HYDRODYNAMIC MODELS FOR A TWO-BAND NONZERO-TEMPERATURE QUANTUM FLUID

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In this paper a hydrodynamic set of equations is derived from a Schrödinger-like model for the dynamics of electrons in a two-band semiconductor, via the Madelung ansatz. A diffusive scaling allows to attain a drift-diffusion formulation.

1. Introduction

Recent advances in semiconductor devices design have compelled the scientific community to provide theoretical models that take fully into account the quantum dynamics of carriers. For example the Resonant Interband Tunneling Diode (RITD[15]) is built on the quantum effect of tunneling of electrons between conduction and valence bands. Multiband models[11,12] derived from the Schrödinger equation are the starting point of a recent series of articles[3,4,6] that propose a two-band description in terms of Wigner functions. However, in the perspective of numerical simulations, quantum hydrodynamic models[5,7,10] are preferable, since they involve directly macroscopic quantities and they admit natural boundary conditions. The Madelung equations constitute the fluiddynamical equivalent of the Schrödinger equation and they are formally identical to the Euler equations for a perfect fluid at zero temperature, apart for the Bohm potential[9]. Analogously, two-band zero-temperature quantum fluiddynamical models[1,2] can be derived by applying the Madelung ansatz either to the two-band Schrödinger-like model introduced by Kane[11], or to the MEF (Multiband Envelope Function) model[13]; the latter one, at difference with the Kane model, seems to be reliable also in presence of heterostructures and impurities of the semiconductor material. Here, the derivation[2] is extended to the case when the electron ensemble is described by mixed states: Madelung-like equations for each band are recovered, coupled by "interband terms" and containing also temperature terms, as expected by comparison with the single-band mixed-state case[8]. A two-band drift-diffusion system is attained in the zero-relaxation time limit and the equations for each band differ from the QDD[14] only for the coupling interband terms.

2. Nonzero-temperature hydrodynamic model

In order to derive a nonzero-temperature model[8], let us describe an electron ensemble by a mixed quantum state, i.e. by a sequence of pure states constituting an orthonormal basis for the electron ensemble state space, with occupation probabilities $\lambda_k \geq 0, k \in \mathbb{N}_0$, such that $\sum_k \lambda_k = 1$. In a "macroscopic" description[13], a pure state of the system can be individuated by $\{\psi_n\}_{n\in\mathbb{N}_0}$ with ψ_n wave-function of the n-th band and $n(x) = \sum_n |\psi_n|^2(x)$ and $J(x) = \mathrm{Im} \sum_n \overline{\psi_n}(x)\nabla\psi_n(x)$. Since we restrict to a conduction-valence band description, we individuate the k-th pure state by two wave-functions ψ_c^k, ψ_v^k, that are solutions of the (rescaled version of) MeF[13] system

$$\begin{cases} i\epsilon \dfrac{\partial \psi_c^k}{\partial t} = -\dfrac{\epsilon^2}{2}\Delta\psi_c^k + (V_c + V)\psi_c^k - \epsilon^2\, K\, \psi_v^k, \\ i\epsilon \dfrac{\partial \psi_v^k}{\partial t} = \quad \dfrac{\epsilon^2}{2}\Delta\psi_v^k + (V_v + V)\psi_v^k - \epsilon^2\, K\, \psi_c^k, \end{cases} \tag{1}$$

where $K = P \cdot \nabla V$, P is the interband momentum matrix, V is the electrostatic potential, V_c, V_v are the minimum and maximum of the conduction and the valence band energy, respectively, and ϵ is the Planck constant. Then, by using the Madelung ansatz $\psi_b^k = \sqrt{n_b^k}\exp\left(iS_b^k/\epsilon\right)$ with the band-index $b = c, v$, the hydrodynamic system corresponding to Eqs. (1) reads

$$\begin{cases} \dfrac{\partial n_c^k}{\partial t} + \ \mathrm{div} J_c^k = -2\epsilon K\ \mathrm{Im}\, n_{cv}^k, \\ \dfrac{\partial n_v^k}{\partial t} - \ \mathrm{div} J_v^k = \quad 2\epsilon K\ \mathrm{Im}\, n_{cv}^k, \\ \dfrac{\partial J_c^k}{\partial t} + \ \mathrm{div}\left(\dfrac{J_c^k \otimes J_c^k}{n_c^k}\right) - n_c^k \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_c^k}}{2\sqrt{n_c^k}}\right) + n_c^k\nabla V \\ \qquad\qquad = \ \epsilon^2 \nabla K\ \mathrm{Re}\ n_{cv}^k + \epsilon K\ \mathrm{Re}\ \left(n_{cv}^k(u_v^k - \overline{u}_c^k)\right)\ , \\ \dfrac{\partial J_v^k}{\partial t} - \ \mathrm{div}\left(\dfrac{J_v^k \otimes J_v^k}{n_v^k}\right) + n_v^k \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_v^k}}{2\sqrt{n_v^k}}\right) + n_v^k\nabla V \\ \qquad\qquad = \ \epsilon^2 \nabla K\ \mathrm{Re}\ n_{cv}^k - \epsilon K\ \mathrm{Re}\ \left(n_{cv}^k(u_v^k - \overline{u}_c^k)\right)\ , \\ \epsilon\nabla\sigma^k = \dfrac{J_v^k}{n_v^k} - \dfrac{J_c^k}{n_c^k}\,, \end{cases} \tag{2}$$

