are equal.

Equations (47) and (49) completely describe the time evolution of all the components of the Wigner function in a two-band model with the parabolic-band approximation and in the absence of external fields. Note that these evolution equations are uncoupled.

Multiband model in the Luttinger-Kohn approximation

As we have already seen in Section 3.2, the Luttinger-Kohn model [LK55] considers the carrier populations near minima (or maxima) of the energy bands and it is therefore to be used in conjunction with the parabolic-band approximation. For the Bloch states near the minimum (or maximum) of the band, the Bloch functions $u_n(x,k)$ are replaced with the set of functions $u_n(x,k_n)$, i.e. the Bloch functions at the bottom (or top) of the band, here assumed at $k = k_n$. The functions $\mathrm{e}^{ikx}u_n(x,k_n)$, after a suitable normalization, also form a complete set (see Ref. [LK55] and see also Section 3.2) and any wave function can be expanded in their basis. In this Section, we use the Luttinger-Kohn basis for expressing the Floquet projections f_{mn} of the Wigner function and for writing the evolution equations. The action of the free Hamiltonian is treated in the parabolic-band approximation.

If the $n-$th band has an extremum at $k = k_n$, we can approximate the Bloch waves as

$$\langle x \,|\, nk\rangle = b_n(x,k) \approx u_n(x,k_n)\,\mathrm{e}^{ikx}. \quad (50)$$

Since the functions $u_n(x,k_n)$ are periodic functions with period a, we can introduce their Fourier expansion,

$$u_n(x,k_n) = \sum_{n'=-\infty}^{\infty} \widehat{U}^n_{n'}\mathrm{e}^{iK_{n'}x},$$

where, $K_n = 2\pi n/a$ are vectors of the reciprocal lattice with $K_{-n} = -K_n$. After evaluating the coefficients Φ_{mn} and the integral kernel W_{mn} in this basis, and after carrying out the integration over the momentum variables k and k', one obtains for the Floquet projection f_{mn} of the Wigner function:

$$\begin{aligned} f_{mn}(x,p) = 4\pi \sum_{m'n'm''n''} & \widehat{U}^m_{m'} \widehat{U}^{n*}_{n'} \widehat{U}^{m*}_{m''} \widehat{U}^n_{n''} \mathrm{e}^{i(K_{m'}-K_{n'})x} \\ & \times \mathcal{H}\left(\frac{\pi}{a} - \left|\frac{p}{\hbar} - \frac{K_{m'}+K_{n'}}{2}\right|\right) \\ & \times \int dx' \frac{\sin 2[\pi/a - |p/\hbar - (K_{m'}+K_{n'})/2|](x-x')}{x-x'} \\ & \times f\left(x', p - \hbar\frac{K_{m'}+K_{n'}-K_{m''}-K_{n''}}{2}\right) \mathrm{e}^{-i(K_{m''}-K_{n''})x'}, \end{aligned}$$

where the integrals are performed over the whole real line and $\mathcal{H}$ is the Heaviside function. The evolution equations have been formulated for the case of two energy bands in the parabolic band approximation. If m_0 and m_1 are the effective masses for band 0 and band 1 respectively and k_0 and k_1 are the values of the crystal momentum at which band 0 and band 1 attain their minimum, we have that

$$\frac{\partial f_{00}}{\partial t} + \frac{p-\hbar k_0}{m_0}\frac{\partial f_{00}}{\partial x} + \frac{i}{\hbar}(\overline{\Theta}_{00} f)(x,p) = 0 \tag{51}$$

$$\frac{\partial f_{11}}{\partial t} + \frac{p-\hbar k_1}{m_1}\frac{\partial f_{11}}{\partial x} + \frac{i}{\hbar}(\overline{\Theta}_{11} f)(x,p) = 0, \tag{52}$$

$$\begin{aligned} i\hbar\frac{\partial f_{01}}{\partial t} = & \left\{\left[\epsilon_0(k_0) + \frac{(p-\hbar k_0)^2}{2m_0}\right] - \left[\epsilon_1(k_1) + \frac{(p-\hbar k_1)^2}{2m_1}\right]\right\} f_{01}(x,p) \\ & - \frac{i\hbar}{2}\left[\frac{p-\hbar k_0}{m_0} + \frac{p-\hbar k_1}{m_1}\right]\frac{\partial f_{01}}{\partial x} - \frac{1}{8}\left(\frac{\hbar^2}{m_0} - \frac{\hbar^2}{m_1}\right)\frac{\partial^2 f_{01}}{\partial x^2} \\ & + (\overline{\Theta}_{01} f)(x,p), \end{aligned} \tag{53}$$

where $\overline{\Theta}_{mn}$ is an operator acting on the whole Wigner function f and, recalling definition (42), is given by

$$\begin{aligned} (\overline{\Theta}_{mn} f)(x,p,t) &= \int\int dx' d\eta \widehat{W}_{mn}(x,p,x',-\eta)\delta V(x',\eta)\widehat{f}(x',\eta,t) \\ &= 4\pi \sum_{m'n'm''n''} \widehat{U}^m_{m'} \widehat{U}^{n*}_{n'} \widehat{U}^{m*}_{m''} \widehat{U}^n_{n''} \mathrm{e}^{i(K_{m'}-K_{n'})x} \mathcal{H}\left(\frac{\pi}{a} - \left|\frac{p}{\hbar} - \frac{K_{m'}+K_{n'}}{2}\right|\right) \\ &\times \int dx' \mathrm{e}^{-i(K_{m''}-K_{n''})x'} \frac{\sin 2[\pi/a - |p/\hbar - (K_{m'}+K_{n'})/2|](x-x')}{x-x'} \\ &\times \int d\eta \delta V(x',\eta) \mathrm{e}^{-i(p-(K_{m'}+K_{n'}-K_{m''}-K_{n''})/2)\eta/\hbar} \widehat{f}(x',\eta,t). \end{aligned} \tag{54}$$

A two-band model with empty-lattice eigenfunctions

A different simplification of the transport equations can be obtained by using the Bloch functions of the "empty lattice", that is periodic plane waves. Here, we consider only the two lowest energy bands, given by

$$\epsilon_0(k) = \frac{\hbar^2 k^2}{2m} \tag{55}$$

$$\epsilon_1(k) = \frac{\hbar^2}{2m}[\mathcal{H}(k)(k-K)^2 + \mathcal{H}(-k)(k+K)^2], \tag{56}$$

with $K = 2\pi/a$ and m the bare electron mass, and whose eigenfunctions are

$$\Psi_{0k}(x) = \langle x \,|\, 0k\rangle = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{ikx} \tag{57}$$

$$\Psi_{1k}(x) = \langle x \,|\, 1k\rangle = \frac{1}{\sqrt{2\pi}}(\mathcal{H}(k)\mathrm{e}^{-iKx} + \mathcal{H}(-k)\mathrm{e}^{iKx})\mathrm{e}^{ikx}. \tag{58}$$

