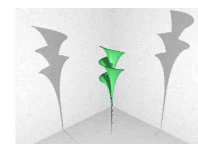
Beyond the effective-mass approximation: multi-band models of semiconductor devices



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- GNFM Research Project: *"Mathematical Models for Microelectronics"*, 2004
- MIUR-COFIN: *"Mathematical problems of Kinetic Theories"*, 2002.

The effective-mass approximation

Most of mathematical models of quantum transport in semiconductor devices makes use of the so-called *effective-mass approximation*.

This amounts to substituting the true Hamiltonian

$$H = -\frac{\hbar^2}{2m}\Delta + V_{\mathrm{per}} + V$$

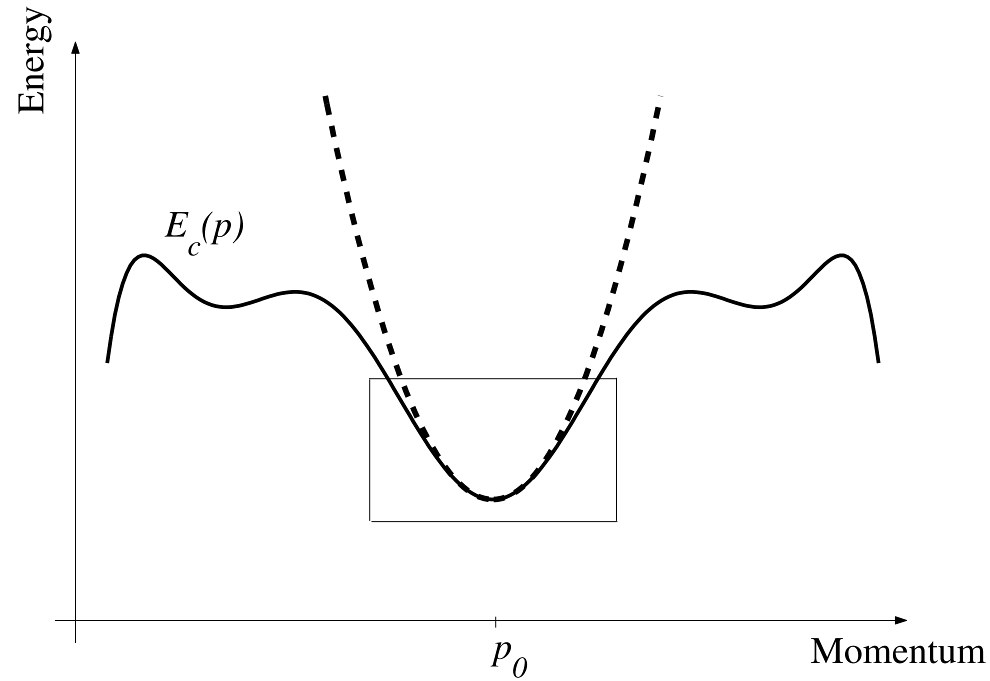
with the following:

$$H_{\mathrm{me}} = -\frac{\hbar^2}{2}\nabla^{\mathrm{T}}\mathbb{M}^{-1}\nabla + V$$

The effective-mass approximation (continued)

The effctive-mass tensor $\mathbb{M}$ arises from a parabolic approximation of the conduction band:

