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

Giuseppe Alì
Istituto per le Applicazioni del Calcolo
CNR - 80131 Napoli

Giovanni Frosali
Dip. di Matematica Applicata "G.Sansone"
Università di Firenze - 50139 Firenze

Physical description of the KANE MODEL.

The Kane model consists into a couple of Schrödinger-like equations for the conduction and the valence band envelope functions.

Let $\psi_c(x,t)$ be the conduction band electron envelope function and $\psi_v(x,t)$ be the valence band electron envelope function

$$\begin{cases} i\hbar\dfrac{\partial\psi_c}{\partial t} = -\dfrac{\hbar^2}{2m}\Delta\psi_c + V_c\psi_c - \dfrac{\hbar^2}{m}P\cdot\nabla\psi_v \\[2ex] i\hbar\dfrac{\partial\psi_v}{\partial t} = -\dfrac{\hbar^2}{2m}\Delta\psi_v + V_v\psi_v + \dfrac{\hbar^2}{m}P\cdot\nabla\psi_v \end{cases}$$

- m is the bare mass of the carriers,
- V_c (V_v) is the minimum (maximum) of the conduction (valence) band energy
- P is the coupling coefficient between the two bands (the matrix element of the gradient operator between the Bloch functions)

SCALING

In order to rewrite the Kane system in a dimensionless form, we introduce the rescaled Planck constant

$$\epsilon = \frac{\hbar}{\alpha} \quad \text{where} \quad \alpha = \frac{m x_R^2}{t_R}$$

by using x_R and t_R as characteristic (scalar) lenght and time variables.

We rescale $t' = \frac{t}{t_R}$, $x' = \frac{x}{x_R}$

and we leave the mass m unchanged. The band energy can be rescaled, taking new potential units $V_0 = \frac{m x_R^2}{t_R^2}$.

The original coupling coefficient is a reciprocal of a characteristic lenght

$$P' = P x_R$$

.

THE SCALED KANE SYSTEM

$$\begin{cases} i\epsilon \dfrac{\partial \psi_c}{\partial t} &= -\dfrac{\epsilon^2}{2}\Delta\psi_c + V_c\psi_c - \epsilon^2 P\cdot\nabla\psi_v\,, \\ i\epsilon \dfrac{\partial \psi_v}{\partial t} &= -\dfrac{\epsilon^2}{2}\Delta\psi_v + V_v\psi_v + \epsilon^2 P\cdot\nabla\psi_c\,. \end{cases}$$

- **WIGNER APPROACH**

- **HYDRODYNAMIC APPROACH**

The first aim of this paper is to derive the **hydrodynamic version** of the Kane system using the WKB method.

Using this approach the hydrodynamic limit is valid only for pure states, (quantum system at zero temperature).

The HYDRODYNAMIC quantities

Look for solutions in the form

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

We introduce the particle densities

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

Then $n = \overline{\psi}_c \psi_c + \overline{\psi}_v \psi_v$ is exactly the electron density in conduction and valence bands.

It is natural to write the coupling terms in a more manageable way, introducing the complex quantity

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

with

$$\sigma := \frac{S_v - S_c}{\epsilon}.$$

We define quantum mechanical electron current densities

$$J_{ij} = \epsilon \text{ Im } \left(\overline{\psi}_i \nabla \psi_j\right) .$$

When $i = j$, we recover the classical current densities

$$J_c := \text{ Im } \left(\epsilon \overline{\psi}_c \nabla \psi_c\right) = n_c \nabla S_c,$$
$$J_v := \text{ Im } \left(\epsilon \overline{\psi}_v \nabla \psi_v\right) = n_v \nabla S_v \,.$$

It is easy to get

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

We introduce the **complex velocities**

$$u_c := \frac{\epsilon\nabla\psi_c}{\psi_c} = \frac{\epsilon\nabla\sqrt{n_c}}{\sqrt{n_c}} + i\nabla S_c,$$
$$u_v := \frac{\epsilon\nabla\psi_v}{\psi_v} = \frac{\epsilon\nabla\sqrt{n_v}}{\sqrt{n_v}} + i\nabla S_v.$$

