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ON THE DRIFT-DIFFUSION MODEL FOR A TWO-BAND QUANTUM FLUID AT ZERO-TEMPERATURE

ПРО МОДЕЛЬ ПЕРЕНОСУ ДИФУЗІЇ ДЛЯ ДВОЗОННОЇ КВАНТОВОЇ РІДИНИ ПРИ НУЛЬОВІЙ ТЕМПЕРАТУРІ

By using a scale transformation, we obtain hydrodynamic equations in the quasiclassical approximation from the two-band Schrödinger equation.

За допомогою масштабного перетворення одержано гідродинамічні рівняння у квазікласичному наближенні з двокомпонентного рівняння Шредінгера.

1. Introduction. In the recent literature there is a growing interest for diodes in which the valence band electrons play a relevant role in the current flow, such as Interband Resonant Tunneling Diodes [1 – 3]. Correspondingly, the effort in the theoretical study of multiband models has increased [4 – 8]. The typical band diagram structure of a tunneling diode is characterized by a band alignment such that the valence band at the positive side of the semiconductor device lies above the conduction band at the negative one.

Correspondingly, one of the simplest multiband model, introduced by E. O. Kane in the early 60's [9], includes only two energy bands of the device material, separated by a forbidden region. It consists of two coupled Schrödinger-like equations for the conduction and the valence band wave (envelope) functions. The coupling term is derived with the $\mathbf{k} \cdot \mathbf{p}$ perturbation method [10, 11], which relies on the assumption that, for a reliable description, it is sufficient solve of the single-electron Schrödinger equation in the neighbourhood of the bottom and the top of the conduction and the valence bands, respectively, since most of the electrons and holes are located there. This model is successfully employed for simulations [2, 3]; in particular, it is suitable for investigations on the bulk properties of semiconductors, such as band nonparabolicity and optical properties.

Nevertheless, the approximation of the original multiband problem by the two-band Kane model has not a clear physical interpretation; indeed, the corresponding equations result to be coupled even in absence of an external potential. Moreover the choice of the envelope functions is subtle: in the literature are present various methods based on partial diagonalization of the Kane Hamiltonian (such as Luttinger effective-mass models); however, they don't give satisfactory results when nonperiodic potentials are present [12]. The method proposed in [8], instead, is based on the use of the Wannier envelope functions, and the "multiband envelope function" model obtained is reliable even when the symmetry of the crystal is broken by an external potential (standing for heterostructures, impurities, e.g.), since the elements of the basis are located at the crystal sites.

Already, in the (semi-)classical framework, a hydrodynamic formulation is recommended, because of the lower computational cost of the implementation. In the quantum framework, many works in the literature are devoted to quantum hydrodynamic formulation, [13, 14] e.g. In a recent work [15], Ali and Frosali have developed a method to extend the derivation of quantum hydrodynamic models from a (single-band) Schrödinger

equation [13] to the Kane model. There, they have obtained a closed system of hydrodynamic equations for a two-band quantum fluid.

The method formulated in [15] is suitable to be applied to the multiband envelope function model in [8] as well, and that is precisely the content of the present work. After introducing (Section 2) the two-band envelope function model, in Section 3 we derive the corresponding fluid-dynamical system for particle and current densities, using the Madelung transform. In Section 4, we perform a drift-diffusive scaling and we end up with a closed set of equations which are the analog of the zero-temperature quantum drift-diffusion model for a two-band envelope function system. In the last section, we compare our model with the one obtained in [15] and we discuss briefly many open problems in the two-band quantum hydrodynamical model, such as closure and numerical experiments.