$$\mathbb{M}^{-1} = \mathrm{Hess}(E_c)_{|p_0}$$

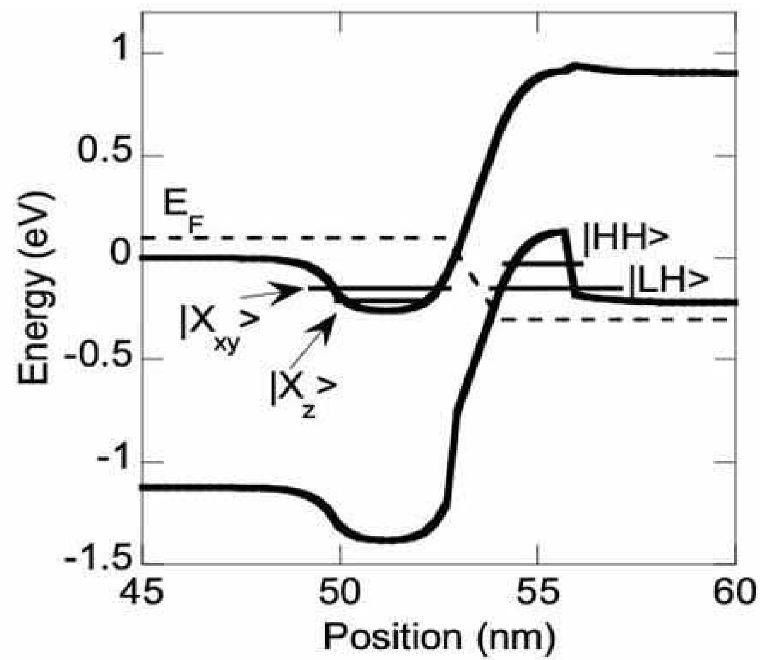


- In such approximation the electron[hole] belongs exclusively to the conduction[valence] band.

Interband devices

The effective-mass approximation is unable to describe interband tunneling, a quantum effect which plays an important role in modern devices.

Scheme of the interband diode developed by P. Berger's team (Ohio State University, USA)



Multi-band models

We need therefore to go beyond the effective-mass approximation and consider more suitable models in which the electron[hole] “feels the presence” of at least two-bands.

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1 - two-band Kane model:

$$H_{\mathrm{Kane}} = \begin{pmatrix} -\frac{\hbar^2}{2m}\Delta + E_g + V & -\frac{\hbar^2}{m} K \cdot \nabla \\ \frac{\hbar^2}{m} K \cdot \nabla & -\frac{\hbar^2}{2m}\Delta + V \end{pmatrix}$$

E. Kane, *J. Phys. Chem. Solids*, 1959

Multi-band models

We need therefore to go beyond the effective-mass approximation and consider more suitable models in which the electron[hole] “feels the presence” of at least two bands.

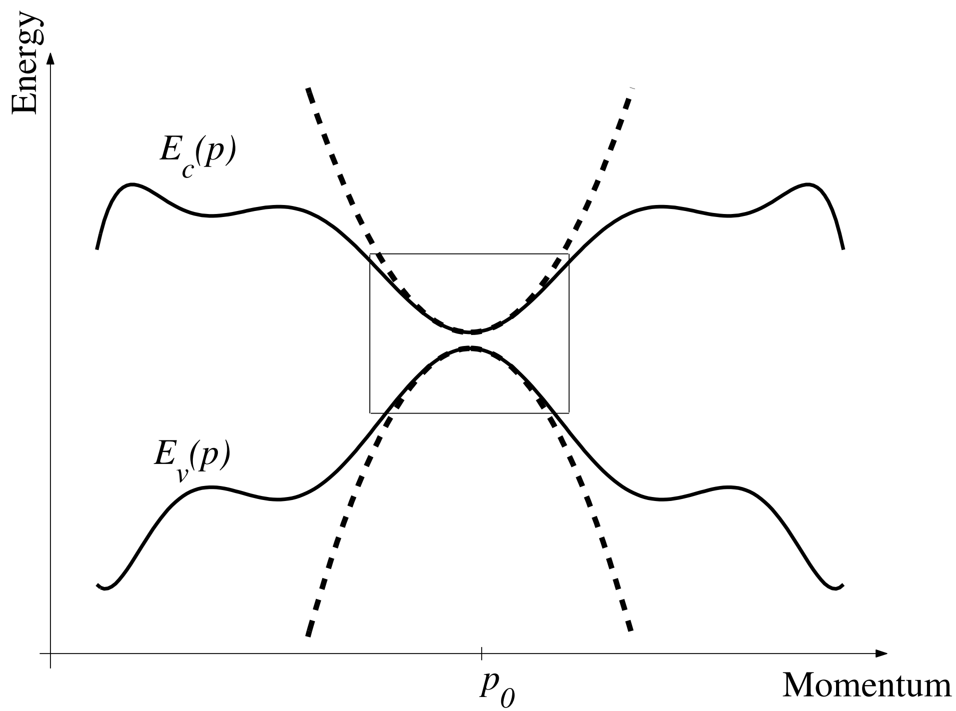
2 - two-band order-1 M-M model:

$$H_{\text{M-M}} = \begin{pmatrix} -\frac{\hbar^2}{2m_1^*}\Delta + E_g + V & \frac{\hbar^2}{mE_g} K \cdot \nabla V \\ \frac{\hbar^2}{mE_g} K \cdot \nabla V & -\frac{\hbar^2}{2m_2^*}\Delta + V \end{pmatrix}$$

