# DERIVATION of Quantum Hydrodynamic Models from the Wigner equations

The equations for the moments of the Wigner functions can be derived by multiplying the equations of Wigner system, by 1, $v$ and $v^2$ and by integrating over the velocity space.

## Definition of macroscopic quantities

**Quantum mechanical probability densities** $n_{cc}$ and $n_{vv}$ for the positions of electrons in band of conduction and valence. The **interband terms** $n_{cv}$ and $n_{vc}$ are complex functions such that $n_{cv} = \overline{n_{vc}}$.

$$n_{ij}(x,t) \;=\; \int_{-\infty}^{+\infty} w_{ij}(x,v,t)dv\,, \quad i,j = c,v\,.$$

Similarly we define the **current densities** by the first moments of the Wigner functions, with the classical meaning of the conduction (valence) current densities $J_{cc}$ ($J_{vv}$).

$$J_{ij} = -q \int_{-\infty}^{+\infty} v w_{ij}(x,v,t)dv\,, \quad i,j = c,v\,.$$

For $i,j = c,v$, the set of moments is

$$
\begin{aligned}
n_{ij}(x,t) &= \int_{-\infty}^{+\infty} w_{ij}(x,v,t)dv\,, \\
J_{ij}(x,t) &= -q \int_{-\infty}^{+\infty} v w_{ij}(x,v,t)dv\,, \\
\mathcal{E}_{ij}(x,t) &= \frac{m}{2} \int_{-\infty}^{+\infty} v^2 w_{ij}(x,v,t)dv, \\
M_{ij}^{(3)}(x,t) &= \int_{-\infty}^{+\infty} v^3 w_{ij}(x,v,t)dv \\
\ldots \qquad & \ldots \qquad \ldots
\end{aligned}
$$

# The total particle density

For the two-band Schrödinger-like Kane model, **the total density** is

$$\mathbf{n_{tot}}(x,t) = |\psi|^2 = |\psi_c|^2 + |\psi_v|^2 = n_{cc}(x,t) + n_{vv}(x,t)\,.$$

In general we know that **the quantum continuity equation** reads as follows

$$\frac{\partial|\psi|^2}{\partial t} = -\,\mathrm{div}\,J$$

where

$$J(x) = \frac{i\hbar}{2m}(\psi\nabla\bar{\psi} - \bar{\psi}\nabla\psi)\ .$$

For the **two-band model** the continuity equation takes the form

$$\boxed{\frac{\partial\ (\mathbf{n_{cc}} + \mathbf{n_{vv}})}{\partial t} = \ \mathrm{div}\ (\mathbf{J_{tot}})}$$

where the total **current density** for the two-band system is

$$\mathbf{J_{tot}}(x,t) \ = \ J_{cc} + J_{vv} - \frac{\hbar P}{m}\,\mathrm{Re}\,\mathbf{n_{cv}}$$

The equations for the current (first moments of equations) contain the second order moments, $\mathcal{E}_{ij}(x,t)$, interpreted as **energy terms.**

A **simple quantum hydrodynamical model** is obtained directly from the first two moments, by manipulating the energy term appearing under the divergence symbol and taking into account that

$$\begin{aligned} \frac{\partial \mathcal{E}_{ij}}{\partial x} &= \frac{m}{2q^2}\frac{\partial}{\partial x}\left(\frac{J_{ij}^2}{n_{ij}}\right) - \frac{\hbar^2}{4m} n_{ij} \frac{\partial}{\partial x}\left[\frac{1}{\sqrt{n_{ij}}}\frac{\partial^2 \sqrt{n_{ij}}}{\partial x^2}\right] \\ &+ \frac{\hbar^2}{2m}\frac{\partial}{\partial x}\Big(n_{ij}T_{ij}\Big) , \end{aligned}$$

with $i,j = c,v$.

The quantum correction term $\frac{1}{\sqrt{n_{ij}}}\frac{\partial^2 \sqrt{n_{ij}}}{\partial x^2}$ can be interpreted as internal self-potential, the so-called **Bohm potential.**

The **''temperatures''** $T_{ij}$ are defined by the operators $P_\pm = \frac{1}{2}\frac{\partial}{\partial x} \pm i\frac{mv}{\hbar}$ , as

$$T_{ij} = \frac{< P_+ P_- w_{ij} >}{< w_{ij} >} - \frac{< P_+ w_{ij} >< P_- w_{ij} >}{< w_{ij} >^2},$$

where $< \cdot >$ means average.

The closure of the previous equations system can be done using the **isothermal assumption.**

The closure can be performed also by using the **thermal equilibrium Wigner functions** for the two-band semiconductor model, in the case of the Kane Hamiltonian, [barletti2003].

# FINAL COMMENTS

In this contribution, we present only the first preliminary results. The future research is oriented towards the closure and the numerical validation of the model.

- The set of Madelung-type equations is closed. The system obtained from Wigner is **not closed**.

- **Closure conditions**.

  – Thermodynamic equilibrium

  – Chapman-Enskog expansion

  – MEP (Maximum entropy principle)

- **Non-smooth** potentials.

- **Numerical validation** of QHD models

- **Comparison** with other models and with experiments.