We name the real and imaginary part of u_c **osmotic velocity and current velocity** respectively:

$$u_{\mathrm{os},i} := \frac{\epsilon \nabla \sqrt{n_i}}{\sqrt{n_i}}, \qquad u_{\mathrm{el},i} := \nabla S_i = \frac{J_i}{n_i}. \quad i = c, v\,, \tag{9}$$

so that

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

Hence osmotic velocity and current velocity can be expressed in terms of n_c, n_v, J_c and J_v.

CHOICE of the hydrodynamic quantities:

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**.**

HYDRODYNAMIC formulation of the Kane model

Taking account of the wave form and using the first equation of the Kane system, we find

$$\begin{aligned} \frac{\partial n_c}{\partial t} &= \overline{\psi}_c \frac{\partial \psi_c}{\partial t} + \psi_c \frac{\partial \overline{\psi}_c}{\partial t} \\ &= -\nabla \cdot \text{ Im } \left(\epsilon \overline{\psi}_c \nabla \psi_c \right) - 2P \cdot \text{ Im } \left(\epsilon \overline{\psi}_c \nabla \psi_v \right). \end{aligned}$$

Analogously for $\frac{\partial n_v}{\partial t}$.

Then, the previous equations become

$$\begin{cases} \dfrac{\partial n_c}{\partial t} + \nabla \cdot J_c = -2P \cdot \text{ Im } \left(\epsilon \overline{\psi}_c \nabla \psi_v \right) \\ \dfrac{\partial n_v}{\partial t} + \nabla \cdot J_v = \quad 2P \cdot \text{ Im } \left(\epsilon \overline{\psi}_v \nabla \psi_c \right) \end{cases} \tag{10}$$

and using the definitions of osmotic and current velocities:

$$\begin{aligned}\epsilon\overline{\psi}_c \nabla\psi_v &= n_{cv} u_v \\ &= \sqrt{n_c}\sqrt{n_v}\,(\cos\sigma + i\sin\sigma)(u_{\mathrm{os},v} + i u_{\mathrm{el},v})\end{aligned}$$

we have

$$\begin{cases} \dfrac{\partial n_c}{\partial t} + \nabla\cdot J_c = -2\ \mathrm{Im}\ (n_{cv} P\cdot u_v) \\ \dfrac{\partial n_v}{\partial t} + \nabla\cdot J_v = \quad 2\ \mathrm{Im}\ (\overline{n}_{cv} P\cdot u_c)\ , \end{cases} \tag{12}$$

Summing the equations in (12), we obtain the **balance law**

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

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

Next, we derive equations for **phases** S_c, S_v, obtaining a system equivalent to the coupled Schrödinger equations.

To obtain a system of coupled equations for the **currents**, we get

$$\frac{\partial J_c}{\partial t} = \sum_j \frac{\epsilon^2}{2}\frac{\partial}{\partial x_j} \text{ Re}\left(\overline{\psi}_c \nabla \frac{\partial \psi_c}{\partial x_j} - \nabla \psi_c \frac{\partial \overline{\psi}_c}{\partial x_j}\right) - \overline{\psi}_c \psi_c \nabla V_c$$

$$+\epsilon^2 \text{ Re}\left[\overline{\psi}_c \nabla (P \cdot \nabla \psi_v) - \nabla \psi_c (P \cdot \nabla \overline{\psi}_v)\right].$$

(similar equation for J_v).

The left-hand sides of such equations can be put in a more familiar form introducing the Bohm potentials for each band

$$\text{div}\left(\nabla\sqrt{n_i} \otimes \nabla\sqrt{n_i} - \frac{1}{4}\nabla \otimes \nabla n_i\right) = -\frac{n_i}{2}\nabla\left[\frac{\Delta\sqrt{n_i}}{\sqrt{n_i}}\right],$$

The correction terms $\dfrac{\epsilon^2}{2}\dfrac{\Delta\sqrt{n_i}}{\sqrt{n_i}} \quad i = c, v$, can be called the **quantum Bohm potential** for each band.