By using this basis in the definition (39) of the multiband Wigner function, one obtains for the band projections f_{mn} (see [DBJ03b] for the details):

$$f_{00}(x,p) = \frac{1}{\pi}\mathcal{H}\left(\frac{K}{2} - \left|\frac{p}{\hbar}\right|\right)\int \frac{\sin 2(K/2 - |p/\hbar|)(x-x')}{x-x'} f(x',p)dx' \tag{59}$$

$$\begin{aligned} f_{01}(x,p) = \frac{1}{\pi}\int \Bigg[& \widetilde{\mathcal{H}}\left(-\frac{3\hbar K}{4}, p, 0\right)\mathrm{e}^{i(\alpha_1+\alpha_2+K)(x-x')}\frac{\sin(\alpha_2-\alpha_1)(x-x')}{x-x'} \\ & + \widetilde{\mathcal{H}}\left(0, p, \frac{3\hbar K}{4}\right)\mathrm{e}^{i(\alpha_3+\alpha_4-K)(x-x')}\frac{\sin(\alpha_4-\alpha_3)(x-x')}{x-x'}\Bigg] \\ & \times f(x',p)dx' \end{aligned} \tag{60}$$

$$\begin{aligned} f_{11}(x,p) = \frac{1}{\pi}\int \Bigg[& \widetilde{\mathcal{H}}\left(-\hbar K, p, -\frac{\hbar K}{2}\right)\frac{\sin 2(K/4 - |p/\hbar + 3K/4|)(x-x')}{x-x'} \\ & + \widetilde{\mathcal{H}}\left(\frac{\hbar K}{2}, p, \hbar K\right)\frac{\sin 2(K/4 - |p/\hbar - 3K/4|)(x-x')}{x-x'} \\ & + 2\mathcal{H}\left(\frac{K}{4} - \left|\frac{p}{\hbar}\right|\right)\frac{\sin 2(K/4 - |p/\hbar|)(x-x')}{x-x'}\cos\frac{3}{2}K(x-x')\Bigg] \\ & \times f(x',p)dx'. \end{aligned} \tag{61}$$

where the function $\widetilde{\mathcal{H}}(a,x,b) \equiv \mathcal{H}(x-a)\mathcal{H}(b-x)$ has been introduced, and

$$\alpha_1(p) = -\frac{K}{2} + \left|\frac{p}{\hbar} + \frac{K}{2}\right| \qquad \alpha_2(p) = \frac{K}{4} - \left|\frac{p}{\hbar} + \frac{K}{4}\right|$$

$$\alpha_3(p) = -\frac{K}{4} + \left|\frac{p}{\hbar} - \frac{K}{4}\right| \qquad \alpha_4(p) = \frac{K}{2} - \left|\frac{p}{\hbar} - \frac{K}{2}\right|.$$

The time evolution of the Floquet projections of the Wigner function is given by:

$$\frac{\partial f_{00}}{\partial t} + \frac{p}{m}\frac{\partial f_{00}}{\partial x} + \frac{i}{\hbar}(\overline{\Theta}_{00} f)(x,p) = 0$$
$$\frac{\partial f_{11}}{\partial t} + \frac{p}{m}\frac{\partial f_{11}}{\partial x} + \frac{i}{\hbar}(\overline{\Theta}_{11} f)(x,p) = 0,$$
$$\frac{\partial f_{01}}{\partial t} + \frac{p}{m}\frac{\partial f_{01}}{\partial x} + \frac{i}{\hbar}(\overline{\Theta}_{01} f)(x,p) = 0,$$

where $\overline{\Theta}$ is an operator acting on the total Wigner function f and is given by

$$(\overline{\Theta}_{00} f)(x,p) = \frac{1}{\pi}\mathcal{H}\left(\frac{\pi}{a} - \left|\frac{p}{\hbar}\right|\right)\int \frac{\sin 2(\pi/a - |p/\hbar|)(x-x')}{x-x'} \times \int \delta V(x',\eta)\widehat{f}(x',\eta,t)\mathrm{e}^{-ip\eta/\hbar}\,d\eta\,dx'$$

$$(\overline{\Theta}_{01} f)(x,p) = \frac{1}{\pi}\int \left[\widetilde{\mathcal{H}}\left(-\frac{3\hbar K}{4}, p, 0\right)\mathrm{e}^{i(\alpha_1+\alpha_2+K)(x-x')}\frac{\sin(\alpha_2-\alpha_1)(x-x')}{x-x'} + \widetilde{\mathcal{H}}\left(0, p, \frac{3\hbar K}{4}\right)\mathrm{e}^{i(\alpha_3+\alpha_4-K)(x-x')}\frac{\sin(\alpha_4-\alpha_3)(x-x')}{x-x'}\right] \times \int \delta V(x',\eta)\widehat{f}(x',\eta,t)\mathrm{e}^{-ip\eta/\hbar}\,d\eta\,dx'$$

$$(\overline{\Theta}_{11} f)(x,p) = \frac{1}{\pi}\int \left[\widetilde{\mathcal{H}}\left(-\hbar K, p, -\frac{\hbar K}{2}\right)\frac{\sin 2(K/4 - |p/\hbar + 3K/4|)(x-x')}{x-x'} + \widetilde{\mathcal{H}}\left(\frac{\hbar K}{2}, p, \hbar K\right)\frac{\sin 2(K/4 - |p/\hbar - 3K/4|)(x-x')}{x-x'} + 2\mathcal{H}\left(\frac{K}{4} - \left|\frac{p}{\hbar}\right|\right)\frac{\sin 2(K/4 - |p/\hbar|)(x-x')}{x-x'}\cos\frac{3}{2}K(x-x')\right] \times \int \delta V(x',\eta)\widehat{f}(x',\eta,t)\mathrm{e}^{-ip\eta/\hbar}\,d\eta\,dx'$$

Equations (59)-(61) show that the Floquet projections of the Wigner function given by this model are functions with compact support and cover different portions of the phase space. The support of the projection f_{00} on the lower band, for example, corresponds to the first Brillouin zone; the supports of the other projections are larger and extend beyond the first Brillouin zone. The equations of this two-band model are very hard to approach numerically, because of the presence of convolution integrals of highly oscillatory functions.