O. Morandi & M. Modugno, 2004 (to appear).

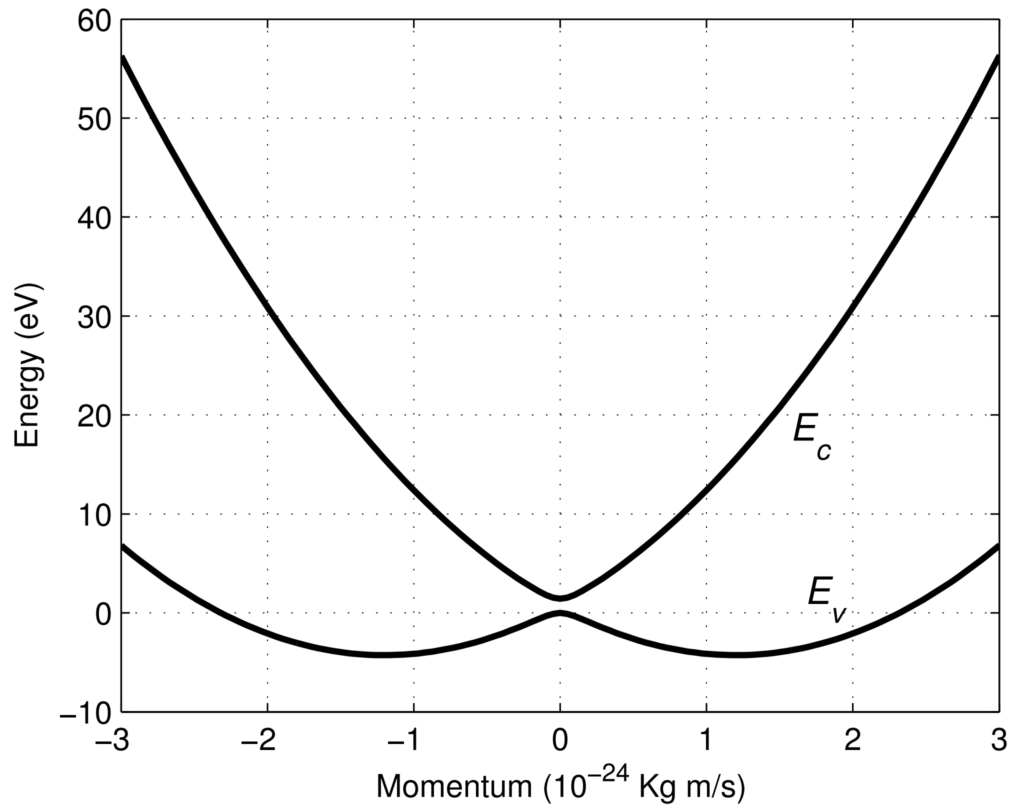
Multi-band models (continued)

All these models furnish an approximation of the real multi-band dispersion relation:



Multi-band models (continued)

As an example, here is the dispersion relation computed with the Kane Hamiltonian for GaAs:



Research program

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- Applications to electronic devices and BEC

The Wigner transform

The Wigner transform

$$w(r,p) = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} \rho\Big(r + \frac{\xi}{2}, r - \frac{\xi}{2}\Big)\, \mathrm{e}^{-i\xi\cdot p/\hbar}\, d\xi$$

is a unitary mapping of $L^2(\mathbb{R}^3 \times \mathbb{R}^3, \mathbb{C})$ into itself.

It allows a *quasi-kinetic formulation of statistical QM*.