Moreover the right-hand sides of the previous equations can be expressed in terms of the hydrodynamic quantities, using the following relations for $i, j = c, v$

$$\begin{array}{rcl} \epsilon\,\overline{\psi}_i(P\cdot\nabla\psi_j) & = & n_{ij}\,P\cdot u_j \\ \epsilon^2\nabla\overline{\psi}_i(P\cdot\nabla\psi_j) & = & n_{ij}\,P\cdot u_j\,\overline{u_i}\,. \end{array}$$

Finally the resulting system takes the following form

$$\left\{ \begin{array}{l} \dfrac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\dfrac{J_c\otimes J_c}{n_c}\right) - n_c\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c\nabla V_c \\ \qquad\qquad\qquad = \ \ \epsilon\nabla\ \mathrm{Re}\ (n_{cv}P\cdot u_v) - 2\ \mathrm{Re}\ (n_{cv}P\cdot u_v\overline{u}_c)\,, \\ \\ \dfrac{\partial J_v}{\partial t} + \ \mathrm{div}\left(\dfrac{J_v\otimes J_v}{n_v}\right) - n_v\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v\nabla V_v \\ \qquad\qquad\qquad = -\epsilon\nabla\ \mathrm{Re}\ (\overline{n}_{cv}P\cdot u_c) + 2\ \mathrm{Re}\ (\overline{n}_{cv}P\cdot u_c\overline{u}_v)\,. \end{array} \right. \tag{13}$$

It is important to notice that, differently from the uncoupled model, (12) and (13) are not equivalent to the original equations, **due to the presence of** σ.

There are many ways to "close" the system, in order to obtain an extension of the classical Madelung fluid equations to a **two-band quantum fluids** .

(12) and (13) can be supplemented with the constraint

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

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

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

n_{cv}, u_v, and u_v are given by the hydrodynamic quantities n_c, n_v, J_c, J_v, and σ.

The DRIFT-DIFFUSIVE scaling

It is customary to introduce a relaxation time term in order to simulate all the mechanisms which force the system towards the statistical mechanical equilibrium.

We rewrite the current equations in the previous system as

$$\begin{cases} \dfrac{\partial J_c}{\partial t} + \text{ div}\left(\dfrac{J_c \otimes J_c}{n_c}\right) - n_c \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c \nabla V_c \\ \qquad\qquad = \quad \epsilon \nabla \text{ Re}\left(n_{cv} P \cdot u_v\right) - 2 \text{ Re}\left(n_{cv} P \cdot u_v \overline{u}_c\right) - \dfrac{J_c}{\tau}, \\ \dfrac{\partial J_v}{\partial t} + \text{ div}\left(\dfrac{J_v \otimes J_v}{n_v}\right) - n_v \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v \nabla V_v \\ \qquad\qquad = -\epsilon \nabla \text{ Re}\left(\overline{n}_{cv} P \cdot u_c\right) + 2 \text{ Re}\left(\overline{n}_{cv} P \cdot u_c \overline{u}_v\right) - \dfrac{J_v}{\tau}, \end{cases} \tag{16}$$

where τ is a relaxation time, which we assume equal for the two bands.