5.3 Envelope-function based statistical models

An alternative approach to statistical models based on the Wigner picture starts from an envelope-function model, such as the Kane model (23) or the

M-M model (29) and then applying the Wigner transformation (32) directly to the envelope functions (Ψ_c and Ψ_v in the former case, Φ_c and Φ_v in the latter).

For a two-band model we need a 2×2 matrix of Wigner functions (Wigner matrix), defined as the component-wise Wigner transform:

$$w_{ij}(x,p) = (\mathcal{W}\,\rho_{ij})\,(x,p), \qquad i,j \in \{c,v\},$$

where $\mathcal{W}$ denotes the Wigner transformation (32) and ρ_{ij} is an envelope-function density matrix (i.e., in the pure-state case, it is given by $\rho_{ij}(x,x') = \Psi_i(x)\,\overline{\Psi}_j(x')$ for the Kane model and by $\rho_{ij}(x,x') = \Phi_i(x)\,\overline{\Phi}_j(x')$ for the M-M model). The self-adjointness of the density operator implies the Hermiticity of the Wigner matrix for any fixed (x,p):

$$\rho_{ij}(x,x') = \overline{\rho_{ji}(x',x)} \implies w_{ij}(x,p) = \overline{w_{ji}(x,p)}.$$

The evolution equation for the Wigner matrix in the case of the Kane model (23) is

$$\begin{aligned}
\left(\frac{\partial}{\partial t} + \frac{p}{m}\cdot\nabla_x + \frac{i}{\hbar}\Theta[V_{cc}]\right) w_{cc} &= -\frac{i\hbar K}{2m}\cdot\nabla_x(w_{cv}-w_{vc}) - \frac{K\cdot p}{m}(w_{cv}+w_{vc}) \\
\left(\frac{\partial}{\partial t} + \frac{p}{m}\cdot\nabla_x + \frac{i}{\hbar}\Theta[V_{cv}]\right) w_{cv} &= \frac{i\hbar K}{2m}\cdot\nabla_x(w_{cc}+w_{vv}) + \frac{K\cdot p}{m}\,(w_{cc}-w_{vv}) \\
\left(\frac{\partial}{\partial t} + \frac{p}{m}\cdot\nabla_x + \frac{i}{\hbar}\Theta[V_{vc}]\right) w_{vc} &= -\frac{i\hbar K}{2m}\cdot\nabla_x(w_{cc}+w_{vv}) + \frac{K\cdot p}{m}\,(w_{cc}-w_{vv}) \\
\left(\frac{\partial}{\partial t} + \frac{p}{m}\cdot\nabla_x + \frac{i}{\hbar}\Theta[V_{vv}]\right) w_{vv} &= -\frac{i\hbar K}{2m}\cdot\nabla_x(w_{cv}-w_{vc}) + \frac{K\cdot p}{m}\,(w_{cv}+w_{vc})
\end{aligned} \tag{62}$$

where we put

$$V_{ij}(x,\xi) = (E_i+V)\left(x+\frac{\xi}{2}\right) - (E_j+V)\left(x-\frac{\xi}{2}\right), \quad i,j\in\{c,v\}, \tag{63}$$

and the pseudo-differential operator, in the present three-dimensional case, is given by

$$(\Theta[\phi]f)\,(x,p) = \frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^6} \mathrm{e}^{-i(p-p')\cdot\xi/\hbar}\,\phi(x,\xi)\,f(x,p')\,d\xi\,dp'. \tag{64}$$

The system (62) has been studied from a mathematical point of view in [BFZ03]. The Wigner matrix describing thermal equilibrium of the Kane model has been analyzed in Ref. [Bar04a].

The evolution equation for the Wigner matrix in the case of the M-M model (4.2) is

$$
\begin{aligned}
&\left(\frac{\partial}{\partial t} + p\cdot \mathbb{M}_c^{-1}\nabla_x + \frac{i}{\hbar}\Theta[V_{cc}]\right) w_{cc} = \Theta[F_-]w_{cv} - \Theta[F_+]w_{vc}\\
&\left(\frac{\partial}{\partial t} + p\cdot \frac{\mathbb{M}_c^{-1}+\mathbb{M}_v^{-1}}{2}\nabla_x - \frac{i\hbar}{4}\nabla_x\cdot\frac{\mathbb{M}_c^{-1}-\mathbb{M}_v^{-1}}{2}\nabla_x + \frac{ip}{\hbar}\cdot\frac{\mathbb{M}_c^{-1}-\mathbb{M}_v^{-1}}{2}p\right) w_{cv}\\
&\qquad = -\frac{i}{\hbar}\Theta[V_{cv}]w_{cv} + \Theta[F_-]w_{cc} - \Theta[F_+]w_{vv}\\
&\left(\frac{\partial}{\partial t} + p\cdot \frac{\mathbb{M}_c^{-1}+\mathbb{M}_v^{-1}}{2}\nabla_x + \frac{i\hbar}{4}\nabla_x\cdot\frac{\mathbb{M}_c^{-1}-\mathbb{M}_v^{-1}}{2}\nabla_x - \frac{ip}{\hbar}\cdot\frac{\mathbb{M}_c^{-1}-\mathbb{M}_v^{-1}}{2}p\right) w_{vc}\\
&\qquad = -\frac{i}{\hbar}\Theta[V_{vc}]w_{vc} - \Theta[F_+]w_{cc} + \Theta[F_-]w_{vv}\\
&\left(\frac{\partial}{\partial t} + p\cdot \mathbb{M}_v^{-1}\nabla_x + \frac{i}{\hbar}\Theta[V_{vv}]\right) w_{vv} = -\Theta[F_+]w_{cv} + \Theta[F_-]w_{vc}
\end{aligned}
\tag{65}
$$

where we put

$$
F_\pm(x,\xi) = \frac{\nabla V\cdot P}{mE_g}\left(x \pm \frac{\xi}{2}\right),
$$

and the symbols V_{ij} are still given by (63). From eq. (26) we see that that P and, consequently, $F_\pm$ are purely imaginary, so that the following relations hold:

$$
\overline{\Theta[F_\pm]w_{ij}} = -\Theta[F_\mp]w_{ji}, \qquad i,j\in\{c,v\}.
$$

