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Quantum hydrodynamic equations arising from the Wigner-Kane model

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Mathematical modeling for semiconductor devices has relied, from the beginning, on a **fluid dynamical approach**, in terms of macroscopic quantities (charge density, current, energy, ...).

When the quantum aspects become not negligible or even predominant, it is useful to formulate semi-classical models in terms of macroscopic variables **(quantum hydrodynamic models)**.

Interesting results are present in literature (Gardner, Jüngel, Markowich, Ringhofer, Unterreiter, etc.). Published results are generally devoted to single-band problems.

In this work we face the problem of a fluid dynamical formulation for a semiconductor device characterized by a **two–band (i.e. conduction and valence band) structure, where the carriers dynamics is driven by interband tunneling.**

Physical description of the Kane model. Let $\psi_c(x,t)$ be the conduction band electron wave (envelope) function and $\psi_v(x,t)$ be the valence band electron wave (envelope) function.

In the one-dimensional case, **the Kane model** reads as follows [kane56]:

$$\begin{cases} i\hbar\dfrac{\partial\psi_c}{\partial t} &= \left[-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}+V_c\right]\psi_c-\dfrac{\hbar^2}{m}P\dfrac{\partial\psi_v}{\partial x} \\ i\hbar\dfrac{\partial\psi_v}{\partial t} &= \left[-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}+V_v\right]\psi_v+\dfrac{\hbar^2}{m}P\dfrac{\partial\psi_c}{\partial x} \end{cases}.$$

where m is the bare mass of the carriers, V_c and V_v are the minimum of the conduction band energy and maximum of the valence band energy respectively, and P is the **coupling coefficient** given by

$$P=\frac{m}{\hbar}\sqrt{\frac{m-m^*}{2mm^*}E_g}$$

which is obtained through the energy dispersion relation and where m^* is the effective electron mass depending, through the $x-$coordinate, on the layer composition, but otherwise isotropic, and $E_g = V_c - V_v$ is the $x-$dependent gap energy.

According to **the envelope function theory** approach it is sufficient to study the evolution of the so-called envelope function because it is not necessary to find the exact evolution of the full wave equation.

The **envelope function** is a smooth function which can be obtained by replacing the wave function by its average in each primitive cell.

Formulation of the Kane model in terms of Wigner functions

We define **the density matrix** $\rho_{ij}(r,s,t) = \bar{\psi}_i(r,t)\psi_j(s,t) \quad i,j = c,v\,.$

Taking formally the derivatives with respect to time t in the density matrix element and using Kane eqs. lead to a **set of four coupled evolution equations** for the density matrix elements ρ_{ij}.

The Wigner function is defined by the **inverse Fourier transformation**

$$w_{i,j}(x,v,t) = \mathcal{F}^{-1}\rho_{i,j}\left(x + \frac{\hbar}{2m}\eta, x - \frac{\hbar}{2m}\eta\right)\ .$$

$$\Downarrow$$

Then we obtain the following system, which is **the Wigner function formulation of the Kane model**

$$\begin{cases} i\hbar\dfrac{\partial w_{cc}}{\partial t} = -i\hbar v\dfrac{\partial w_{cc}}{\partial x} + \Theta_{cc}w_{cc} + \dfrac{\hbar}{2m}P\left[\dfrac{\partial w_{vc}}{\partial x} - \dfrac{\partial w_{cv}}{\partial x}\right] - i\hbar Pv\left[w_{vc} + w_{cv}\right] \\ i\hbar\dfrac{\partial w_{cv}}{\partial t} = -i\hbar v\dfrac{\partial w_{cv}}{\partial x} + \Theta_{vc}w_{cv} + \dfrac{\hbar^2}{2m}P\left[\dfrac{\partial w_{vv}}{\partial x} + \dfrac{\partial w_{cc}}{\partial x}\right] - i\hbar Pv\left[w_{vv} - w_{cc}\right] \\ i\hbar v\dfrac{\partial w_{vv}}{\partial t} = -i\hbar v\dfrac{\partial w_{vv}}{\partial x} + \Theta_{vv}w_{vv} - \dfrac{\hbar^2}{2m}P\left[\dfrac{\partial w_{cv}}{\partial x} - \dfrac{\partial w_{vc}}{\partial x}\right] + i\hbar Pv\left[w_{cv} + w_{vc}\right] \end{cases}$$

where

$$\Theta_{ij}w_{ij} = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\left[V_j\left(x - \frac{\hbar}{2m}\eta, t\right) - V_i\left(x + \frac{\hbar}{2m}\eta, t\right)\right] w_{ij}(x, v', t)\cdot \mathrm{e}^{i(v-v')\eta}d\eta dv'$$

with $i, j = c, v$.