A two-band diffusive model of electron transport in semiconductors

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Outline

1. The quantum kinetic model
2. Scaling the model
3. Quantum diffusive limit
4. Semiclassical limit
5. Numerical experiments
6. Conclusions and future work
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1. The quantum kinetic model
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6. Conclusions and future work
The quantum kinetic model

The Hamiltonian I

An electron moving in a semiconductor crystal, with two relevant energy bands, is approximately described by the \( k \cdot p \)-type Hamiltonian

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

where \( V \) is the “external” electrostatic potential, \( E_g \) is the band-gap and \( K = (K_1, K_2, K_3) \) is the matrix element of the gradient operator between the Bloch functions of the upper (+) and lower (−) band:

\[
K = \int_{\text{lattice cell}} \bar{u}_+(x) \nabla u_-(x) \, dx
\]
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where $V$ is the “external” electrostatic potential, $E_g$ is the band-gap and $K = (K_1, K_2, K_3)$ is the matrix element of the gradient operator between the Bloch functions of the upper (+) and lower (−) band:

$$K = \int_{\text{lattice cell}} \overline{u}_+(x) \nabla u_-(x) \, dx$$
The Hamiltonian II

Putting $\alpha = \hbar K/m$ and $\gamma = E_g/2$, the symbol $h(x, p)$ of $H$ can be written

\[
h(x, p) = \left(\frac{p^2}{2m} + V(x)\right)\sigma_0 + \alpha \cdot p \sigma_2 + \gamma \sigma_3
\]

\[
= h_0(x, p)\sigma_0 + \vec{h}(p) \cdot \vec{\sigma},
\]

where

\[
h_0(x, p) = \frac{p^2}{2m} + V(x), \quad \vec{h}(p) = (0, \alpha \cdot p, \gamma), \quad \vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3).
\]

and $\sigma_i$ are the Pauli matrices

\[
\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]
Mixed states: the operator description

The quantum statistical state of the system (mixed state) is described by a time-dependent, self-adjoint, positive and trace-class operator $S(t), \ t \geq 0$.

Similarly to the Hamiltonian $H$, the operator $S(t)$ acts on the Hilbert space $L^2(\mathbb{R}^3, \mathbb{C}^2)$ (i.e. it is a $2 \times 2$ matrix of operators).

The evolution of $S(t)$ is given by the von Neumann equation

\[ i\hbar \partial_t S(t) = [H, S(t)] \]
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The evolution of $S(t)$ is given by the von Neumann equation

$$i\hbar \frac{\partial}{\partial t} S(t) = [H, S(t)]$$
Mixed states: the Wigner description

The phase-space description of the state $S(t)$ is given by the $2 \times 2$ Wigner matrix $w$, defined by

$$w_{ij}(t) = \text{Op}_\hbar^{-1} [S_{ij}(t)], \quad w_{ij}(t) = w_{ij}(x, p, t),$$

where $\text{Op}_\hbar^{-1}$ denotes the Wigner transform (inverse of the Weyl quantization $\text{Op}_\hbar$).

The matrix $w(x, p, t) = w_{ij}(x, p, t)$ is hermitian and, therefore, can be decomposed in the Pauli basis with real coefficients $w_k$:

$$w = w_0 \sigma_0 + \vec{w} \cdot \vec{\sigma}, \quad \vec{w} = (w_1, w_2, w_3).$$
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Wigner equation

It can be proved that the von Neumann equation leads to the following system for the Pauli-Wigner functions \((w_0, \vec{w})\):

\[
\left( \partial_t + \frac{p}{m} \cdot \nabla_x + \Theta \hbar[V] \right) w_0 + \alpha \cdot \nabla_x w_2 = 0,
\]

\[
\left( \partial_t + \frac{p}{m} \cdot \nabla_x + \Theta \hbar[V] \right) \vec{w} + \alpha \cdot \nabla_x w_0 \vec{e}_2 - \frac{2}{\hbar} \hbar(p) \times \vec{w} = 0,
\]

where \(\hbar(p) = (0, \alpha \cdot p, \gamma)\), \(\vec{e}_2 = (0, 1, 0)\) and \(\Theta \hbar[V]\) is the pseudo-differential operator

\[
\Theta \hbar[V] = \frac{i}{\hbar} \left[ V \left( x + \frac{i\hbar}{2} \nabla_p \right) - V \left( x - \frac{i\hbar}{2} \nabla_p \right) \right]
\]
Wigner-BGK (WBGK) equation