In analogy with the **classical diffusive limit** for a one-band system, we introduce the scaling

$$t \to \frac{t}{\tau}, \qquad J_c \to \tau J_c, \qquad J_v \to \tau J_v\,. \tag{17}$$

Consequently, the phase difference has to rescaled in a such way that

$$\sigma \to \tau\sigma\,.$$

Then, we have

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

Moreover, the coupling terms has to be tackled with much care, as follows

$$n_{cv} P\cdot u_v \to \sqrt{n_c}\sqrt{n_v} P \cdot u_{os,v} + i\sqrt{n_c}\sqrt{n_v}\left(\sigma P \cdot u_{os,v} + P \cdot u_{el,v}\right)\tau + O(\tau^2).$$

Formally, as τ tends to zero, the hydrodynamic system with the current equations (16) reduces to

$$\begin{cases} \dfrac{\partial n_c}{\partial t} + \mathrm{div} J_c = -2\sqrt{n_c}\sqrt{n_v}\left(\sigma P \cdot u_{os,v} + P \cdot u_{el,v}\right), \\ \dfrac{\partial n_v}{\partial t} + \mathrm{div} J_v = -2\sqrt{n_c}\sqrt{n_v}\left(\sigma P \cdot u_{os,c} - P \cdot u_{el,c}\right), \\ J_c = n_c \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) - n_c \nabla V_c + \epsilon\,\nabla\left(\sqrt{n_c}\sqrt{n_v} P \cdot u_{os,v}\right) - 2\sqrt{n_c}\sqrt{n_v} P\cdot u_{os,v} u_{os,c}, \\ J_v = n_v \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) - n_v \nabla V_v - \epsilon\nabla\left(\sqrt{n_c}\sqrt{n_v} P \cdot u_{os,c}\right) + 2\sqrt{n_c}\sqrt{n_v} P\cdot u_{os,c} u_{os,v} \\ \epsilon\nabla\sigma = \dfrac{J_v}{n_v} - \dfrac{J_c}{n_c}. \end{cases} \tag{19}$$

Finally, after having expressed the osmotic and current velocities, in terms of the other hydrodynamic quantities, we have

$$\begin{cases} \dfrac{\partial n_c}{\partial t} + \mathrm{div} J_c = -2\epsilon\sigma\sqrt{n_c} P \cdot \nabla\sqrt{n_v} - 2\dfrac{\sqrt{n_c}}{\sqrt{n_v}} P \cdot J_v, \\ \dfrac{\partial n_v}{\partial t} + \mathrm{div} J_v = -2\epsilon\sigma\sqrt{n_v} P \cdot \nabla\sqrt{n_c} + 2\dfrac{\sqrt{n_v}}{\sqrt{n_c}} P \cdot J_c, \\ J_c = n_c \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) - n_c \nabla V_c + \epsilon^2 \nabla\left(\sqrt{n_c} P \cdot \nabla\sqrt{n_v}\right) - 2\epsilon^2 P \cdot \nabla\sqrt{n_v} \nabla\sqrt{n_c}\,, \\ J_v = n_v \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) - n_v \nabla V_v - \epsilon^2 \nabla\left(\sqrt{n_v} P \cdot \nabla\sqrt{n_c}\right) + 2\epsilon^2 P \cdot \nabla\sqrt{n_c} \nabla\sqrt{n_v} \\ \epsilon\nabla\sigma = \dfrac{J_v}{n_v} - \dfrac{J_c}{n_c}\,. \end{cases} \tag{20}$$

This system represents the zero-temperature **QUANTUM DRIFT-DIFFUSION MODEL** for a Kane system.

NONZERO TEMPERATURE hydrodynamic model

We consider an electron ensemble which is represented by a mixed quantum mechanical state, with a view to obtaining a nonzero temperature model for a Kane system. A mixed state is a sequence of single states with occupation probabilities $\lambda_k, k = 0, 1, 2, \ldots \; k \in \mathbb{N}$ for the $k-$th single state.