where $J_b^k = n_b^k \nabla S_b^k$, $u_b^k = \epsilon \nabla \sqrt{n_b^k}/\sqrt{n_b^k} + i\, J_b^k/n_b^k$, $\sigma^k = (S_v^k - S_c^k)/\epsilon$ and $n_{cv}^k = \sqrt{n_c^k}\sqrt{n_v^k}\,\exp(i\sigma^k)$. In the mixed-state description[8], densities and currents corresponding to the bands are $n_b := \sum_k \lambda_k n_b^k$, $J_b := \sum_k \lambda_k J_b^k$, $u_b := \epsilon\nabla\sqrt{n_b}/\sqrt{n_b} + iJ_b/n_b = \epsilon u_{\mathrm{os},b} + i u_{\mathrm{el},b}$, while the "interband" quantities are $\sigma := \sum_k \lambda_k \sigma^k$ and $n_{cv} := \sqrt{n_c}\sqrt{n_v}\exp(i\sigma)$. Observe that we assume V_b to be constant, as in the derivation[13] of Eqs. (1). Multiplying Eqs. (2) by λ_k and summing over k, we find the equations for the hydrodynamic quantities n_b, J_b, and σ

$$\begin{cases} \dfrac{\partial n_c}{\partial t} + \ \mathrm{div} J_c = -2\epsilon K \ \mathrm{Im}\, R_{cv}, \\ \dfrac{\partial n_v}{\partial t} - \ \mathrm{div} J_v = \ \ 2\epsilon K \ \mathrm{Im}\, R_{cv}, \\ \dfrac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\dfrac{J_c \otimes J_c}{n_c} + n_c\theta_c\right) - n_c \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c \nabla V \\ \qquad\qquad = \epsilon^2 \nabla K\, \mathrm{Re}\, R_{cv} + \epsilon^2 K \ \mathrm{Re}\ Q_{cv}, \\ \dfrac{\partial J_v}{\partial t} - \ \mathrm{div}\left(\dfrac{J_v \otimes J_v}{n_v} + n_v\theta_v\right) + n_v \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v \nabla V \\ \qquad\qquad = \epsilon^2 \nabla K\, \mathrm{Re}\, R_{cv} - \epsilon^2 K \ \mathrm{Re}\ Q_{cv}, \\ \epsilon\nabla\sigma = \displaystyle\sum_k \lambda_k \left(\dfrac{J_v^k}{n_v^k} - \dfrac{J_c^k}{n_c^k}\right), \end{cases} \tag{3}$$

with $R_{cv} = \sum_k \lambda_k n_{cv}^k$, $Q_{cv} = \sum_k \lambda_k n_{cv}^k \left(u_v^k - \overline{u_c^k}\right)$. In analogy with the one-band case[8], we introduce the temperatures $\theta_b = \theta_{\mathrm{os},b} + \theta_{\mathrm{el},b}$, $b = c, v$, with the osmotic parts $\theta_{\mathrm{os},b}$ defined by

$$\theta_{\mathrm{os},b} = \sum_k \lambda_k \frac{n_b^k}{n_b} (u_{\mathrm{os},b}^k - u_{\mathrm{os},b}) \otimes (u_{\mathrm{os},b}^k - u_{\mathrm{os},b})$$

and the current temperatures $\theta_{\mathrm{el},b}$ defined correspondingly. If we call

$$\alpha := \sum_k \lambda_k \frac{n_{cv}^k}{n_{cv}}, \quad \beta_v := \sum_k \lambda_k \frac{n_{cv}^k}{n_{cv}} (u_v^k - u_v), \quad \beta_c := \sum_k \lambda_k \frac{\overline{n_{cv}^k}}{\overline{n_{cv}}} (u_c^k - u_c),$$

the coupling terms contain $R_{cv} = \alpha n_{cv}$, $Q_{cv} = n_{cv}\left[\alpha(u_v - \overline{u_c}) + \beta_v - \overline{\beta_c}\right]$. In order to find a relation between α, β_v and β_c and the hydrodynamic quantities, we take the gradient of α and use the definition of n_{cv}, u_c, u_v and the identity

$$\frac{\epsilon\nabla n_{cv}}{n_{cv}} - u_v - \overline{u_c} = i\left(\epsilon\nabla\sigma - \frac{J_v}{n_v} + \frac{J_c}{n_c}\right).$$