In the special case of constant and opposite effective-masses,

$$
\mathbb{M}_c = m^* I, \qquad \mathbb{M}_v = -m^* I,
$$

the above system reduces to

$$
\begin{aligned}
&\left(\frac{\partial}{\partial t} + \frac{p}{m^*}\cdot\nabla_x + \frac{i}{\hbar}\Theta[V_{cc}]\right) w_{cc} = \Theta[F_-]w_{cv} - \Theta[F_+]w_{vc}\\
&\left(\frac{\partial}{\partial t} - \frac{i\hbar}{4m^*}\nabla_x^2 + \frac{ip^2}{\hbar m^*} + \frac{i}{\hbar}\Theta[V_{cv}]\right) w_{cv} = \Theta[F_-]w_{cc} - \Theta[F_+]w_{vv}\\
&\left(\frac{\partial}{\partial t} + \frac{i\hbar}{4m^*}\nabla_x^2 - \frac{ip^2}{\hbar m^*} + \frac{i}{\hbar}\Theta[V_{vc}]\right) w_{vc} = -\Theta[F_+]w_{cc} + \Theta[F_-]w_{vv}\\
&\left(\frac{\partial}{\partial t} - \frac{p}{m^*}\cdot\nabla_x + \frac{i}{\hbar}\Theta[V_{vv}]\right) w_{vv} = -\Theta[F_+]w_{cv} + \Theta[F_-]w_{vc}\,,
\end{aligned}
\tag{66}
$$

(see also Ref. [FM05]). The negative effective-mass introduced in this model has the effect of making the Hamiltonian unbounded from below. As it is well known, such a Hamiltonian is not very good, especially for statistical purposes (the thermal equilibrium states are ill-defined). However, the correct interpretation is that (66) should be considered just as an approximation of the true dynamics for small values of the momentum p.

6 Hydrodynamic models

It is universally recognized that the hydrodynamic approach presents important properties both from the theoretical and the numerical point of view because it gives an interpretation of the transport phenomenon by macroscopic quantities and it produces many advantages from the computational point of view.

The literature on hydrodynamic models is very broad, both in classical as well as in semiclassical and quantum framework.

Some very interesting results have been achieved, proposing quantum hydrodynamic equations, able to describe the behaviour of nanometric devices like resonant tunneling diodes. Here, we restrict ourselves to describing the hydrodynamic versions of the Kane model and of the M-M model.

Most of the results published in the literature refer to single-band problems. The generalization to multiband models presents several difficulties. Among others, the definition of the macroscopic quantities with a realistic physical meaning and the difficulty in imposing boundary conditions.

In this review we give an insight into the classical derivation of a two-band quantum fluid. As we have said, the above-mentioned multiband models are based on the single electron Schrödinger equation, and the resulting equations are essentially linear. By applying the WKB method, it is possible to derive a zero-temperature hydrodynamic version of the Schrödinger two-band models.

When it is desirable to model the dynamics of a family of electrons, the statistical description requires the introduction of a sequence of mixed states, with an attached occupation probability. In this case, the WKB method leads to a sequence of hydrodynamic equations. Starting from it, it is possible to derive a set of equations for certain macroscopic averaged quantities. These hydrodynamic equations share a similar structure with the corresponding equations for a single electron, the only difference being the appearance of terms that can be interpreted as thermal tensors, and of additional source terms. These new terms depend on all states, so the system is not closed unless appropriate closure conditions are provided. It is clear that the final hydrodynamic model with temperature is by no means equivalent to the original quantum model. We could say that the nonlinearity of the resulting hydrodynamic model is "genuine" and is the price to pay for keeping only a finite number of equations.

6.1 The hydrodynamic quantities

In order to obtain hydrodynamic versions of the kinetic models described in the previous sections, one possibility is to follow the general hydrodynamic approach to quantum mechanics due to Madelung [LL77]. This approach consists in writing the wave function in the quasi-classical form $a \exp\left(\frac{iS}{\epsilon}\right)$, where a is called the amplitude and S/ϵ the phase. With this approach, the hydrodynamic limit is valid only for pure states, that is to say, it is valid only for

a quantum system at zero temperature. In the case of a two-band model, we have

$$\psi_a(x,t) = \sqrt{n_a(x,t)}\exp\left(\tfrac{iS_a(x,t)}{\epsilon}\right), \quad a = c, v. \tag{67}$$

where the squared amplitude has the physical meaning of the probability density of finding the "particle" at some point in space, and the gradient of the phase corresponds to the classical velocity of the "particle".

In the framework of two-band models, the densities

$$n_{ab} = \overline{\psi}_a \psi_b,$$

are introduced, where ψ_a, with $a = c, v$, is the envelope function for the conduction and the valence band, respectively. When $a = b$, the quantities $n_{ab} = n_a = |\psi_a|^2$ are real and represent the position probability densities of the conduction band and of the valence band electrons, albeit only in an approximate sense, since ψ_c and ψ_v are envelope functions which mix the Bloch states. Nevertheless, $n = \overline{\psi}_c\psi_c + \overline{\psi}_v\psi_v$ is exactly the total electron density in the conduction and in the valence band, and, as expected, it satisfies a continuity equation. When $a \neq b$, the density $\overline{\psi}_a\psi_b$ is a complex quantity, which does not have a precise physical meaning. Despite of this, as it will become clear in the next section, the complex quantities $\overline{\psi}_a\psi_b$ appear explicitly in the evolution equation for the total density n.

It is customary, after (67), to write the coupling terms in a more convenient way, by introducing the complex quantity

$$n_{cv} = \overline{\psi}_c\psi_v = \sqrt{n_c}\sqrt{n_v}\, e^{i\sigma}, \tag{68}$$

where σ is the phase difference defined by

$$\sigma = \frac{S_v - S_c}{\epsilon}\,. \tag{69}$$

In this way, in order to study a zero-temperature quantum hydrodynamic model, we need to use only the three quantities n_c, n_v and σ to characterize the zero order moments.

The situation is more involved for the current densities. In analogy to the one-band case, we introduce the quantum mechanical electron current densities

$$J_{ab} = \epsilon\ \mathrm{Im}\ \left(\overline{\psi}_a\nabla\psi_b\right)\,. \tag{70}$$

It is natural to recover the classical current densities,

$$J_c = \ \mathrm{Im}\ \left(\epsilon\overline{\psi}_c\nabla\psi_c\right) = n_c\nabla S_c, \quad J_v = \ \mathrm{Im}\ \left(\epsilon\overline{\psi}_v\nabla\psi_v\right) = n_v\nabla S_v\,, \tag{71}$$

whose physical meaning is clear.

