Zero-temperature QUANTUM HYDRODYNAMIC EQUATIONS (Madelung fluid equations)

Direct approach from the Schrödinger-type equations.

Special solution. We look for solution of the (scaled) Kane model

$$\begin{cases} i\epsilon \dfrac{\partial \psi_c}{\partial t} = -\epsilon^2 \dfrac{\partial^2 \psi_c}{\partial x^2} + V_c \psi_c + i\epsilon^2 P \dfrac{\partial \psi_v}{\partial x} \\ \\ i\epsilon \dfrac{\partial \psi_v}{\partial t} = -\epsilon^2 \dfrac{\partial^2 \psi_v}{\partial x^2} + V_v \psi_v + i\epsilon^2 P \dfrac{\partial \psi_c}{\partial x} \end{cases}$$

in the following form

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

where

n_c and n_v are the electron and hole densities

S_c and S_v are the phases of the "wave" functions

$$J_{ij}(x,t) = \epsilon \mathrm{Im}\left[\overline{\psi_i}(x,t)\psi_j'(x,t)\right], \qquad i,j = c,v$$

The equations for the densities n_c and n_v and the phases S_c and S_v take the form

$$
\left\{
\begin{aligned}
&\frac{\partial n_c}{\partial t} = -\frac{\partial}{\partial x}\left(n_c \frac{\partial S_c}{\partial x}\right) + \epsilon P \frac{\sqrt{n_c}}{\sqrt{n_v}} \frac{\partial n_v}{\partial x} \cos\left(\frac{S_v - S_c}{\epsilon}\right) \\
&\qquad - 2P\sqrt{n_v}\sqrt{n_c}\frac{\partial S_v}{\partial x} \sin\left(\frac{S_v - S_c}{\epsilon}\right) \\
&\frac{\partial n_v}{\partial t} = -\frac{\partial}{\partial x}\left(n_v \frac{\partial S_v}{\partial x}\right) + \epsilon P \frac{\sqrt{n_v}}{\sqrt{n_c}} \frac{\partial n_c}{\partial x} \cos\left(\frac{S_c - S_v}{\epsilon}\right) \\
&\qquad - 2P\sqrt{n_c}\sqrt{n_v}\frac{\partial S_c}{\partial x} \sin\left(\frac{S_c - S_v}{\epsilon}\right) \\
&\frac{\partial S_c}{\partial t} + \frac{1}{2}\left(\frac{\partial S_c}{\partial x}\right)^2 + V_c - \frac{\epsilon^2}{2}\left(\frac{1}{\sqrt{n_c}}\frac{\partial^2 \sqrt{n_c}}{\partial x^2}\right) \\
&\qquad - \epsilon P \frac{\sqrt{n_v}}{\sqrt{n_c}} \frac{\partial S_v}{\partial x} \cos\left(\frac{S_v - S_c}{\epsilon}\right) \\
&\qquad - \epsilon^2 P \frac{1}{2} \frac{1}{\sqrt{n_v}\sqrt{n_c}} \frac{\partial n_v}{\partial x} \sin\left(\tfrac{S_v - S_c}{\epsilon}\right) = 0 \\
&\frac{\partial S_v}{\partial t} + \frac{1}{2}\left(\frac{\partial S_v}{\partial x}\right)^2 + V_v - \frac{\epsilon^2}{2}\left(\frac{1}{\sqrt{n_v}}\frac{\partial^2 \sqrt{n_v}}{\partial x^2}\right) \\
&\qquad - \epsilon P \frac{\sqrt{n_c}}{\sqrt{n_v}} \frac{\partial S_c}{\partial x} \cos\left(\frac{S_c - S_v}{\epsilon}\right) \\
&\qquad - \epsilon^2 p \frac{1}{2} \frac{1}{\sqrt{n_c}\sqrt{n_v}} \frac{\partial n_c}{\partial x} \sin\left(\tfrac{S_c - S_v}{\epsilon}\right) = 0\,.
\end{aligned}
\right.
$$

The additional unknown

$$\mathsf{S}_{cv} = \sin\left(\frac{S_c - S_v}{\epsilon}\right), \qquad \mathsf{C}_{cv} = \cos\left(\frac{S_c - S_v}{\epsilon}\right),$$

can be manipulated in order to obtain links with the current densities J_c, J_v,

$$\frac{\partial}{\partial x}\mathsf{S}_{cv} = \frac{1}{\epsilon}\mathsf{C}_{cv}\left(\frac{J_c}{n_c} - \frac{J_v}{n_v}\right),$$

$$\frac{\partial}{\partial x}\mathsf{C}_{cv} = -\frac{1}{\epsilon}\mathsf{S}_{cv}\left(\frac{J_c}{n_c} - \frac{J_v}{n_v}\right).$$