2. A two-band envelope function system. Let $\psi_c(x, t)$ be the conduction band envelope function and $\psi_v(x, t)$ be the valence band envelope function. The multiband envelope function model in the two-band time-dependent case reads as follows:

$$\begin{aligned} i\hbar \frac{\partial \psi_c}{\partial t} &= -\frac{\hbar^2}{2m^*} \Delta \psi_c + (V_c + V) \psi_c - \frac{\hbar^2}{m} \frac{P \cdot \nabla V}{E_g} \psi_v, \\ i\hbar \frac{\partial \psi_v}{\partial t} &= \frac{\hbar^2}{2m^*} \Delta \psi_v + (V_v + V) \psi_v - \frac{\hbar^2}{m} \frac{P \cdot \nabla V}{E_g} \psi_c. \end{aligned} \quad (2.1)$$

This model will be considered in \mathbb{R}^3 . Here, i is the imaginary unit, \hbar is the reduced Planck constant, m^* is the isotropic effective mass of both the conduction and valence band electrons, which we suppose to be equal, and m is the bare mass of the carriers. Moreover, V is the electrostatic potential, V_c and V_v are the minimum and the maximum of the conduction and the valence band energy, respectively. The last two quantities depend, through the x -coordinate, on the layer composition, while their difference $E_g = V_c - V_v$, which is called gap energy, is supposed to be constant. The coupling coefficient between the two bands P represents the momentum operator matrix element between the corresponding Wannier functions.

For the derivation of model (2.1) in the framework of the Bloch theory, we refer the reader to [8].

We recall that, for anisotropic materials, the inverse of the isotropic effective mass should be replaced by an inverse mass tensor. We make use of the following scaling: after choosing a (scalar) characteristic length scale x_R and a characteristic time scale t_R , we introduce the rescaled Planck constant

$$\epsilon = \frac{\hbar}{\alpha},$$

with the dimensional parameter

$$\alpha = \frac{m^* x_R^2}{t_R},$$

and the rescaled time and space variables $t' = \frac{t}{t_R}$, $x' = \frac{x}{x_R}$ componentwise.

In the adimensional version of (2.1), the masses m and m^* are kept unchanged, since they appear in a ratio, while the band energy can be rescaled by $V_R = \frac{m^* x_R^2}{t_R^2}$.

A dimensional argument shows that the original coupling coefficient is a reciprocal of a characteristic length, thus $P' = P x_R$, componentwise.

Hence, dropping the prime, we get the following two-band envelope function model, which will be the object of our study:

$$\begin{aligned} i\epsilon \frac{\partial \psi_c}{\partial t} &= -\frac{\epsilon^2}{2} \Delta \psi_c + (V_c + V) \psi_c - \epsilon^2 K \psi_v, \\ i\epsilon \frac{\partial \psi_v}{\partial t} &= \frac{\epsilon^2}{2} \Delta \psi_v + (V_v + V) \psi_v - \epsilon^2 K \psi_c, \end{aligned} \quad (2.2)$$

where $K = \frac{m^* P \cdot \nabla V}{m E_g}$.

3. Derivation of the fluidynamical model. The simplest way to derive a fluidynamical formulation of the evolution equations for particle and current densities is the (classically used) Madelung transform. Since our model consists of two coupled Schrödinger equations, we decompose the wave (envelope) functions for conduction and valence bands into their amplitudes $\sqrt{n_c}$, $\sqrt{n_v}$ and phases S_c , S_v , defined by the relations

$$\begin{aligned} \psi_c(x, t) &= \sqrt{n_c(x, t)} \exp\left(\frac{iS_c(x, t)}{\epsilon}\right), \\ \psi_v(x, t) &= \sqrt{n_v(x, t)} \exp\left(\frac{iS_v(x, t)}{\epsilon}\right). \end{aligned} \quad (3.1)$$

For more details on the notation see Section 2 of [15], where the same procedure is applied to the two-band Kane model.