The introduction of the complex quantity (68) allows to write $\epsilon\overline{\psi}_a\nabla\psi_b$ in (70) as

$$\epsilon\overline{\psi}_c\nabla\psi_v = n_{cv}u_v, \qquad \epsilon\overline{\psi}_v\nabla\psi_c = \overline{n}_{cv}u_c, \tag{72}$$

where the complex velocities u_c and u_v are given by

$$u_c = u_{\mathrm{os},c} + iu_{\mathrm{el},c}, \quad u_v = u_{\mathrm{os},v} + iu_{\mathrm{el},v}. \tag{73}$$

with $u_{\mathrm{os},c}$ and $u_{\mathrm{os},v}$ the so-called osmotic velocity and current velocity given by

$$u_{\mathrm{os},a} = \frac{\epsilon\nabla\sqrt{n_a}}{\sqrt{n_a}}, \qquad u_{\mathrm{el},a} = \nabla S_a = \frac{J_c}{n_a}\,, a = c, v. \tag{74}$$

In analogy with the single-band case we have defined the osmotic and current velocities as complex quantities which can be expressed solely by means of n_c, n_v, J_c and J_v. In addition, the coupling term n_{cv} has been defined by introducing the phase difference σ. We note that

$$\epsilon\nabla n_{cv} = n_{cv}(\overline{u}_c + u_v). \tag{75}$$

Coming back to the choice of the hydrodynamic quantities, we maintain that, for a zero-temperature quantum hydrodynamic system, it is sufficient to take the usual quantities n_c, n_v, J_c and J_v, plus the phase difference σ. This will be confirmed in the next section.

6.2 Hydrodynamic version of the Kane system

The Kane model was introduced in Section 4.1 by using envelope functions. Before introducing the hydrodynamic form, we rewrite it by using dimensionless variables. To this aim we introduce the rescaled Planck constant $\epsilon = \hbar/\alpha$, where the dimensional parameter α is given by $\alpha = mx_R^2/t_R$, by using x_R and t_R as characteristic (scalar) length and time variables. The band energy can be rescaled by taking new potential units $V_0 = mx_R^2/t_R^2$. A dimensional argument shows that the original coupling coefficient is a reciprocal of a characteristic lenght, thus the coefficient is scaled by Kx_R, componentwise.

Hence, dropping the primes and without changing the name of the variables, we get the following scaled Kane system, which will be the object of our study:

$$\begin{aligned} i\epsilon\frac{\partial\psi_c}{\partial t} &= -\frac{\epsilon^2}{2}\Delta\psi_c + V_c\psi_c - \epsilon^2 K\cdot\nabla\psi_v \\ i\epsilon\frac{\partial\psi_v}{\partial t} &= -\frac{\epsilon^2}{2}\Delta\psi_v + V_v\psi_v + \epsilon^2 K\cdot\nabla\psi_c\,, \end{aligned} \tag{76}$$

where K is the rescaled coupling interband coefficient, ϵ is the rescaled Planck constant, $V_c = E_c + V$ and $V_v = E_v + V$. In the Kane model the coupling parameter has to be considered constant. In realistic heterostructure semiconductor devices, the parameter K, approximatively expressed in terms of the effective electron mass and the energy gap, depends on the layer composition through the spatial coordinates.

Taking into account the wave form (67) and using the equations of system (76), time derivation of $n_a, a = c, v$ gives immediately

$$\begin{aligned} \frac{\partial n_c}{\partial t} + \nabla \cdot J_c &= -2K \cdot \text{ Im } (n_{cv} u_v) \\ \frac{\partial n_v}{\partial t} + \nabla \cdot J_v &= \quad 2K \cdot \text{ Im } (\overline{n}_{cv} u_c) \,, \end{aligned} \tag{77}$$

where (71) has been used for J_c and J_v. We remark that the right-hand side of (77), containing the terms $n_{cv}u_v$ and $\overline{n}_{cv}u_c$, can be expressed in terms of osmotic and current velocities, and the phase difference σ.

Adding the equations in (77) and using the identity $\text{Im}\,(\epsilon\overline{\psi}_c \nabla\psi_v) - \text{Im}\,(\epsilon\overline{\psi}_v \nabla\psi_c) = \epsilon\nabla \text{ Im}\, n_{cv}$, we obtain the balance law for the total density

$$\frac{\partial}{\partial t}(n_c + n_v) + \nabla \cdot (J_c + J_v + 2\epsilon K \text{ Im}\, n_{cv}) = 0 \,,$$

which is just the quantum counterpart of the classical continuity equation.

The derivation of the equations for the phases S_c, S_v, and consequently for J_c and J_v, is more involved.

Referring the reader to the original paper [AF05] for more details, the equations for the currents take the form

$$\begin{aligned} \frac{\partial J_c}{\partial t} + \text{ div} \left(\frac{J_c \otimes J_c}{n_c} + \epsilon^2 \nabla\sqrt{n_c} \otimes \nabla\sqrt{n_c} - \frac{\epsilon^2}{4} \nabla \otimes \nabla n_c \right) + n_c \nabla V_c \\ = \epsilon^2 \text{ Re } \left[\nabla(\overline{\psi}_c (K \cdot \nabla\psi_v)) - 2\nabla\overline{\psi}_c (K \cdot \nabla\psi_v) \right] . \end{aligned} \tag{78}$$

$$\begin{aligned} \frac{\partial J_v}{\partial t} + \text{ div} \left(\frac{J_v \otimes J_v}{n_v} + \epsilon^2 \nabla\sqrt{n_v} \otimes \nabla\sqrt{n_v} - \frac{\epsilon^2}{4} \nabla \otimes \nabla n_v \right) + n_v \nabla V_v \\ = -\epsilon^2 \text{ Re } \left[\nabla(\overline{\psi}_v (K \cdot \nabla\psi_c)) - 2\nabla\overline{\psi}_v (K \cdot \nabla\psi_c) \right] . \end{aligned} \tag{79}$$

The left-hand sides of the equations for the currents can be put in a more familiar form by using the identity

$$\text{div} \left(\nabla\sqrt{n_a} \otimes \nabla\sqrt{n_a} - \frac{1}{4} \nabla \otimes \nabla n_a \right) = -\frac{n_a}{2} \nabla \left[\frac{\Delta\sqrt{n_a}}{\sqrt{n_a}} \right] , \quad a = c, v.$$