Summarizing, we have the set of equations, which are the **zero-temperature quantum hydrodynamic equations**:

$$\frac{\partial n_c}{\partial t} = -\frac{\partial J_c}{\partial x} + \epsilon P \frac{\sqrt{n_c}}{\sqrt{n_v}} \frac{\partial n_v}{\partial x} \mathsf{C}_{cv} + 2P \frac{\sqrt{n_c}}{\sqrt{n_v}} J_v \, \mathsf{S}_{cv}$$

$$\frac{\partial n_v}{\partial t} = -\frac{\partial J_v}{\partial x} + \epsilon P \frac{\sqrt{n_v}}{\sqrt{n_c}} \frac{\partial n_c}{\partial x} \mathsf{C}_{cv} - 2P \frac{\sqrt{n_v}}{\sqrt{n_c}} J_c \, \mathsf{S}_{cv}$$

$$\begin{aligned}
&\frac{\partial J_c}{\partial t} + \frac{\partial}{\partial x}\left(\frac{{J_c}^2}{n_c}\right) + n_c \frac{\partial V_c}{\partial x} - \frac{\epsilon^2}{2} n_c \frac{\partial}{\partial x}\left(\frac{1}{\sqrt{n_c}} \frac{\partial^2 \sqrt{n_c}}{\partial x^2}\right) \\
&\quad - \epsilon P \, n_c \frac{\partial}{\partial x}\left(\frac{J_v}{\sqrt{n_c n_v}}\right) \mathsf{C}_{cv} + \epsilon^2 \frac{P}{2} n_c \frac{\partial}{\partial x}\left(\frac{1}{\sqrt{n_c n_v}} \frac{\partial n_v}{\partial x}\right) \mathsf{S}_{cv} \\
&\quad - \epsilon P \frac{n_c J_v}{\sqrt{n_c n_v}} \frac{\partial \mathsf{C}_{cv}}{\partial x} + \epsilon^2 P n_c \frac{1}{2} \frac{1}{\sqrt{n_c n_v}} \frac{\partial n_v}{\partial x} \frac{\partial \mathsf{S}_{cv}}{\partial x} = 0
\end{aligned}$$

$$\begin{aligned}
&\frac{\partial J_v}{\partial t} + \frac{\partial}{\partial x}\left(\frac{{J_v}^2}{n_c}\right) + n_v \frac{\partial V_v}{\partial x} - \frac{\epsilon^2}{2} n_v \frac{\partial}{\partial x}\left(\frac{1}{\sqrt{n_v}} \frac{\partial^2 \sqrt{n_v}}{\partial x^2}\right) \\
&\quad - \epsilon P \, n_v \frac{\partial}{\partial x}\left(\frac{J_c}{\sqrt{n_c n_v}}\right) \mathsf{C}_{cv} - \epsilon^2 \frac{P}{2} n_v \frac{\partial}{\partial x}\left(\frac{1}{\sqrt{n_c n_v}} \frac{\partial n_c}{\partial x}\right) \mathsf{S}_{cv} \\
&\quad - \epsilon P \, n_v \frac{J_c}{\sqrt{n_c n_v}} \frac{\partial \mathsf{C}_{cv}}{\partial x} - \epsilon^2 P \, n_v \frac{1}{2} \frac{1}{\sqrt{n_c n_v}} \frac{\partial n_c}{\partial x} \frac{\partial \mathsf{S}_{cv}}{\partial x} = 0
\end{aligned}$$

For $\epsilon = 0 (\hbar = 0)$ **classical Euler equations.**

It is easy to verify the **CONTINUITY EQUATION**

$$\frac{\partial\ \mathbf{n_{tot}(x,t)}}{\partial t} = -\,\mathrm{div}\,\mathbf{J_{tot}}$$

where **the total density** is

$$\mathbf{n_{tot}(x,t)} = n_c(x,t) + n_v(x,t)\,.$$

and **the total particle current density** is

$$\mathbf{J_{tot}}(x,t) = J_c(x,t) + J_v(x,t) - 2\epsilon P\ \mathrm{Re}\ \left(\bar{\psi}_c \psi_v\right)$$

with

$$\mathrm{Re}\ \left(\bar{\psi}_c \psi_v\right) = \sqrt{n_c\, n_v}\cos\left(\frac{S_v - S_c}{\epsilon}\right)$$