Accordingly

$$\epsilon\nabla\sigma - \frac{J_v}{n_v} + \frac{J_c}{n_c} = \frac{i}{\alpha}\left(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\right) . \tag{4}$$

The last equation of system (3) can be rephrased as

$$\epsilon\nabla\sigma = \frac{J_v}{n_v} - \frac{J_c}{n_c} + \sum_k \lambda_k \left(\frac{J_v^k}{n_v^k} - \frac{J_v}{n_v}\right) - \sum_k \lambda_k \left(\frac{J_c^k}{n_c^k} - \frac{J_c}{n_c}\right) \tag{5}$$

and, by comparison of (4) with (5), we get

$$\sum_k \lambda_k \left(\frac{J_v^k}{n_v^k} - \frac{J_v}{n_v}\right) - \sum_k \lambda_k \left(\frac{J_c^k}{n_c^k} - \frac{J_c}{n_c}\right) = \frac{i}{\alpha}\left(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\right) ,$$

then $\mathrm{Re}\left\{\left(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\right)/\alpha\right\} = 0$. Accordingly, Eqs. (3) can be written as

$$\begin{cases} \dfrac{\partial n_c}{\partial t} + \ \mathrm{div} J_c = -2\epsilon K \ \mathrm{Im}\,(\alpha n_{cv}), \\ \dfrac{\partial n_v}{\partial t} - \ \mathrm{div} J_v = \quad 2\epsilon K \ \mathrm{Im}\,(\alpha n_{cv}), \\ \dfrac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\dfrac{J_c \otimes J_c}{n_c} + n_c\theta_c\right) - n_c\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c\nabla V \\ \qquad = \epsilon^2\nabla K \ \mathrm{Re}\,(\alpha n_{cv}) + \epsilon^2 K \ \mathrm{Re}\,\left(n_{cv}\left[\alpha(u_v - \overline{u_c}) + \beta_v - \overline{\beta_c}\right]\right), \\ \dfrac{\partial J_v}{\partial t} - \ \mathrm{div}\left(\dfrac{J_v \otimes J_v}{n_v} + n_v\theta_v\right) + n_v\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v\nabla V \\ \qquad = \epsilon^2\nabla K \ \mathrm{Re}\,(\alpha n_{cv}) - \epsilon^2 K \ \mathrm{Re}\,\left(n_{cv}\left[\alpha(u_v - \overline{u_c}) + \beta_v - \overline{\beta_c}\right]\right), \\ \epsilon\nabla\sigma - \dfrac{J_v}{n_v} + \dfrac{J_c}{n_c} = - \ \mathrm{Im}\left\{\dfrac{1}{\alpha}\left(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\right)\right\}. \end{cases} \tag{6}$$

The terms on the right hand side of the equations determine the coupling. The system is not closed: the quantities α, β_c and β_v are not expressed in terms of the hydrodynamic quantites, but they are linked by

$$\mathrm{Re}\left\{\left(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\right)/\alpha\right\} = 0. \tag{7}$$

In addition, we must assign constitutive relations for the tensors θ_c and θ_v. A simple class of closure conditions can be obtained by assuming $\alpha = \alpha(n_c, n_v, \sigma)$ and taking

$$\beta_c = 2n_c\frac{\partial\bar\alpha}{\partial n_c}u_{\mathrm{os},c} - \frac{\partial\bar\alpha}{\partial\sigma}u_{\mathrm{el},c}, \quad \beta_v = 2n_v\frac{\partial\alpha}{\partial n_v}u_{\mathrm{os},v} + \frac{\partial\alpha}{\partial\sigma}u_{\mathrm{el},v}. \tag{8}$$

Then $\epsilon\nabla\alpha - \beta_v - \overline{\beta_c} = 0$, thus Eq. (7) is fulfilled and moreover $\epsilon\nabla\sigma - J_v/n_v + J_c/n_c = 0$. For the temperatures we assume $n_b\theta_b = p_b(n_b)I$, where I is the identity tensor and the functions p_c, p_v are pressures. In particular, we can take $p_b = \theta^0 n_b$, as for an ideal gas in isothermal conditions, and $\alpha = 1, \beta_c = \beta_v = 0$ (which follows, e.g., from $n_{cv}^k \simeq n_{cv}$). Accordingly, we obtain the simplest two-band isothermal QHD model