The $k-$th state for the Kane system is described by the solutions of the system

$$\left\{ \begin{array}{lcl} i\epsilon \dfrac{\partial \psi_c^k}{\partial t} & = & -\dfrac{\epsilon^2}{2}\Delta \psi_c^k + V_c \psi_c^k - \epsilon^2 P \cdot \nabla \psi_v^k \,, \\ i\epsilon \dfrac{\partial \psi_v^k}{\partial t} & = & -\dfrac{\epsilon^2}{2}\Delta \psi_v^k + V_v \psi_v^k + \epsilon^2 P \cdot \nabla \psi_c^k \,. \end{array} \right. \tag{21}$$

Using the **Madelung-type transform**, under the assumption of positivity of the densities n_c^k and n_v^k,

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

the previous system is equivalent to

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

we define

$$J_i^k = n_i^k \nabla S_i^k, \quad \sigma^k = \frac{S_v^k - S_c^k}{\epsilon},$$

$$n_{cv}^k = \sqrt{n_c^k}\sqrt{n_v^k}\,\mathsf{exp}\left(i\sigma^k\right), \quad u_i^k = \frac{\epsilon\nabla\sqrt{n_i^k}}{\sqrt{n_i^k}} + i\frac{J_i^k}{n_i^k}.$$

The densities and the currents corresponding to the two mixed states can be defined as

$$n_i := \sum_{k=0}^{\infty} \lambda_k n_i^k, \quad J_i := \sum_{k=0}^{\infty} \lambda_k J_i^k\,.$$

We also define

$$\sigma := \sum_{k=0}^{\infty} \lambda_k \sigma^k, \quad n_{cv} := \sqrt{n_c}\sqrt{n_v}\,\mathsf{exp}(i\sigma), \quad u_i := \frac{\epsilon\nabla\sqrt{n_i}}{\sqrt{n_i}} + i\frac{J_i}{n_c}.$$

Multiplying by λ_k and summing over k, we find

$$
\left\{
\begin{aligned}
&\frac{\partial n_c}{\partial t} + \mathrm{div} J_c = -2 \ \mathrm{Im}\ R_c, \\
&\frac{\partial n_v}{\partial t} + \mathrm{div} J_v = \quad 2 \ \mathrm{Im}\ R_v, \\
&\frac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\frac{J_c \otimes J_c}{n_c} + n_c \theta_c\right) - n_c \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c \nabla V_c \\
&\qquad\qquad\qquad\qquad\qquad\qquad = \quad \epsilon \nabla \ \mathrm{Re}\, R_c - 2P\cdot \ \mathrm{Re}\ Q_{cv}, \\
&\frac{\partial J_v}{\partial t} + \ \mathrm{div}\left(\frac{J_v \otimes J_v}{n_v} + n_v \theta_v\right) - n_v \nabla \left(\frac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v \nabla V_v \\
&\qquad\qquad\qquad\qquad\qquad\qquad = -\epsilon \nabla \ \mathrm{Re}\, R_v + 2P\cdot \ \mathrm{Re}\ Q_{vc}, \\
&\epsilon \Delta \sigma = \nabla \left(\sum_{k=0}^{\infty} \lambda_k \left(\frac{J_v^k}{n_v^k} - \frac{J_c^k}{n_c^k} \right) \right) \ ,
\end{aligned}
\right.
\tag{23}
$$

with

$$R_i = \sum_{k=0}^{\infty} \lambda_k n_{ij}^k P \cdot u_j^k, \qquad Q_{ij} = \sum_{k=0}^{\infty} \lambda_k \overline{n_{ij}^k} u_j^k \otimes \overline{u_j^k}, \quad i,j = c,v.$$

Analogously with the one-band case, new terms containing the total temperature θ_c and θ_v, for each band, appear.

The temperature tensors $\theta_c = \theta_{os,c} + \theta_{el,c}$ and $\theta_v = \theta_{os,v} + \theta_{el,v}$ are the sum of osmotic temperature and electron current temperature,

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

We write

$$R_c = P \cdot n_{cv}(\alpha u_v + \beta_v), \qquad R_v = P \cdot \overline{n_{cv}}(\overline{\alpha}\, u_c + \beta_c), \tag{24}$$

with

$$\alpha := \sum_{k=0}^{\infty} \lambda_k \frac{n_{cv}^k}{n_{cv}}, \qquad \beta_i := \sum_{k=0}^{\infty} \lambda_k \frac{n_{ij}^k}{n_{ij}} (u_i^k - u_i), \quad i, j = c, v.$$