The correction terms

$$\frac{\epsilon^2}{2} \frac{\Delta\sqrt{n_a}}{\sqrt{n_a}}, \quad a = c, v \,,$$

can be identified with the quantum Bohm potentials for each band, because they can be interpreted as internal self-consistent potentials, in analogy with the single-band case. The right-hand sides can be further expressed in terms of the hydrodynamic quantities, obtaining the final system

$$\begin{aligned}
&\frac{\partial J_c}{\partial t} + \operatorname{div}\left(\frac{J_c \otimes J_c}{n_c}\right) - n_c \nabla\left(\frac{\epsilon^2 \Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c \nabla V_c \\
&\qquad\qquad = \quad \epsilon \nabla \operatorname{Re}\left(n_{cv} K \cdot u_v\right) - 2 \operatorname{Re}\left(n_{cv} K \cdot u_v \overline{u}_c\right), \\
&\frac{\partial J_v}{\partial t} + \operatorname{div}\left(\frac{J_v \otimes J_v}{n_v}\right) - n_v \nabla\left(\frac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v \nabla V_v \\
&\qquad\qquad = -\epsilon \nabla \operatorname{Re}\left(\overline{n}_{cv} K \cdot u_c\right) + 2 \operatorname{Re}\left(\overline{n}_{cv} K \cdot u_c \overline{u}_v\right).
\end{aligned} \tag{80}$$

It is evident that the equations for the conduction and the valence band are coupled. Also, because of the presence of σ, it is necessary to "close" the system, in order to obtain an extension of the classical Madelung fluid equations to a two-band quantum fluid. In this context, we choose the following constraint

$$\epsilon \nabla \sigma = \frac{J_v}{n_v} - \frac{J_c}{n_c}. \tag{81}$$

Now we are in position to rewrite the hydrodynamic system (80) as follows

$$\begin{aligned}
&\frac{\partial n_c}{\partial t} + \operatorname{div} J_c = -2K \cdot \operatorname{Im}\left(n_{cv} u_v\right), \\
&\frac{\partial n_v}{\partial t} + \operatorname{div} J_v = \quad 2K \cdot \operatorname{Im}\left(\overline{n}_{cv} u_c\right), \\
&\frac{\partial J_c}{\partial t} + \operatorname{div}\left(\frac{J_c \otimes J_c}{n_c}\right) - n_c \nabla\left(\frac{\epsilon^2 \Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c \nabla V_c \\
&\qquad\qquad = \quad \epsilon \nabla \operatorname{Re}\left(n_{cv} K \cdot u_v\right) - 2 \operatorname{Re}\left(n_{cv} K \cdot u_v \overline{u}_c\right), \\
&\frac{\partial J_v}{\partial t} + \operatorname{div}\left(\frac{J_v \otimes J_v}{n_v}\right) - n_v \nabla\left(\frac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v \nabla V_v \\
&\qquad\qquad = -\epsilon \nabla \operatorname{Re}\left(\overline{n}_{cv} K \cdot u_c\right) + 2 \operatorname{Re}\left(\overline{n}_{cv} K \cdot u_c \overline{u}_v\right), \\
&\epsilon \nabla \sigma = \frac{J_v}{n_v} - \frac{J_c}{n_c},
\end{aligned} \tag{82}$$

where n_{cv}, u_v, and u_v are expressed in the terms of the hydrodynamic quantities n_c, n_v, J_c, J_v, and σ by (68) and (73).

6.3 The nonzero-temperature case

The extension of the previous analysis to an electron ensemble requires a quantum statistical mechanics treatment. According to the general discussion at the beginning of Section 5, it is possible to represent an electron ensemble as a mixed quantum mechanical state given by a sequence of pure states Ψ_k, with occupation probabilities $\lambda^k \geq 0$, so that $\sum_k \lambda^k = 1$. In the two-band case, each pure state is represented by a couple of envelope-functions, ψ_c^k and ψ_v^k and, therefore, we shall extend the definition of the hydrodynamic

quantities as a superposition, with weights λ^k, of the corresponding pure-state quantities. For example, the density will be $n_a = \sum_k \lambda^k \overline{\psi}_a^k \psi_a^k$, for $a = c, v$.

In the sequel we shall work at the formal level, and we refer to the equations found in [AF05]. The k-th state for the Kane system is described by the solutions of the system

$$\begin{aligned} i\epsilon \frac{\partial \psi_c^k}{\partial t} &= -\frac{\epsilon^2}{2} \Delta \psi_c^k + V_c \psi_c^k - \epsilon^2 K \cdot \nabla \psi_v^k \,, \\ i\epsilon \frac{\partial \psi_v^k}{\partial t} &= -\frac{\epsilon^2}{2} \Delta \psi_v^k + V_v \psi_v^k + \epsilon^2 K \cdot \nabla \psi_c^k \,. \end{aligned} \tag{83}$$

Using the expressions (67) for each state k in (83),

$$\psi_c^k = \sqrt{n_c^k} \exp\left(iS_c^k/\epsilon\right), \qquad \psi_v^k = \sqrt{n_v^k} \exp\left(iS_v^k/\epsilon\right),$$

under the assumption of positivity of the densities n_c^k and n_v^k, a hydrodynamic system analogous to (82) is obtained for each state k. The densities and the currents corresponding to the two mixed states for conduction and valence electrons can be defined as

$$\begin{aligned} n_c &= \sum_{k=0}^{\infty} \lambda^k n_c^k, \quad n_v = \sum_{k=0}^{\infty} \lambda^k n_v^k, \\ J_c &= \sum_{k=0}^{\infty} \lambda^k J_c^k, \quad J_v = \sum_{k=0}^{\infty} \lambda^k J_v^k \,. \end{aligned}$$

We also define

$$\begin{aligned} \sigma &= \sum_{k=0}^{\infty} \lambda^k \sigma^k, \quad n_{cv} = \sqrt{n_c}\sqrt{n_v} \exp(i\sigma), \\ u_c &= \frac{\epsilon \nabla \sqrt{n_c}}{\sqrt{n_c}} + i\frac{J_c}{n_c}, \quad u_v = \frac{\epsilon \nabla \sqrt{n_v}}{\sqrt{n_v}} + i\frac{J_v}{n_v}. \end{aligned}$$