$$\begin{cases} \dfrac{\partial n_c}{\partial t} + \ \mathrm{div} J_c = -2\epsilon K \ \mathrm{Im}\, n_{cv}, \\ \dfrac{\partial n_v}{\partial t} - \ \mathrm{div} J_v = \quad 2\epsilon K \ \mathrm{Im}\, n_{cv}\,, \\ \dfrac{\partial J_c}{\partial t} + \ \mathrm{div} \dfrac{J_c \otimes J_c}{n_c} + \theta^0 \nabla n_c - n_c \nabla \left(\dfrac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} - V \right) \\ \qquad\qquad = \epsilon^2 \nabla K \ \mathrm{Re}\ n_{cv} + \epsilon^2 K \ \mathrm{Re}\ (n_{cv} \,(u_v - \overline{u_c})), \\ \dfrac{\partial J_v}{\partial t} - \ \mathrm{div} \dfrac{J_v \otimes J_v}{n_v} + \theta^0 \nabla n_v + n_v \nabla \left(\dfrac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} + V \right) \\ \qquad\qquad = \epsilon^2 \nabla K \ \mathrm{Re}\ n_{cv} - \epsilon^2 K \ \mathrm{Re}\ (n_{cv} \,(u_v - \overline{u_c})), \\ \epsilon \nabla \sigma - \dfrac{J_v}{n_v} + \dfrac{J_c}{n_c} = 0\,. \end{cases} \tag{9}$$

Here, the only peculiarity of the mixed-state case is the presence of the temperature terms.

3. The drift-diffusion model

Now we perform the zero-relaxation time limit of the hydrodynamic models recovered. First, we start from Eqs. (9), we add relaxation terms for the currents and we introduce the diffusive scaling

$$t \to \frac{t}{\tau}, \quad J_c \to \tau J_c, \quad J_v \to \tau J_v, \tag{10}$$

that leads to the ansatz $\sigma \to \sigma_0 + \tau\sigma$, where σ_0 is a constant phase to be determined. In the limit $\tau \to 0$ the system reads

$$\begin{cases} \dfrac{\partial n_c}{\partial t} + \ \mathrm{div} J_c = -2\epsilon K \sqrt{n_c}\sqrt{n_v}\sigma, \\ \dfrac{\partial n_v}{\partial t} - \ \mathrm{div} J_v = \quad 2\epsilon K \sqrt{n_c}\sqrt{n_v}\sigma, \\ J_c = -\,\theta^0 \nabla n_c + n_c \left\{ \nabla \left[\dfrac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} - V + \epsilon^2 \dfrac{\sqrt{n_v}}{\sqrt{n_c}} K \right] \right\}, \\ J_v = \quad \theta^0 \nabla n_v - n_v \left\{ \nabla \left[\dfrac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} + V - \epsilon^2 \dfrac{\sqrt{n_c}}{\sqrt{n_v}} K \right] \right\}, \\ \epsilon \nabla \sigma - \dfrac{J_v}{n_v} + \dfrac{J_c}{n_c} = 0, \end{cases} \tag{11}$$

where $\sigma_0 = 0$, due to the limit of the first equation. Alternatively, we start from the isothermal version of the Eqs. (6), closed with $\alpha = \alpha(n_c, n_v)$, $\beta_c := 2n_c \frac{\partial \overline{\alpha}}{\partial n_c} u_{\mathrm{os},c}$, $\beta_v := 2n_v \frac{\partial \alpha}{\partial n_v} u_{\mathrm{os},v}$, we add relaxation terms for the currents and we consider the diffusive scaling in Eq. (10), with $\sigma_0 = 0$. In the limit $\tau \to 0$, we get $\mathrm{Im}\ \alpha = 0$ and the isothermal QDD system reads

$$\begin{cases} \dfrac{\partial n_c}{\partial t} + \ \mathrm{div} J_c = -2\epsilon K \sqrt{n_c}\sqrt{n_v}\alpha\sigma, \\ \dfrac{\partial n_v}{\partial t} - \ \mathrm{div} J_v = \ \ 2\epsilon K \sqrt{n_c}\sqrt{n_v}\alpha\sigma, \\ J_c = -\theta^0 \nabla n_c + n_c \left\{ \nabla \left[\dfrac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} - V \right] + \epsilon^2 \alpha \nabla \left[\dfrac{\sqrt{n_v}}{\sqrt{n_c}} K \right] \right\} + \\ \qquad\qquad + \epsilon^2 (\beta_v - \beta_c) \sqrt{n_v}\sqrt{n_c} K, \\ J_v = \ \ \theta^0 \nabla n_v - n_v \left\{ \nabla \left[\dfrac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} + V \right] - \epsilon^2 \alpha \nabla \left[\dfrac{\sqrt{n_c}}{\sqrt{n_v}} K \right] \right\} + \\ \qquad\qquad - \epsilon^2 (\beta_v - \beta_c) \sqrt{n_c}\sqrt{n_v} K, \\ \epsilon \nabla \sigma - \dfrac{J_v}{n_v} + \dfrac{J_c}{n_c} = 0. \end{cases}$$

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