E. Wigner, *Phys. Rev.*, 1932

The Wigner equation

The quantum Liouville equation

$$i\hbar\,\partial_t\,\rho = \left[-\frac{\hbar^2}{2m}\Delta + V, \rho\right]$$

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The quantum Liouville equation

$$i\hbar\,\partial_t\,\rho = \Big[-\frac{\hbar^2}{2m}\Delta + V, \rho\Big]$$

is equivalent to the Wigner equation

$$\partial_t\,w + \frac{1}{m}\,\nabla_r \cdot p\,w = \frac{1}{i\hbar}\Big[V\Big(r + \frac{i\hbar}{2}\nabla_p\Big) - V\Big(r - \frac{i\hbar}{2}\nabla_p\Big)\Big]\,w$$

How MB Transport Eqs. should look like?

Single band case (no discrete degrees of freedom):

$$S = \sum_k \lambda_k \, \psi^k(x)\overline{\psi^k(y)} \quad \xrightarrow{\text{Wigner transform}} \quad w(r,p)$$

mixed state — Wigner function

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Multi-band/spin case (one discrete degree of freedom):

$$S = \sum_k \lambda_k \, \psi_i^k(x)\overline{\psi_j^k(y)} \quad \xrightarrow{\text{Wigner transform}} \quad w_{ij}(r,p)$$

mixed state — Wigner matrix

where $w_{ij}(r,p) = \overline{w_{ji}(r,p)}$.

How MBTE should look like? (contd.)

Now assume $1 \leq i, j \leq 2$ and recall that the Pauli matrices

$$\boldsymbol{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are a orthonormal basis of 2×2 hermitian matrices over $\mathbb{R}$.

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Thus, we can decompose the Wigner matrix $\boldsymbol{W} = (w_{ij})$ as:

$$\boxed{\boldsymbol{W} = w_0\,\boldsymbol{\sigma}_0 + w_1\,\boldsymbol{\sigma}_1 + w_2\,\boldsymbol{\sigma}_2 + w_3\,\boldsymbol{\sigma}_3}$$

where the functions w_k are real.

How MBTE should look like? (contd.)

Explicitly:

$$\begin{cases} w_0 = \frac{1}{2}\left(w_{11} + w_{22}\right) \\ w_1 = \mathrm{Re}\, w_{12} = \mathrm{Re}\, w_{21} \\ w_2 = -\mathrm{Im}\, w_{12} = \mathrm{Im}\, w_{21} \\ w_3 = \frac{1}{2}\left(w_{11} - w_{22}\right) \end{cases}$$

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Putting $\langle w \rangle(r) = \int w(r,p)\,dp$, we have

$$\langle w_0 \rangle^2 = \langle w_1 \rangle^2 + \langle w_2 \rangle^2 + \langle w_3 \rangle^2, \quad \text{for a pure state,}$$

$$\langle w_0 \rangle^2 \geq \langle w_1 \rangle^2 + \langle w_2 \rangle^2 + \langle w_3 \rangle^2, \quad \text{for a mixed state,}$$

in analogy with Stokes parameters describing a polarized light beam.

Interpretation

For $i = 0, 1, 2, 3$ we have

$$\mathrm{Tr}(S\boldsymbol{\sigma}_i) = \sum_{k=0}^{3} \int w_k(r,p)\, dr\, dp\, \mathrm{Tr}(\boldsymbol{\sigma}_k \boldsymbol{\sigma}_i)$$

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$$\int w_0(r,p)\, dr\, dp = 1$$

and, for $i = 1, 2, 3$,

$$\int w_i(r,p)\, dr\, dp = \frac{1}{2} \times \textit{“spin” expectation in direction } i$$

Interpretation (continued)

In the case of Kane or M-M model:

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The Wigner function w_3 can thus be given a local meaning:

$$\frac{\langle w_3 \rangle}{\langle w_0 \rangle} =$$ *local expectation of band-index.*

Dynamics

The Kane Hamiltonian can be decomposed as follows:

$$H = \big(-\tfrac{1}{2}\Delta + V \big)\boldsymbol{\sigma}_0 - iK \cdot \nabla\, \boldsymbol{\sigma}_2 + E_g\, \boldsymbol{\sigma}_3$$

where we put $\hbar = m = 1$.

Assume for simplicity that we are describing electrons in a bulk crystal (constant E_g and K.)

Thus the dynamics of Wigner functions is given by the following set of equations.