These quantities are not independent:

$$\frac{1}{i\alpha}\left(\epsilon \nabla \alpha - \beta_v - \overline{\beta_c}\right) = -\epsilon \nabla \sigma + \frac{J_v}{n_v} - \frac{J_c}{n_c},$$

Next, in order to obtain an expression of the coupling terms between the two bands by a sort of temperature tensors, we write

$$\begin{aligned} Q_{cv} &= n_{cv} \left(\alpha u_v \otimes \overline{u_c} + \beta_v \otimes \overline{u_c} + u_v \otimes \overline{\beta_c} + \theta_{cv}\right), \\ Q_{vc} &= \overline{n_{cv}} \left(\overline{\alpha} u_c \otimes \overline{u_v} + \beta_c \otimes \overline{u_v} + u_c \otimes \overline{\beta_v} + \theta_{vc}\right), \end{aligned}$$

with

$$\theta_{cv} := \sum_{k=0}^{\infty} \lambda_k \frac{n_{cv}^k}{n_{cv}} (u_v^k - u_v) \otimes (\overline{u_c^k} - \overline{u_c}),$$

In conclusion, using the new quantities defined above, system (23) can be written as

$$
\begin{cases}
\dfrac{\partial n_c}{\partial t} + \mathrm{div} J_c = -\,2P\cdot\ \mathrm{Im}\,[n_{cv}\,(\alpha u_v + \beta_v)], \\
\dfrac{\partial n_v}{\partial t} + \mathrm{div} J_v = \quad 2P\cdot\ \mathrm{Im}\,[\overline{n_{cv}}\,(\overline{\alpha}\,u_c + \beta_c)], \\
\dfrac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\dfrac{J_c \otimes J_c}{n_c} + n_c\theta_c\right) - n_c\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c\nabla V_c \\
\qquad\qquad = \ \epsilon\, P\cdot\nabla\ \mathrm{Re}\ (n_{cv}(\alpha u_v + \beta_v)) \\
\qquad\qquad -\,2P\cdot\ \mathrm{Re}\ \Big(n_{cv}(\alpha u_v \otimes \overline{u_c} + \beta_v \otimes \overline{u_c} + u_v \otimes \overline{\beta_c} + \theta_{cv})\Big), \\
\dfrac{\partial J_v}{\partial t} + \ \mathrm{div}\left(\dfrac{J_v \otimes J_v}{n_v} + n_v\theta_v\right) - n_v\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v\nabla V_v \\
\qquad\qquad = -\epsilon\, P\cdot\nabla\ \mathrm{Re}\ (\overline{n_{cv}}\,(\overline{\alpha} u_c + \beta_c)) \\
\qquad\qquad +\,2P\cdot\ \mathrm{Re}\ \Big(\overline{n_{cv}}\,(\overline{\alpha} u_c \otimes \overline{u_v} + \beta_c \otimes \overline{u_v} + u_c \otimes \overline{\beta_v} + \theta_{vc})\Big), \\
\epsilon\nabla\sigma - \dfrac{J_v}{n_v} + \dfrac{J_c}{n_c} = -\ \mathrm{Im}\ \left\{\dfrac{1}{\alpha}\Big(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\Big)\right\}.
\end{cases}
\tag{25}
$$

FINAL REMARKS

We have derived a set of **quantum hydrodynamic equations from the two-band Kane model.**

This system, which can be considered as a **nonzero-temperature quantum fluid model**, is not closed.

In addition to other quantities, we have the tensors θ_c, θ_v, θ_{cv} and θ_{vc} (only the first ones are similar to the **temperature tensor** of kinetic theory).

- Closure of the quantum hydrodynamic system
- Poor physical meaning of the envelope functions
- New basis for more physical envelope functions
- Heterogeneous materials
- Numerical treatment