By using the first equation of the two-band envelope function system (2.2), we find

$$\frac{\partial n_c}{\partial t} = \bar{\psi}_c \frac{\partial \psi_c}{\partial t} + \psi_c \frac{\partial \bar{\psi}_c}{\partial t} = -\nabla \cdot \text{Im}(\epsilon \bar{\psi}_c \nabla \psi_c) - 2K \text{Im}(\epsilon \bar{\psi}_c \psi_v).$$

In a similar way, we get the equation for the evolution of n_v . Then, the previous equations become

$$\begin{aligned} \frac{\partial n_c}{\partial t} + \nabla \cdot \text{Im}(\epsilon \bar{\psi}_c \nabla \psi_c) &= -2K \text{Im}(\epsilon \bar{\psi}_c \psi_v), \\ \frac{\partial n_v}{\partial t} - \nabla \cdot \text{Im}(\epsilon \bar{\psi}_v \nabla \psi_v) &= 2K \text{Im}(\epsilon \bar{\psi}_c \psi_v), \end{aligned} \quad (3.2)$$

and by using the definition of current density, we get

$$\begin{aligned} \frac{\partial n_c}{\partial t} + \nabla \cdot J_c &= -2K \text{Im}(\epsilon \bar{\psi}_c \psi_v), \\ \frac{\partial n_v}{\partial t} - \nabla \cdot J_v &= 2K \text{Im}(\epsilon \bar{\psi}_c \psi_v). \end{aligned} \quad (3.3)$$

Summing the equations in (3.3), we obtain the balance law for the total density,

$$\frac{\partial}{\partial t}(n_c + n_v) + \nabla \cdot (J_c - J_v) = 0. \quad (3.4)$$

We remark that, in contrast with the Kane model, currents due to the interband terms do not appear in the conservation of the total density.

Next, we derive equations for phases S_c , S_v . Using systems (2.2) and (3.2), we get

$$\begin{aligned} \frac{\partial S_c}{\partial t} &= -i\epsilon \frac{\partial}{\partial t} \ln\left(\frac{\psi_c}{\sqrt{n_c}}\right) = -i\epsilon \left(\frac{1}{\psi_c} \frac{\partial \psi_c}{\partial t} - \frac{1}{2n_c} \frac{\partial n_c}{\partial t}\right) = \\ &= \frac{\epsilon^2}{2n_c} (\nabla \cdot \text{Re}(\bar{\psi}_c \nabla \psi_c) - \nabla \bar{\psi}_c \cdot \nabla \psi_c) - (V_c + V) + \frac{\epsilon^2}{n_c} K \text{Re}(\bar{\psi}_c \psi_v). \end{aligned}$$

It is possible to rewrite the previous equation as

$$\frac{\partial S_c}{\partial t} = -\frac{1}{2} |\nabla S_c|^2 + \frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} - (V_c + V) + \frac{\epsilon^2}{n_c} K \operatorname{Re} (\bar{\psi}_c \psi_v).$$

A similar equation can be derived for S_v . The resulting system is

$$\begin{aligned} \frac{\partial S_c}{\partial t} + \frac{1}{2} |\nabla S_c|^2 - \frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} + (V_c + V) &= \frac{\epsilon^2}{n_c} K \operatorname{Re} (\bar{\psi}_c \psi_v), \\ \frac{\partial S_v}{\partial t} - \frac{1}{2} |\nabla S_v|^2 + \frac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} + (V_v + V) &= \frac{\epsilon^2}{n_v} K \operatorname{Re} (\bar{\psi}_c \psi_v). \end{aligned} \quad (3.5)$$

Equations (3.2) and (3.5) are equivalent to the coupled Schrödinger equations in (2.2).

We would like to replace system (3.5) with one of coupled equations for the currents.

We can evaluate

$$\begin{aligned} \frac{\partial J_c}{\partial t} &= \epsilon \operatorname{Im} \left(\bar{\psi}_c \nabla \frac{\partial \psi_c}{\partial t} + \nabla \psi_c \frac{\partial \bar{\psi}_c}{\partial t} \right) = \\ &= \sum_j \frac{\epsilon^2}{2} \frac{\partial}{\partial x_j} \operatorname{Re} \left(\bar{\psi}_c \nabla \frac{\partial \psi_c}{\partial x_j} - \nabla \psi_c \frac{\partial \bar{\psi}_c}{\partial x_j} \right) - \bar{\psi}_c \psi_c \nabla V_c + \\ &+ \epsilon^2 \nabla K \operatorname{Re} (\bar{\psi}_c \psi_v) + \epsilon^2 K \operatorname{Re} \left[\nabla (\bar{\psi}_c \psi_v) - 2 \nabla \bar{\psi}_c \psi_v \right]. \end{aligned} \quad (3.6)$$