A model taking account of collisional effects can be obtained by adding BGK-like terms to the previous equations:

\[
\begin{align*}
\left( \partial_t + \frac{p}{m} \cdot \nabla_x + \Theta_{\hbar}[V] \right) w_0 + \alpha \cdot \nabla_x w_2 &= - \frac{w_0 - g_0}{\tau_c} \\
\left( \partial_t + \frac{p}{m} \cdot \nabla_x + \Theta_{\hbar}[V] \right) \vec{w} + \alpha \cdot \nabla_x w_0 \vec{e}_2 - \frac{2}{\hbar} \vec{h}(p) \times \vec{w} &= - \frac{\vec{w} - \vec{g}}{\tau_c}.
\end{align*}
\]

Here, \( \tau_c \) is a relaxation time and \((g_0, \vec{g})\) are suitable local-equilibrium Wigner functions, to be specified later on.
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Scaled WBGK equation

The scaled version of the WBGK equation reads as follows:

\[
(\tau \partial_t + p \cdot \nabla_x + \Theta_{\epsilon}[V]) w_0 + \epsilon \alpha \cdot \nabla_x w_2 = -\frac{w_0 - g_0}{\tau}
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\[
(\tau \partial_t + p \cdot \nabla_x + \Theta_{\epsilon}[V]) \vec{w} + \epsilon \alpha \cdot \nabla_x w_0 \vec{e}_2 - 2\hbar(p) \times \vec{w} = -\frac{\vec{w} - \vec{g}}{\tau}.
\]

Here we have introduced two small, dimensionless, parameters:

\[
\epsilon = \frac{\hbar}{p_0 x_0} - \text{semiclassical \ parameter (scaled relaxation time)},
\]

\[
\tau = \frac{p_0 \tau_c}{m x_0} - \text{diffusive \ parameter (scaled Planck constant)}
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(where \(x_0\) and \(p_0 = \sqrt{mk_B T}\) are reference length and momentum).
 scaling the model

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Physical regime

We want to study the behaviour of the system when $\tau$ and $\epsilon$ are small.

The physical meaning is that we assume to be in a diffusive (many collisions) and semiclassical (small Planck constant) regime.

Moreover, we are assuming that the bands are “almost parabolic” (which is the case, e.g., of a semiconductor superlattice). In fact, the scaled energy bands are:

$$E_{\pm}(p) = \frac{1}{2} |p|^2 \pm \epsilon \sqrt{(\alpha \cdot p)^2 + \gamma^2} = \frac{1}{2} |p|^2 \pm \epsilon |\vec{h}(p)|.$$
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\[ \tau \rightarrow 0, \quad \epsilon \sim 1. \]

To this aim we adopt the Chapman-Enskog method.

We need to choose a suitable local equilibrium, represented by the Wigner functions \( (g_0, \tilde{g}) \), used to define the BGK collisional operator in the WBGK equation.
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Local equilibrium I

We assume that *collisions do not produce band-crossing*.

Hence, the BGK operator is assumed to locally conserve the two band densities:

\[
n_{\pm}(x, t) = (N_{\pm}w)(x, t) = \int_{\mathbb{R}^3} \left[ w_0(x, p, t) \pm \vec{v}(p) \cdot \vec{w}(x, p, t) \right] dp
\]

where

\[
\vec{v}(p) = \frac{\vec{h}(p)}{|\vec{h}(p)|} = (0, \alpha \cdot p, \gamma)/\sqrt{(\alpha \cdot p)^2 + \gamma^2}.
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Then, \( g = (g_0, \vec{g}) \) should satisfy the moment condition

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N_{\pm}g = n_{\pm} = N_{\pm}w
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Local equilibrium II

By using the *quantum maximum-entropy principle* it can be shown that two “band chemical potentials” $\mu_{\pm}(x, t)$ exist such that the (scaled) local-equilibrium Wigner function $g^\epsilon = (g_0^\epsilon, \tilde{g}^\epsilon)$ is given by

$$g^\epsilon = \text{Op}_\epsilon^{-1} \left[ \exp(-H_{\mu}^\epsilon) \right]$$

where $H_{\mu}^\epsilon$ is the quantization of

$$h_{\mu}^\epsilon(x, p, t) = [h_0(x, p) + \mu_0(x, t)]\sigma_0 + \epsilon|\tilde{h}(p)| + \mu_s(x, t)]\vec{\nu}(p) \cdot \vec{\sigma},$$

and

$$\mu_0 = \mu_+ + \mu_-, \quad \mu_s = \mu_+ - \mu_-.$$
The moment condition

\[ \mathcal{N}_\pm g = n_\pm = \mathcal{N}_\pm w \]

allows (in principle) to express \( \mu_\pm \) in function of \( n_\pm \).