In terms of "interband" densities and current densities

$$\begin{aligned}
\frac{\partial n_c}{\partial t} &= -\frac{\partial J_c}{\partial x} + \frac{\epsilon p}{2}\frac{\partial}{\partial x}\left(n_{cv} + n_{vc}\right) + iP\left[J_{cv}(x,t) - J_{vc}(x,t)\right] \\
\frac{\partial n_v}{\partial t} &= -\frac{\partial J_v}{\partial x} + \frac{\epsilon p}{2}\frac{\partial}{\partial x}\left(n_{vc} + n_{cv}\right) - iP\left[J_{cv}(x,t) - J_{vc}(x,t)\right]
\end{aligned}$$

with $\mathbf{J_{tot}}(x,t) =$

$$J_c(x,t) + J_v(x,t) - \epsilon\,P\ \left[n_{cv}(x,t) + n_{vc}(x,t)\right]$$

$$
\left\{
\begin{aligned}
\frac{\partial}{\partial t}(\text{ Re }\mathbf{n_{cv}}) = & -\frac{1}{2}\frac{1}{\mathbf{n_c}}(\text{ Re }\mathbf{n_{cv}})\left[\frac{\partial \mathbf{J_{cc}}}{\partial x} + \frac{\partial}{\partial x|_v}(\text{ Re }\mathbf{n_{cv}})\right] \\
& -\frac{1}{2}\frac{1}{\mathbf{n_v}}(\text{ Re }\mathbf{n_{cv}})\left[\frac{\partial \mathbf{J_{vv}}}{\partial x} + \frac{\partial}{\partial x|_c}(\text{ Re }\mathbf{n_{cv}})\right] \\
& +\frac{1}{2\epsilon}\text{ Im }\mathbf{n_{cv}}\left(\frac{\mathbf{J_{vv}}^2}{\mathbf{n_v}^2} - \frac{\mathbf{n_{cc}}^2}{\mathbf{n_c}^2}\right) + \frac{1}{\epsilon}\text{ Im }\mathbf{n_{cv}}\,(V_v - V_c) \\
& +\frac{\epsilon}{2}\text{ Im }\mathbf{n_{cv}}\left(\frac{1}{\sqrt{n_c}}\frac{\partial^2\sqrt{n_c}}{\partial x^2} - \frac{1}{\sqrt{n_v}}\frac{\partial^2\sqrt{n_v}}{\partial x^2}\right) \\
& -\frac{1}{2}\text{ Im }\mathbf{n_{cv}}\left(\frac{1}{\mathbf{n_{vv}}}\frac{\partial}{\partial x|_c}(\text{ Im }\mathbf{n_{cv}}) + \frac{1}{\mathbf{n_{cc}}}\frac{\partial}{\partial x|_v}(\text{ Im }\mathbf{n_{cv}})\right) \\
\frac{\partial}{\partial t}(\text{ Im }\mathbf{n_{cv}}) = & -\frac{1}{2}\frac{1}{\mathbf{n_c}}(\text{ Im }\mathbf{n_{cv}})\left[\frac{\partial \mathbf{J_{cc}}}{\partial x} + \frac{\partial}{\partial x|_v}(\text{ Re }\mathbf{n_{cv}})\right] \\
& = -\frac{1}{2}\frac{1}{\mathbf{n_v}}(\text{ Im }\mathbf{n_{cv}})\left[\frac{\partial \mathbf{J_{vv}}}{\partial x} + \frac{\partial}{\partial x|_c}(\text{ Re }\mathbf{n_{cv}})\right] \\
& +\frac{1}{2\epsilon}\text{ Re }\mathbf{n_{cv}}\left(\frac{\mathbf{J_{vv}}^2}{\mathbf{n_v}^2} - \frac{\mathbf{J_{cc}}^2}{\mathbf{n_c}^2}\right) + \frac{1}{\epsilon}\text{ Re }\mathbf{n_{cv}}\,(V_v - V_c) \\
& +\frac{\epsilon}{2}\text{ Re }\mathbf{n_{cv}}\left(\frac{1}{\sqrt{n_c}}\frac{\partial^2\sqrt{n_c}}{\partial x^2} - \frac{1}{\sqrt{n_v}}\frac{\partial^2\sqrt{n_v}}{\partial x^2}\right) \\
& -\frac{1}{2}\text{ Re }\mathbf{n_{cv}}\left(\frac{1}{\mathbf{n_{vv}}}\frac{\partial}{\partial x|_c}(\text{ Im }\mathbf{n_{cv}}) + \frac{1}{\mathbf{n_{cc}}}\frac{\partial}{\partial x|_v}(\text{ Im }\mathbf{n_{cv}})\right)
\end{aligned}
\right.
$$

The previous equations are the

ZERO-TEMPERATURE QUANTUM HYDRODYNAMIC EQUATIONS for a TWO-BAND electron system.

In order to obtain a **nonzero temperature**, we consider MIXED STATES.