Using standard identities, eq. (3.6) can be rewritten in the more familiar form

$$\begin{aligned} \frac{\partial J_c}{\partial t} + \operatorname{div} \left(\frac{J_c \otimes J_c}{n_c} + \epsilon^2 \nabla \sqrt{n_c} \otimes \nabla \sqrt{n_c} - \frac{\epsilon^2}{4} \nabla \otimes \nabla n_c \right) + n_c (\nabla V_c + \nabla V) &= \\ = \epsilon^2 \nabla K \operatorname{Re} (\bar{\psi}_c \psi_v) + \epsilon^2 K \operatorname{Re} \left[\nabla (\bar{\psi}_c \psi_v) - 2 \nabla \bar{\psi}_c \psi_v \right]. \end{aligned} \quad (3.7)$$

Similarly, for J_v we find

$$\begin{aligned} \frac{\partial J_v}{\partial t} - \operatorname{div} \left(\frac{J_v \otimes J_v}{n_v} + \epsilon^2 \nabla \sqrt{n_v} \otimes \nabla \sqrt{n_v} - \frac{\epsilon^2}{4} \nabla \otimes \nabla n_v \right) + n_v (\nabla V_v + \nabla V) &= \\ = \epsilon^2 \nabla K \operatorname{Re} (\bar{\psi}_c \psi_v) + \epsilon^2 K \operatorname{Re} \left[\nabla (\bar{\psi}_c \psi_v) - 2 \bar{\psi}_c \nabla \psi_v \right]. \end{aligned} \quad (3.8)$$

The left-hand sides of the equations for the currents can be reformulated by the following identity:

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

The correction terms

$$\frac{\epsilon^2}{2} \frac{\Delta \sqrt{n_i}}{\sqrt{n_i}} \quad i = c, v,$$

can be interpreted as internal self-potentials for each band and are called quantum Bohm potentials.

In addition, the right-hand sides of equations (3.7), (3.8) can be expressed in terms of the hydrodynamic quantities, by using the relations and definitions we recall here (cf. [15]):

$$\bar{\psi}_i \nabla \psi_j = \sqrt{n_i} \sqrt{n_j} \exp \left(i \frac{S_j - S_i}{\epsilon} \right) \left(\epsilon \frac{\nabla \sqrt{n_j}}{\sqrt{n_j}} + i \nabla S_j \right), \quad (3.9)$$

$$n_{cv} := \overline{\psi}_c \psi_v = \sqrt{n_c} \sqrt{n_v} e^{i\sigma}, \tag{3.10}$$

where σ is the phase difference defined by $\sigma := \frac{S_v - S_c}{\epsilon}$,

$$u_c := \frac{\epsilon \nabla \psi_c}{\psi_c} = \underbrace{\frac{\epsilon \nabla \sqrt{n_c}}{\sqrt{n_c}}}_{u_{os,c}} + i \underbrace{\nabla S_c}_{u_{el,c}}, \quad u_v := \frac{\epsilon \nabla \psi_v}{\psi_v} = \underbrace{\frac{\epsilon \nabla \sqrt{n_v}}{\sqrt{n_v}}}_{u_{os,v}} + i \underbrace{\nabla S_v}_{u_{el,v}}, \tag{3.11}$$

$$\epsilon \nabla n_{cv} = n_{cv} (u_v + \overline{u}_c). \tag{3.12}$$

Thus,

$$\begin{aligned} \frac{\partial J_c}{\partial t} + \operatorname{div} \left(\frac{J_c \otimes J_c}{n_c} \right) - n_c \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} \right) + n_c (\nabla V_c + \nabla V) = \\ = \epsilon^2 \nabla K \operatorname{Re} (\overline{\psi}_c \psi_v) + \epsilon K \operatorname{Re} (n_{cv} (u_v - \overline{u}_c)), \end{aligned} \tag{3.13}$$