Dynamics (continued)

$$\begin{cases} \big(\partial_t + p \cdot \nabla_r + i\Theta_V\big) w_0 = -K \cdot \nabla_r w_2 \\ \big(\partial_t + p \cdot \nabla_r + i\Theta_V\big) w_1 = -E_g w_2 + 2K \cdot p\, w_3 \\ \big(\partial_t + p \cdot \nabla_r + i\Theta_V\big) w_2 = -K \cdot \nabla_r w_0 + E_g w_1 \\ \big(\partial_t + p \cdot \nabla_r + i\Theta_V\big) w_3 = -2K \cdot p\, w_1 \end{cases}$$

where

$$\Theta_V = V\big(r + \tfrac{i\hbar}{2}\nabla_p\big) - V\big(r - \tfrac{i\hbar}{2}\nabla_p\big)$$

Plane-wave dynamics

A statistical superimposition of plane waves corresponds in the Wigner picture to a *space-homogeneous Wigner function*.

Assuming space-homogeneity and $V(r) = \vec{F} \cdot r$, the previous equations reduce to

$$\begin{cases} \left(\partial_t - \vec{F} \cdot \nabla_p\right) w_0 = 0 \\ \left(\partial_t - \vec{F} \cdot \nabla_p\right) w_1 = -E_g w_2 + 2K \cdot p \, w_3 \\ \left(\partial_t - \vec{F} \cdot \nabla_p\right) w_2 = E_g w_1 \\ \left(\partial_t - \vec{F} \cdot \nabla_p\right) w_3 = -2K \cdot p \, w_1 \end{cases}$$

Plane-wave dynamics (continued)

Putting

$$\vec{w} := (w_1, w_2, w_3) \quad \text{and} \quad \vec{B}(p) := (0,\ 2K \cdot p,\ E_g)$$

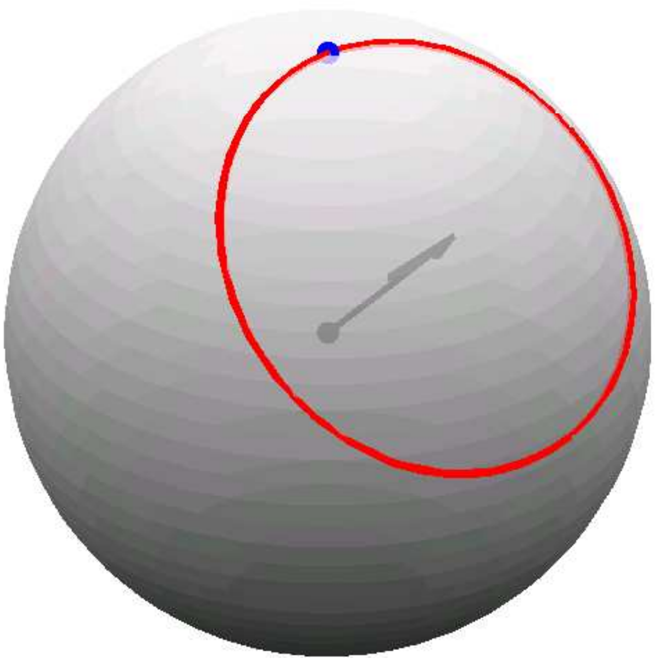
the “spinorial part” of the previous system can be presented in the following simple form:

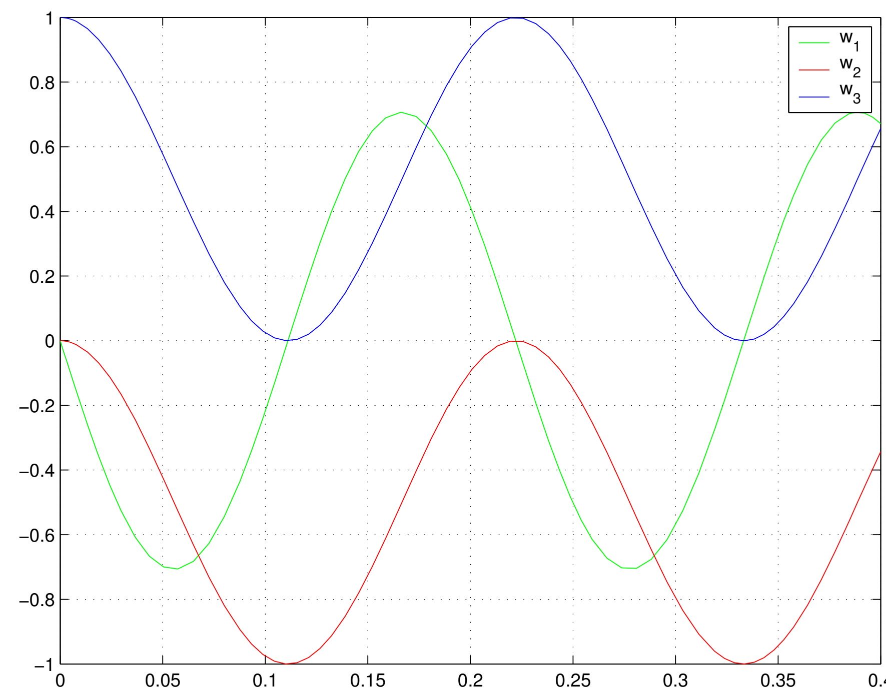
$$\boxed{\left(\partial_t - \vec{F} \cdot \nabla_p\right)\vec{w} = \vec{B}(p) \wedge \vec{w}}$$

