

On the zero-temperature quantum hydrodynamic model for the two-band Kane system

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In this paper we derive a hydrodynamic formulation of the following scaled Kane system [1, 2]:

$$\begin{cases} i\epsilon \frac{\partial \psi_c}{\partial t} &= -\frac{\epsilon^2}{2} \Delta \psi_c + V_c \psi_c - \epsilon^2 P \cdot \nabla \psi_v, \\ i\epsilon \frac{\partial \psi_v}{\partial t} &= -\frac{\epsilon^2}{2} \Delta \psi_v + V_v \psi_v + \epsilon^2 P \cdot \nabla \psi_c, \end{cases} \quad (1)$$

where $\psi_c(x, t)$ and $\psi_v(x, t)$ are the conduction and valence band electron envelope functions, the space variable $x \in \mathbb{R}^3$, i is the imaginary unit, ϵ is the rescaled Planck constant, V_c and V_v are the minimum of the rescaled conduction band energy and maximum of the rescaled valence band energy respectively, and P is the coupling coefficient between the two bands given by the matrix element of the gradient operator between the Bloch functions. The Kane model is a simple two-band model for describing the electron dynamics in a material where the tunneling across potential barriers between different bands has to be taken into account. Such a model is of great importance for Resonant Interband Tunneling Diode (RITD), whose properties differ from other devices because of the role played by the valence band electrons [3]. This model, firstly proposed by E.O. Kane in 1956 [1], is widely used in literature. The Kane model, obtained in the frame of the envelope function theory, consists into a couple of Schrödinger-like equations for the conduction and the valence band envelope functions.

In this paper we apply the WKB method, which is a classical way to write the Schrödinger equation in hydrodynamic form. It consists in characterizing the wave function with a quasi-classical limit expression $a \exp\left(\frac{iS}{\epsilon}\right)$, where a is called the amplitude and S/ϵ the phase of the wave.

Another approach to face the problem of a quantum hydrodynamic model is based on the formulation of the Kane model in terms of Wigner functions [4]. The reader interested in quantum hydrodynamic modeling can refer to the papers quoted in the book by Jünger [5].

In our case, we look for solutions of the rescaled system (1) in the form

$$\psi_j(x, t) = \sqrt{n_j(x, t)} \exp\left(\frac{iS_j(x, t)}{\epsilon}\right), \quad j = c, v. \quad (2)$$

The squared amplitude is interpreted as 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 frame of the two band Kane model, we introduce the particle densities

$$n_{ij} = \bar{\psi}_i \psi_j$$

where ψ_i , with $i = c, v$ are the envelope function for the conduction and the valence band. When $i = j$, quantities n_{ij} are real and represent the quantum probability densities for the position of conduction band and valence band electron only in an approximate sense, because ψ_i are envelope functions which mix the Bloch states. Nevertheless, $\rho = \bar{\psi}_c \psi_c + \bar{\psi}_v \psi_v$ is exactly the electron density in conduction and valence band. Moreover we introduce the complex quantity $n_{cv} := \bar{\psi}_c \psi_v = \sqrt{n_c} \sqrt{n_v} e^{i\sigma}$, with $\sigma := \frac{S_v - S_c}{\epsilon}$.

Then we define quantum mechanical electron current densities

$$J_{ij} = \epsilon \operatorname{Im} (\bar{\psi}_i \nabla \psi_j) .$$

When $i = j$, still using the form (2), we recover the classical current densities

$$J_c := \operatorname{Im} (\epsilon \bar{\psi}_c \nabla \psi_c) = n_c \nabla S_c, \quad J_v := \operatorname{Im} (\epsilon \bar{\psi}_v \nabla \psi_v) = n_v \nabla S_v.$$

Also, we introduce the complex velocities u_c and u_v , with

$$u_c = u_{\text{os},c} + i u_{\text{el},c} := \frac{\epsilon \nabla \sqrt{n_c}}{\sqrt{n_c}} + i \nabla S_c, \quad u_v = u_{\text{os},v} + i u_{\text{el},v} := \frac{\epsilon \nabla \sqrt{n_v}}{\sqrt{n_v}} + i \nabla S_v.$$

The real and imaginary part of u_c and u_v are named osmotic velocities and current velocities, respectively, and each one can be expressed in terms of n_c , J_c and n_v , J_v . It is easy to verify that, as hydrodynamic quantities for a zero-temperature quantum hydrodynamic system, it is sufficient to choose the usual quantities n_c , n_v , J_c and J_v , plus the phase difference σ .

The equations for the particle densities n_c and n_v read as follows

$$\begin{cases} \frac{\partial n_c}{\partial t} + \nabla \cdot J_c = -2 \operatorname{Im} (n_{cv} P \cdot u_v), \\ \frac{\partial n_v}{\partial t} + \nabla \cdot J_v = 2 \operatorname{Im} (\bar{n}_{cv} P \cdot u_c). \end{cases} \quad (3)$$

where, by means of the definitions of osmotic and current velocities, we have used $\epsilon \bar{\psi}_c \nabla \psi_v = n_{cv} u_v$ and $\epsilon \bar{\psi}_v \nabla \psi_c = \bar{n}_{cv} u_c$. Summing the equations in (3), we obtain the balance law for the total density (continuity equation)

$$\frac{\partial}{\partial t} (n_c + n_v) + \nabla \cdot (J_c + J_v + 2\epsilon P \operatorname{Im} n_{cv}) = 0.$$

Moreover the resulting system for the currents takes the following form

$$\left\{ \begin{array}{l} \frac{\partial J_c}{\partial t} + \operatorname{div} \left(\frac{J_c \otimes J_c}{n_c} \right) - n_c \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} \right) + n_c \nabla V_c \\ \qquad \qquad \qquad = \epsilon \nabla \operatorname{Re} (n_{cv} P \cdot u_v) - 2 \operatorname{Re} (n_{cv} P \cdot u_v \bar{u}_c), \\ \\ \frac{\partial J_v}{\partial t} + \operatorname{div} \left(\frac{J_v \otimes J_v}{n_v} \right) - n_v \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} \right) + n_v \nabla V_v \\ \qquad \qquad \qquad = -\epsilon \nabla \operatorname{Re} (\bar{n}_{cv} P \cdot u_c) - 2 \operatorname{Re} (\bar{n}_{cv} P \cdot u_c \bar{u}_v). \end{array} \right. \quad (4)$$

In order to close the system and to obtain an extension of the classical Madelung fluid equations, we can add the following elliptic equation for σ ,

$$\epsilon \Delta \sigma = \nabla \cdot \left(\frac{J_v}{n_v} - \frac{J_c}{n_c} \right). \quad (5)$$

Introducing a suitable diffusive scaling and performing the relaxation-time limit, we derive the drift-diffusion equations corresponding to the zero temperature system (3)-(4)-(5). Finally, considering mixed states, we obtain the nonzero temperature hydrodynamic model.

The results presented in this paper are obtained only formally and a more appropriate mathematical investigation is devoted to a future work.

References

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