$$\begin{aligned} \frac{\partial J_v}{\partial t} - \operatorname{div} \left(\frac{J_v \otimes J_v}{n_v} \right) + n_v \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} \right) + n_v (\nabla V_v + \nabla V) = \\ = \epsilon^2 \nabla K \operatorname{Re} (\overline{\psi}_c \psi_v) - \epsilon K \operatorname{Re} (n_{cv} (u_v - \overline{u}_c)). \end{aligned}$$

By exploiting, instead, the definition (3.11) of osmotic velocities $(u_{os,c}, u_{os,v})$ and current velocities $(u_{el,c}, u_{el,v})$, and the relation (3.9), we get

$$\begin{aligned} \frac{\partial J_c}{\partial t} + \operatorname{div} \left(\frac{J_c \otimes J_c}{n_c} \right) - n_c \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} \right) + n_c (\nabla V_c + \nabla V) = \\ = \epsilon^2 \nabla K \operatorname{Re} n_{cv} + \epsilon K \sqrt{n_c} \sqrt{n_v} (\cos \sigma (u_{os,v} - u_{os,c}) - \sin \sigma (u_{el,c} + u_{el,v})), \end{aligned} \tag{3.14}$$

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

Analogously to Ref. [15] and at variance with the uncoupled model, systems (3.3) and (3.14) are not equivalent to the original system (2.2), due to the presence of σ . The way to close systems (3.3) and (3.14) is not unique; one possibility is to use system (3.5) to derive an evolution equation for $\sigma = (S_v - S_c)/\epsilon$, namely

$$\begin{aligned} \epsilon \frac{\partial \sigma}{\partial t} - \frac{1}{2} \left(\left| \frac{J_c}{n_c} \right|^2 + \left| \frac{J_v}{n_v} \right|^2 \right) + \frac{\epsilon^2}{2} \left(\frac{\Delta \sqrt{n_c}}{\sqrt{n_c}} + \frac{\Delta \sqrt{n_v}}{\sqrt{n_v}} \right) - V_c + V_v = \\ = \frac{\epsilon}{2} K \operatorname{Re} (\epsilon \overline{\psi}_c \psi_v) \left(\frac{1}{n_v} - \frac{1}{n_c} \right). \end{aligned} \tag{3.15}$$

Equation (3.15) must be supplemented with the constraint

$$\epsilon \nabla \sigma = \frac{J_v}{n_v} - \frac{J_c}{n_c}. \tag{3.16}$$

It is possible to prove that equations (3.15) and (3.16) are equivalent. Indeed, if we consider equation (3.16), then we can recover σ as a function of the other variables by solving the elliptic equation

$$\epsilon \Delta \sigma = \nabla \cdot \left(\frac{J_v}{n_v} - \frac{J_c}{n_c} \right), \tag{3.17}$$

which can be obtained immediately by derivation of the constraint (3.16).

Another possibility is to regard n_{cv} in system (3.13) as an independent variable, rather than σ . From definition (3.10) and the two-band envelope function system (2.2), we find

$$\begin{aligned} \frac{\partial n_{cv}}{\partial t} &= \psi_v \frac{\partial \bar{\psi}_c}{\partial t} + \bar{\psi}_c \frac{\partial \psi_v}{\partial t} = \\ &= -\frac{i\epsilon}{2} \nabla \cdot (\psi_v \nabla \bar{\psi}_c \bar{\psi}_c \nabla \psi_v - 2 \nabla \psi_v \nabla \bar{\psi}_c) + \\ &+ \frac{i}{\epsilon} (V_c - V_v) \bar{\psi}_c \psi_v - i\epsilon K (\psi_v \bar{\psi}_v - \bar{\psi}_c \psi_c), \end{aligned}$$

which, using (3.9) and the definitions of osmotic and current velocities, leads to

$$\epsilon \frac{\partial n_{cv}}{\partial t} = -\frac{i}{2} \nabla \cdot \nabla n_{cv} - \frac{i}{\epsilon} n_{cv} (\bar{u}_c u_v) + \frac{i}{\epsilon} n_{cv} (V_c - V_v) + i\epsilon K (n_c - n_v). \quad (3.18)$$