A **mixed quantum mechanical state** consists of a sequence of single states with occupation probabilities λ_j, $j = 0, 1, 2, \ldots$ for the $j-$th single state described by the envelope function ψ_c^j (ψ_v^j), **for each index j.**

We look for solutions $\psi_c^j(x,t)$ and $\psi_v^j(x,t)$, as before. We define for the mixed state the carrier densities and the current densities

$$\begin{aligned}
n_c(x) &= \textstyle\sum_{j=0}^{\infty} \lambda^j n_c^j(x) \\
n_v(x) &= \textstyle\sum_{j=0}^{\infty} \lambda^j n_v^j(x) \\
n_{cv}(x) &= \textstyle\sum_{j=0}^{\infty} \lambda^j n_{cv}^j(x) \\
J_c(x) &= \textstyle\sum_{j=0}^{\infty} \lambda^j J_c^j(x) \\
J_v(x) &= \textstyle\sum_{j=0}^{\infty} \lambda^j J_v^j(x) \\
J_{cv}(x) &= \textstyle\sum_{j=0}^{\infty} \lambda^j J_{cv}^j(x)
\end{aligned}$$

- **No problem** for the total quantum continuity equation.

- The "one-band" part of the current densities takes the new form

$$\frac{\partial J_c}{\partial t}+\frac{\partial}{\partial x}\left(\frac{J_c^2}{n_c}+n_c\mathbf{T_{cc}}\right)+n_c\frac{\partial V_c}{\partial x}-\frac{\epsilon^2}{2}n_c\frac{\partial}{\partial x}\left(\frac{1}{\sqrt{n_c}}\frac{\partial^2\sqrt{n_c}}{\partial x^2}\right)$$

where $\mathbf{T_{cc}} = \dfrac{\epsilon^2}{4}\sum_{j=0}^{\infty}\lambda^j\dfrac{n_c^j}{n_c}\left(\dfrac{1}{n_c^j}\dfrac{\partial n_c^j}{\partial x}-\dfrac{1}{n_c}\dfrac{\partial n_c}{\partial x}\right)^2$

$$+\sum_{j=0}^{\infty}\lambda^j\frac{n_c^j}{n_c}\left(\frac{J_c^j}{n_c^j}-\frac{J_c}{n_c}\right)^2$$

and analogously for the valence electrons: J_v, $\mathbf{T_{vv}}$.

For each band, $\mathbf{T_{cc}}$ and $\mathbf{T_{vv}}$ are the total temperature, sum of the **current temperature** ${\mathbf{T_{cc}}}^c$ and ${\mathbf{T_{vv}}}^c$, and the **osmotic temperature** ${\mathbf{T_{cc}}}^{os}$ and ${\mathbf{T_{vv}}}^{os}$.

- More complicated are the nonzero temperature corrections in the "two-band" part of the current density equations.

$$
\begin{aligned}
\mathbf{T}^{\mathbf{c}}_{\mathbf{cv}} &= n_c \sum_{j=0}^{\infty} \lambda^j \frac{n_c^j}{n_c} \left(\frac{J_c^j}{n_c^j} - \frac{J_c}{n_c} \right) \\
&\qquad \left(\frac{1}{n_c^j} \frac{\partial}{\partial x|_v} \left(\text{ Re } n_{cv}^j \right) - \frac{1}{n_c} \frac{\partial}{\partial x|_v} \left(\text{ Re } n_{cv} \right) \right) \\
&\quad - \frac{\epsilon}{2} \sum_{j=0}^{\infty} \lambda^j n_c^j \left(\frac{1}{n_c^j} \frac{\partial n_c^j}{\partial x} - \frac{1}{n_c} \frac{\partial n_c}{\partial x} \right) \\
&\qquad \left(\frac{1}{n_c^j} \frac{\partial}{\partial x|_v} \left(\text{ Im } n_{cv}^j \right) - \frac{1}{n_c} \frac{\partial}{\partial x|_v} \left(\text{ Im } n_{cv} \right) \right)
\end{aligned}
$$

and a similar term with v instead of c.

- The new corrections due to the interband coupling in the evolution of J_{cv} are long and intricated.

TWO-BAND QUANTUM HYDRODYNAMIC MODEL

CONCLUSIONS

1. It is **impossible** to get a system where only the **total quantum current density** appears.

2. The set of equations is **not closed**.

3. **CLOSURE conditions**.

   2.1 **Thermodynamic equilibrium**

   2.2 **Chapman-Enskog** expansion

   2.3 **MEP** (Maximum entropy principle)

4. Numerical validation and comparison with other models and **experimental data**.

5. **Non-smooth** potentials.