$\vec{F} \cdot \nabla_p \, \vec{w} =$ *momentum drift* $\qquad$ $\vec{B}(p) \wedge \vec{w} =$ *band transitions*

Plane-wave dynamics (continued)

Path of a plane wave on the Poincaré sphere:





Moment equations

For $i = 0, 1, 2, 3$, define the local averages:

$$n_i(r) = \int w_i(r,p)\,dp$$

$$j_i(r) = \int p\,w_i(r,p)\,dp$$

$$c_i(r) = \int p \otimes p\,w_i(r,p)\,dp$$

Order-0 moment equations

$$
\begin{cases}
\partial_t n_0 + \nabla \cdot j_0 = -\nabla \cdot K\, n_2 \\
\partial_t n_1 + \nabla \cdot j_1 = -E_g\, n_2 + 2K \cdot j_3 \\
\partial_t n_2 + \nabla \cdot j_2 = -\nabla \cdot K\, n_0 + E_g\, n_1 \\
\partial_t n_3 + \nabla \cdot j_3 = -2K \cdot j_1
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Continuity equation for the total density:

$$\partial_t n_0 + \nabla \cdot (j_0 + K\, n_2) = 0$$

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Continuity equation for the total density:

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$\Longrightarrow \quad K n_2$ = *interband current*

Order-1 moment equations

$$\begin{cases} \partial_t j_0 + \nabla \cdot c_0 + \nabla V n_0 = -\nabla \cdot K \otimes j_2 \\ \partial_t j_1 + \nabla \cdot c_1 + \nabla V n_1 = -E_g j_2 + 2K \cdot c_3 \\ \partial_t j_2 + \nabla \cdot c_2 + \nabla V n_2 = -\nabla \cdot K \otimes j_0 + E_g j_1 \\ \partial_t j_3 + \nabla \cdot c_3 + \nabla V n_3 = -2K \cdot c_1 \end{cases}$$

Where:

$c_i = \frac{j_i \otimes j_i}{n_i} + Q(n_i) + n_i T_i$,

$Q(n_i) = -\frac{\hbar^2}{4} \left(\nabla \otimes \nabla n_i - \frac{(\nabla n_i) \otimes (\nabla n_i)}{n_i} \right)$ = *Bohm term*

T_i = *"temperature" term*

Two-band Madelung equations

Theorem. *If* (w_0, w_1, w_2, w_3) *are the Wigner functions of a pure state, then the temperature terms vanish:*

$$\boxed{T_i \equiv 0, \qquad i = 0, 1, 2, 3.}$$

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$$T_i \equiv 0, \qquad i = 0, 1, 2, 3.$$

Therefore, the order-0 and order-1 moment equations are a *closed* system yelding Madelung-like equations for the Kane model, equivalent to the Schrödinger equation.

E. Madelung, *Zeitschr. f. Phys.*, 1926

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- We have discussed the meaning of the multi-band approach to quantum transport in semiconductor devices.
- We have focused our attention on the description of a 2-B system by means of Wigner functions.
- We have seen the form of 2-B transport equations for the Kane model.
- We have seen the form of 2-B Madelung-like QHD equation for the Kane model.