In addition to (3.18), the complex function n_{cv} must satisfy the constraints

$$\bar{n}_{cv} n_{cv} = n_c n_v, \quad (3.19)$$

$$\epsilon \nabla n_{cv} = (u_v + \bar{u}_c) n_{cv}. \quad (3.20)$$

Alternatively, we can use the identity (3.20) to derive a nonlinear elliptic equation for n_{cv} ,

$$\operatorname{div} \left(\frac{\epsilon \nabla n_{cv}}{n_{cv}} \right) = \operatorname{div} (u_v + \bar{u}_c), \quad (3.21)$$

which must be solved together with the constraint (3.19).

Now we are in position to rewrite the hydrodynamic system as follows:

$$\begin{aligned} \frac{\partial n_c}{\partial t} + \operatorname{div} J_c &= -2\epsilon K \operatorname{Im} n_{cv}, \\ \frac{\partial n_v}{\partial t} - \operatorname{div} J_v &= 2\epsilon K \operatorname{Im} n_{cv}, \\ \frac{\partial J_c}{\partial t} + \operatorname{div} \left(\frac{J_c \otimes J_c}{n_c} \right) - n_c \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} \right) + n_c (\nabla V_c + \nabla V) &= \\ &= \epsilon^2 \nabla K \operatorname{Re} n_{cv} + \epsilon K \operatorname{Re} (n_{cv} (u_v - \bar{u}_c)), \quad (3.22) \\ \frac{\partial J_v}{\partial t} - \operatorname{div} \left(\frac{J_v \otimes J_v}{n_v} \right) + n_v \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} \right) + n_v (\nabla V_v + \nabla V) &= \\ &= \epsilon^2 \nabla K \operatorname{Re} n_{cv} - \epsilon K \operatorname{Re} (n_{cv} (u_v - \bar{u}_c)), \\ \epsilon \nabla \sigma &= \frac{J_v}{n_v} - \frac{J_c}{n_c}, \end{aligned}$$

where n_{cv} , u_v , u_c are expressed in the terms of the hydrodynamic quantities n_c , n_v , J_c , J_v , σ by (3.10) and (3.11). System (3.22) is the extension of the classical Madelung fluid equations to a two-band quantum fluid.

4. The drift-diffusive scaling. In the following we will consider a modified version of the system (3.3), (3.13) and (3.17), with additional relaxation terms for the currents. It is convenient to rewrite this system as

$$\begin{aligned} \frac{\partial n_c}{\partial t} + \operatorname{div} J_c &= -2\epsilon K \operatorname{Im} n_{cv}, \\ \frac{\partial n_v}{\partial t} - \operatorname{div} J_v &= 2\epsilon K \operatorname{Im} n_{cv}, \end{aligned}$$

$$\begin{aligned}
\frac{\partial J_c}{\partial t} + \operatorname{div} \left(\frac{J_c \otimes J_c}{n_c} \right) - n_c \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} \right) + n_c (\nabla V_c + \nabla V) &= \\
= \epsilon^2 \nabla K \operatorname{Re} n_{cv} + \epsilon K \operatorname{Re} (n_{cv}(u_v - \bar{u}_c)) - \frac{J_c}{\tau}, & \quad (4.1) \\
\frac{\partial J_v}{\partial t} - \operatorname{div} \left(\frac{J_v \otimes J_v}{n_v} \right) + n_v \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} \right) + n_v (\nabla V_v + \nabla V) &= \\
= \epsilon^2 \nabla K \operatorname{Re} n_{cv} - \epsilon K \operatorname{Re} (n_{cv}(u_v - \bar{u}_c)) - \frac{J_v}{\tau}, & \\
\epsilon \nabla \sigma = \frac{J_v}{n_v} - \frac{J_c}{n_c}, &
\end{aligned}$$

where τ is a relaxation time, which we assume the same for the two bands. As customary in semiconductor theory, we perform the diffusive limit by introducing the scaling

$$t \rightarrow \frac{t}{\tau}, \quad J_c \rightarrow \tau J_c, \quad J_v \rightarrow \tau J_v. \quad (4.2)$$