Multiplying (82) for the state k by λ^k and summing over k, we find new quantities that must be manipulated with much care. In analogy with the one-band case [GMU95], new terms containing the total temperature θ_c and θ_v, for each band, appear in the current equations. The temperature tensors are defined by the sum of osmotic temperature and electron current temperature

$$\theta_c = \theta_{\mathrm{os},c} + \theta_{\mathrm{el},c} \quad \text{and} \quad \theta_v = \theta_{\mathrm{os},v} + \theta_{\mathrm{el},v}$$

given by

$$\begin{aligned} \theta_{\mathrm{os},c} &= \sum_{k=0}^{\infty} \lambda^k \frac{n_c^k}{n_c} (u_{\mathrm{os},c}^k - u_{\mathrm{os},c}) \otimes (u_{\mathrm{os},c}^k - u_{\mathrm{os},c}), \\ \theta_{\mathrm{el},c} &= \sum_{k=0}^{\infty} \lambda^k \frac{n_c^k}{n_c} (u_{\mathrm{el},c}^k - u_{\mathrm{el},c}) \otimes (u_{\mathrm{el},c}^k - u_{\mathrm{el},c}). \end{aligned}$$

In conclusion our system becomes

$$
\begin{aligned}
&\frac{\partial n_c}{\partial t} + \mathrm{div} J_c = -\,2K\cdot\ \mathrm{Im}\,[n_{cv}\,(\alpha u_v + \beta_v)],\\
&\frac{\partial n_v}{\partial t} + \mathrm{div} J_v = \quad 2K\cdot\ \mathrm{Im}\,[\overline{n_{cv}}\,(\overline{\alpha}\,u_c + \beta_c)],\\
&\frac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\frac{J_c\otimes J_c}{n_c} + n_c\theta_c\right) - n_c\nabla\left(\frac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c\nabla V_c\\
&\qquad\qquad = \ \epsilon\,K\cdot\nabla\ \mathrm{Re}\ (n_{cv}(\alpha u_v + \beta_v))\\
&\qquad\qquad\quad -\,2K\cdot\ \mathrm{Re}\ \left(n_{cv}(\alpha u_v\otimes\overline{u_c} + \beta_v\otimes\overline{u_c} + u_v\otimes\overline{\beta_c} + \theta_{cv})\right),\\
&\frac{\partial J_v}{\partial t} + \ \mathrm{div}\left(\frac{J_v\otimes J_v}{n_v} + n_v\theta_v\right) - n_v\nabla\left(\frac{\epsilon^2\Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v\nabla V_v\\
&\qquad\qquad = -\epsilon\,K\cdot\nabla\ \mathrm{Re}\ (\overline{n_{cv}}\,(\overline{\alpha}u_c + \beta_c))\\
&\qquad\qquad\quad +\,2K\cdot\ \mathrm{Re}\ \left(\overline{n_{cv}}\,(\overline{\alpha}u_c\otimes\overline{u_v} + \beta_c\otimes\overline{u_v} + u_c\otimes\overline{\beta_v} + \theta_{vc})\right),\\
&\epsilon\nabla\sigma - \frac{J_v}{n_v} + \frac{J_c}{n_c} = -\ \mathrm{Im}\left\{\frac{1}{\alpha}\left(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\right)\right\}.
\end{aligned}
\tag{84}
$$

where the new quantities are defined by

$$
\alpha = \sum_{k=0}^{\infty}\lambda^k\frac{n_{cv}^k}{n_{cv}},\qquad \beta_v = \sum_{k=0}^{\infty}\lambda^k\frac{n_{cv}^k}{n_{cv}}(u_v^k - u_v),\qquad \beta_c = \sum_{k=0}^{\infty}\lambda^k\frac{\overline{n_{cv}^k}}{\overline{n_{cv}}}(u_c^k - u_c).
$$

and, in the expression of the coupling terms between the two bands, there appears a of temperature tensor, given by

$$
\begin{aligned}
\theta_{cv} &= \sum_{k=0}^{\infty}\lambda^k\frac{n_{cv}^k}{n_{cv}}(u_v^k - u_v)\otimes(\overline{u_c^k} - \overline{u_c}),\\
\theta_{vc} &= \sum_{k=0}^{\infty}\lambda^k\frac{\overline{n_{cv}^k}}{\overline{n_{cv}}}(u_c^k - u_c)\otimes(\overline{u_v^k} - \overline{u_v}).
\end{aligned}
$$

Equations (84) can be considered as a nonzero-temperature quantum fluid model. The quantities n_{cv}, u_c, and u_v, already present in (82), are expressed in terms of n_c, n_v, J_c, J_v, and σ, while the new quantities α, β_c, and β_v satisfy the relation

$$
\mathrm{Re}\left\{\frac{1}{\alpha}\left(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\right)\right\} = 0
$$

and need appropriate closure relations. Moreover, we must assign constitutive relations for the tensor components θ_c, θ_v, θ_{cv} and θ_{vc}; θ_c and θ_v are formally analogous to the temperature tensor of kinetic theory.

A simple class of closure conditions can be obtained by assigning a function $\alpha = \alpha(n_c, n_v, \sigma)$ and taking

$$\beta_c = 2n_c \frac{\partial \bar{\alpha}}{\partial n_c} u_{\mathrm{os},c} - \frac{\partial \bar{\alpha}}{\partial \sigma} u_{\mathrm{el},c}, \quad \beta_v = 2n_v \frac{\partial \alpha}{\partial n_v} u_{\mathrm{os},v} + \frac{\partial \alpha}{\partial \sigma} u_{\mathrm{el},v}. \tag{85}$$

Then, we have

$$\epsilon \nabla \alpha - \beta_v - \overline{\beta_c} = 0,$$

which implies

$$\epsilon \nabla \sigma - \frac{J_v}{n_v} + \frac{J_c}{n_c} = 0.$$

In particular, it is possible to choose

$$\alpha = 1, \quad \beta_c = \beta_v = 0. \tag{86}$$

We still need to consider the temperature tensors θ_c, θ_v, θ_{cv} and θ_{vc}. Heuristically, following the analogy with the single-band fluid-dynamical model [Jun01], the simplest closure relation is:

$$\theta_c = \frac{1}{n_c} p_c(n_c) I, \quad \theta_v = \frac{1}{n_v} p_v(n_v) I, \quad \theta_{cv} = \theta_{vc} = 0, \tag{87}$$

where I is the identity tensor and the functions p_c and p_v can be interpreted as pressures. In this way we obtain the simplest two-band, isentropic, fluid-dynamical model:

$$\begin{aligned}
&\frac{\partial n_c}{\partial t} + \mathrm{div} J_c = -2K \cdot \mathrm{Im}\,(n_{cv}\, u_v), \\
&\frac{\partial n_v}{\partial t} + \mathrm{div} J_v = \quad 2K \cdot \mathrm{Im}\,(\overline{n_{cv}}\, u_c), \\
&\frac{\partial J_c}{\partial t} + \mathrm{div}\left(\frac{J_c \otimes J_c}{n_c} + p_c(n_c) I\right) - n_c \nabla\left(\frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c \nabla V_c \\
&\qquad\qquad = \epsilon K \cdot \nabla\, \mathrm{Re}\,(n_{cv} u_v) - 2K \cdot \mathrm{Re}\,(n_{cv} u_v \otimes \overline{u_c}), \\
&\frac{\partial J_v}{\partial t} + \mathrm{div}\left(\frac{J_v \otimes J_v}{n_v} + p_v(n_v) I\right) - n_v \nabla\left(\frac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v \nabla V_v \\
&\qquad\qquad = -\epsilon K \cdot \nabla\, \mathrm{Re}\,(\overline{n_{cv}}\, u_c) + 2K \cdot \mathrm{Re}\,(\overline{n_{cv}}\, u_c \otimes \overline{u_v}), \\
&\epsilon \nabla \sigma - \frac{J_v}{n_v} + \frac{J_c}{n_c} = 0.
\end{aligned} \tag{88}$$

