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

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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

\[ H = -\frac{\hbar^2}{2m} \Delta + V_{\text{per}} + V \]

with the following:

\[ H_{\text{me}} = -\frac{\hbar^2}{2} \nabla^T M^{-1} \nabla + V \]
The effective-mass approximation (continued)

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

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

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.
Multi-band models

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1 - two-band Kane model:

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

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:

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

Multi-band models (continued)

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

\[ E_c(p) \]
\[ E_v(p) \]

\[ p_0 \]
Multi-band models (continued)

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

![Graph showing dispersion relation with labels E_v and E_c.]
Research program

- Quantum kinetic theory
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- Quantum kinetic theory
- Nonlinear/dissipative Wigner equations
- MB Wigner equations
- MB thermal equilibrium
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- Spintronics

- Applications to electronic devices and BEC
The Wigner transform

The Wigner transform

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

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

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

The quantum Liouville equation

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

is equivalent to the Wigner equation

\[ \frac{\partial}{\partial t} w + \frac{1}{m} \nabla_r \cdot p \ w = \frac{1}{i\hbar} \left[ V \left( r + \frac{i\hbar}{2} \nabla_p \right) - V \left( r - \frac{i\hbar}{2} \nabla_p \right) \right] w \]
How MB Transport Eqs. should look like?

Single band case (no discrete degrees of freedom):

\[ S = \sum_k \lambda_k \psi^k(x)\overline{\psi^k(y)} \]

Wigner transform \[ w(r, p) \]

mixed state \hspace{1cm} \text{Wigner function}
How MB Transport Eqs. should look like?

Single band case (no discrete degrees of freedom):

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

mixed state \quad \text{Wigner function}

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

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

mixed state \quad \text{Wigner matrix}

where \( w_{ij}(r, p) = w_{ji}(r, p) \).
How MBTE should look like? (contd.)

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

\[
\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

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

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

\[
W = w_0 \sigma_0 + w_1 \sigma_1 + w_2 \sigma_2 + w_3 \sigma_3
\]

where the functions $w_k$ are real.
How MBTE should look like? (contd.)

Explicitly:

\[
\begin{align*}
  w_0 &= \frac{1}{2} (w_{11} + w_{22}) \\
  w_1 &= \text{Re} \, w_{12} = \text{Re} \, w_{21} \\
  w_2 &= -\text{Im} \, w_{12} = \text{Im} \, w_{21} \\
  w_3 &= \frac{1}{2} (w_{11} - w_{22})
\end{align*}
\]
How MBTE should look like? (contd.)

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\end{align*}
\]

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

\[
\begin{align*}
    \langle w_0 \rangle^2 &= \langle w_1 \rangle^2 + \langle w_2 \rangle^2 + \langle w_3 \rangle^2, & \text{for a pure state,} \\
    \langle w_0 \rangle^2 &\geq \langle w_1 \rangle^2 + \langle w_2 \rangle^2 + \langle w_3 \rangle^2, & \text{for a mixed state,}
\end{align*}
\]

in analogy with \textbf{Stokes parameters} describing a polarized light beam.
Interpretation

For \( i = 0, 1, 2, 3 \) we have

\[
\text{Tr}(S\sigma_i) = \sum_{k=0}^{3} \int w_k(r, p) \, dr \, dp \, \text{Tr}(\sigma_k\sigma_i)
\]

which, since \( \text{Tr}(\sigma_k\sigma_i) = 2\delta_{kj} \), implies
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$$\int w_0(r, p) \, dr \, dp = 1$$
Interpretation

For \( i = 0, 1, 2, 3 \) we have

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which, since \( \text{Tr}(\sigma_k \sigma_i) = 2\delta_{kj} \), implies

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

and, for \( i = 1, 2, 3 \),

\[
\int w_i(r, p) \, dr \, dp = \frac{1}{2} \times \text{“spin” expectation in direction } i
\]
Interpretation (continued)

In the case of Kane or M-M model:

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ is the observable "band index"}$$
Interpretation (continued)

In the case of Kane or M-M model:

\[ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \] is the observable “band index”

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

\[ \frac{\langle w_3 \rangle}{\langle w_0 \rangle} = \text{local expectation of band-index}. \]
Dynamics

The Kane Hamiltonian can be decomposed as follows:

\[
H = \left( -\frac{1}{2}\Delta + V \right)\sigma_0 - iK \cdot \nabla \sigma_2 + E_g \sigma_3
\]

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.
where

$$\Theta_V = V\left(r + \frac{i\hbar}{2} \nabla p\right) - V\left(r - \frac{i\hbar}{2} \nabla p\right)$$
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

\[
\begin{cases}
(\partial_t - \vec{F} \cdot \nabla_p) w_0 = 0 \\
(\partial_t - \vec{F} \cdot \nabla_p) w_1 = -E_g w_2 + 2K \cdot p w_3 \\
(\partial_t - \vec{F} \cdot \nabla_p) w_2 = E_g w_1 \\
(\partial_t - \vec{F} \cdot \nabla_p) w_3 = -2K \cdot p w_1
\end{cases}
\]
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:

\[
(\partial_t - \vec{F} \cdot \nabla_p)\vec{w} = \vec{B}(p) \wedge \vec{w}
\]

\[ \vec{F} \cdot \nabla_p \vec{w} = \text{momentum drift} \quad \vec{B}(p) \wedge \vec{w} = \text{band transitions} \]
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

\[
\begin{align*}
\partial_t n_0 + \nabla \cdot j_0 &= -\nabla \cdot K n_2 \\
\partial_t n_1 + \nabla \cdot j_1 &= -E_g n_2 + 2K \cdot j_3 \\
\partial_t n_2 + \nabla \cdot j_2 &= -\nabla \cdot K n_0 + E_g n_1 \\
\partial_t n_3 + \nabla \cdot j_3 &= -2K \cdot j_1
\end{align*}
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\end{cases}
\]

Continuity equation for the total density:

\[
\partial_t n_0 + \nabla \cdot (j_0 + K n_2) = 0
\]
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\[
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\]

Continuity equation for the total density:

\[
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\]

\[\Rightarrow \quad K n_2 = \text{interband current}\]
Order-1 moment equations

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

Where:

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

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

\[
T_i = \text{“temperature” term}
\]
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:

\[
T_i \equiv 0, \quad i = 0, 1, 2, 3.
\]
Two-band Madelung equations

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\[ T_i \equiv 0, \quad i = 0, 1, 2, 3. \]

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

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Conclusions

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Conclusions

- 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.