Consequently, from definition (3.17), the phase difference σ has to be rescaled as

$$\epsilon \nabla \sigma \rightarrow \tau \epsilon \nabla \sigma,$$

and hence

$$\sigma \rightarrow \tau \sigma + \text{constant}.$$

Then, by choosing the constant equal to zero, we have

$$\begin{aligned}
n_{cv} &\rightarrow \sqrt{n_c} \sqrt{n_v} + O(\tau), \\
u_c &\rightarrow \frac{\epsilon \nabla \sqrt{n_c}}{\sqrt{n_c}} + i \frac{J_c}{n_c} \tau, \\
u_v &\rightarrow \frac{\epsilon \nabla \sqrt{n_v}}{\sqrt{n_v}} + i \frac{J_v}{n_v} \tau.
\end{aligned}$$

The coupling term has to be tackled with much care, by writing

$$n_{cv} u_v \rightarrow \sqrt{n_c} \sqrt{n_v} u_{os,v} + i \sqrt{n_c} \sqrt{n_v} (\epsilon \sigma u_{os,v} + u_{el,v}) \tau + O(\tau^2).$$

Formally, as τ tends to zero, after expressing the osmotic and current velocities in terms of the other hydrodynamic quantities, (4.1) reduces to

$$\begin{aligned}
\frac{\partial n_c}{\partial t} + \operatorname{div} J_c &= -2\epsilon \sigma K \sqrt{n_c} \sqrt{n_v}, \\
\frac{\partial n_v}{\partial t} + \operatorname{div} J_v &= 2\epsilon \sigma K \sqrt{n_c} \sqrt{n_v}, \\
J_c &= n_c \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} \right) - n_c (\nabla V_c + \nabla V) + \epsilon^2 \nabla K \sqrt{n_c} \sqrt{n_v} + \\
&\quad + \epsilon^2 K (\sqrt{n_c} \nabla \sqrt{n_v} - \sqrt{n_v} \nabla \sqrt{n_c}), & \quad (4.3) \\
J_v &= -n_v \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} \right) - n_v (\nabla V_v + \nabla V) + \epsilon^2 \nabla K \sqrt{n_c} \sqrt{n_v} + \\
&\quad + \epsilon^2 K (\sqrt{n_v} \nabla \sqrt{n_c} - \sqrt{n_c} \nabla \sqrt{n_v}), \\
\epsilon \nabla \sigma &= \frac{J_v}{n_v} - \frac{J_c}{n_c}.
\end{aligned}$$

This system represents the analog of the zero-temperature, quantum drift-diffusion model for a two-band envelope function system.

5. Conclusions. We can summarize the considerations done during the derivation of our fluidynamical model (3.22), by saying that the two-band envelope function model [8] seems to be more suitable for the formulation of a hydrodynamic system and, consequently, of a drift-diffusion model for a two-band quantum system. As a further confirmation, we remark that in the scaled equations (4.3) the interband current terms have disappeared, making more evident the physical meaning of the model presented. Both the system (3.22) and the its scaled version (4.3) refer to quantum systems described by pure states; however, the procedure can be easily repeated for an appropriate combination of pure states in order to get the corresponding systems for mixed states (cf. [15]). The closure relation chosen is the one proposed for one-band system by Gasser–Markowich [13]; however, a deeper discussion about this problem would be needed and has to be postponed for further investigations. Thus, this contribution is meant to be a preliminary step of a bigger project in which thermal effects will be taken into account as well, and numerical validations will be included.

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