We remark that if the (classical) pressures are linear functions of n_c and n_v equations (88) reduce to the so-called isothermal case.

6.4 Hydrodynamic version of the M-M system

The method used in the previous section is suitable to be applied also to the multiband envelope function model introduced by Modugno and Morandi in [MM05] and described in Section 4.2. However, as we have remarked at the end of Section 5.3, when mixed states become important (namely, for nonzero temperature models), the M-M model has some undesirable features that make the discussion more complicated, beyond the scope of the present review. For this reason we shall restrict ourselves to the zero-temperature case.

By using dimensionless variables, the system (29) reads as follows:

$$\begin{aligned} i\epsilon\frac{\partial\psi_c}{\partial t} &= -\frac{\epsilon^2}{2}\Delta\psi_c + (E_c+V)\psi_c - \epsilon^2\, P\,\psi_v, \\ i\epsilon\frac{\partial\psi_v}{\partial t} &= \quad\frac{\epsilon^2}{2}\Delta\psi_v + (E_v+V)\psi_v - \epsilon^2\, P\,\psi_c, \end{aligned} \tag{89}$$

where P is the rescaled coupling interband coefficient and ϵ is the rescaled Planck constant.

By using the Madelung form (67) for the wave functions, and proceeding in the same way as for the Kane model in Section 6.2, we obtain the hydrodynamic equations for the two-band M-M model

$$\begin{aligned} \frac{\partial n_c}{\partial t} + \nabla\cdot J_c &= -2P\ \mathrm{Im}\ \left(\epsilon\overline{\psi}_c\psi_v\right)\ , \\ \frac{\partial n_v}{\partial t} - \nabla\cdot J_v &= \quad 2P\ \mathrm{Im}\ \left(\epsilon\overline{\psi}_c\psi_v\right)\ . \end{aligned} \tag{90}$$

By summing the two equations in (90), we obtain the balance law for the total density,

$$\frac{\partial\rho}{\partial t} + \nabla\cdot J = 0. \tag{91}$$

where $\rho = n_c + n_v$ is the total density and $J = J_c - J_v$ is the total current.

We remark that, in contrast with the Kane model, interband current terms do not appear in the conservation of the total density.
Next, the equations for the phases S_c, S_v, and the currents J_c and J_v are derived. Referring the reader to the paper [AFM05] for the details, here we only write the equations for the currents in the final form

$$\begin{aligned} &\frac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\frac{J_c\otimes J_c}{n_c}\right) - n_c\nabla\left(\frac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c(\nabla E_c + \nabla V) \\ &= \epsilon^2\nabla P\ \mathrm{Re}\ n_{cv} + \epsilon P\sqrt{n_c}\sqrt{n_v}(\cos\sigma(u_{\mathrm{os},v} - u_{\mathrm{os},c}) - \sin\sigma(u_{\mathrm{el},c} + u_{\mathrm{el},v})), \end{aligned}$$

$$\frac{\partial J_v}{\partial t} - \ \mathrm{div}\left(\frac{J_v \otimes J_v}{n_v}\right) + n_v \nabla\left(\frac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v(\nabla E_v + \nabla V)$$
$$= \epsilon^2 \nabla P \ \mathrm{Re}\ n_{cv} - \epsilon P \sqrt{n_c}\sqrt{n_v}(\cos\sigma(u_{\mathrm{os},v} - u_{\mathrm{os},c}) - \sin\sigma(u_{\mathrm{el},c} + u_{\mathrm{el},v})). \tag{92}$$

Also in this case, we have introduced the internal self-consistent potentials for each band (the Bohm potentials) and the osmotic velocities $(u_{\mathrm{os},c}, u_{\mathrm{os},v})$ and current velocities $(u_{\mathrm{el},c}, u_{\mathrm{el},v})$; σ is again the phase difference defined by $\sigma = \frac{S_v - S_c}{\epsilon}$.

The systems (90) and (92) are not equivalent to the original system (89), due to the presence of σ. By using the constraint (81), we finally obtain the hydrodynamic system

$$\begin{aligned}
&\frac{\partial n_c}{\partial t} + \mathrm{div} J_c = -2\epsilon P \ \mathrm{Im}\, n_{cv},\\
&\frac{\partial n_v}{\partial t} - \mathrm{div} J_v = \quad 2\epsilon P \ \mathrm{Im}\, n_{cv},\\
&\frac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\frac{J_c \otimes J_c}{n_c}\right) - n_c \nabla\left(\frac{\epsilon^2 \Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c(\nabla E_c + \nabla V)\\
&\qquad\qquad = \quad \epsilon^2 \nabla P \ \mathrm{Re}\ n_{cv} + \epsilon P \ \mathrm{Re}\ \ (n_{cv}(u_v - \overline{u}_c))\ ,\\
&\frac{\partial J_v}{\partial t} - \ \mathrm{div}\left(\frac{J_v \otimes J_v}{n_v}\right) + n_v \nabla\left(\frac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v(\nabla E_v + \nabla V)\\
&\qquad\qquad = \quad \epsilon^2 \nabla P \ \mathrm{Re}\ n_{cv} - \epsilon P \ \mathrm{Re}\ \ (n_{cv}(u_v - \overline{u}_c))\ ,\\
&\epsilon \nabla \sigma = \frac{J_v}{n_v} - \frac{J_c}{n_c}\,,
\end{aligned} \tag{93}$$

where n_{cv}, u_v, u_v are expressed in the terms of the hydrodynamic quantities n_c, n_v, J_c, J_v, σ. System (93) is the extension of the classical Madelung fluid equations to a two-band quantum fluid.

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