Then,

\[ g^\epsilon(x, p, t) = g^\epsilon(n_+(x, t), n_-(x, t), p) \]

and \( g^\epsilon \) can be used to close the momentum system by means of the Chapman-Enskog (C-E) procedure.
Local equilibrium III

The moment condition

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and \( g^\epsilon \) can be used to close the momentum system by means of the Chapman-Enskog (C-E) procedure.
Chapman-Enskog procedure I

We can now apply the C-E method to the WBGK equation, that we rewrite in compact form

\[ \tau \partial_t w + T_\epsilon w = \frac{g_\epsilon - w}{\tau}, \]

where

\[ T_\epsilon w = \left( \begin{array}{c}
(p \cdot \nabla_x + \Theta_\epsilon [V]) w_0 + \epsilon \alpha \cdot \nabla_x w_2 \\
(p \cdot \nabla_x + \Theta_\epsilon [V]) \tilde{w} + \epsilon \alpha \cdot \nabla_x w_0 \tilde{e}_2 - 2\hat{h}(p) \times \tilde{w}
\end{array} \right). \]

Expanding \( w = w^{(0)} + \tau w^{(1)} + \cdots \), we obtain

\[ w^{(0)} = g_\epsilon, \]

\[ w^{(1)} = -T_\epsilon w^{(0)} = -T_\epsilon g_\epsilon. \]
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Expanding \( w = w^{(0)} + \tau w^{(1)} + \ldots \), we obtain

\[ w^{(0)} = g^\epsilon, \]
\[ w^{(1)} = -T_\epsilon w^{(0)} = -T_\epsilon g^\epsilon. \]
Applying $N_\pm$ to both sides of the WBGK equation we get an equation for $n_\pm = N_\pm w$

$$\tau \partial_t n_\pm + N_\pm T_\epsilon w = 0$$

Now, substituting $w \approx w^{(0)} + \tau w^{(1)} = g^\epsilon - \tau T_\epsilon g^\epsilon$, at first order we obtain

$$\partial_t n_\pm = N_\pm T_\epsilon T_\epsilon g^\epsilon,$$

which is (in principle) a closed equation because $g^\epsilon = g^\epsilon(n_+, n_-, p)$.

Such equation is our quantum diffusive model of two-band electron transport in semiconductors.
Applying $\mathcal{N}_\pm$ to both sides of the WBGK equation we get an equation for $n_\pm = \mathcal{N}_\pm w$

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Semiclassical expansion of the diffusive model

The quantum diffusive model

\[
\partial_t n_\pm = \mathcal{N}_\pm T_\epsilon T_\epsilon g^\epsilon,
\]

is extremely complicated, especially due to the structure of \(g^\epsilon = g^\epsilon(n_+, n_-, p)\).

However, in most applications the parameter \(\epsilon\) (left untouched so far) is very small and, therefore, the previous model should be semiclassically expanded.

First of all, we have \(T_\epsilon = T_0 + \epsilon T_1 + \cdots\), with

\[
T_0 w = (p \cdot \nabla_x - \nabla V \cdot \nabla p) \left( \begin{array}{c} w_0 \\ \vec{w} \end{array} \right) - 2 \left( \begin{array}{c} 0 \\ \vec{h}(p) \times \vec{w} \end{array} \right)
\]
Semiclassical limit

Semiclassical expansion of the diffusive model

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\[ T_0 w = (p \cdot \nabla_x - \nabla V \cdot \nabla p) \left( \frac{w_0}{\vec{w}} \right) - 2 \left( \frac{0}{\vec{h}(p) \times \vec{w}} \right) \]
Semiclassical expansion of the diffusive model

The quantum diffusive model

\[ \partial_t n_{\pm} = \mathcal{N}_{\pm} \, T_{\epsilon} \, T_{\epsilon} \, g^\epsilon, \]

is extremely complicated, especially due to the structure of \( g^\epsilon = g^\epsilon(n_+, n_-, p) \).

However, in most applications the parameter \( \epsilon \) (left untouched so far) is very small and, therefore, the previous model should be semiclassically expanded.

First of all, we have \( T_{\epsilon} = T_0 + \epsilon T_1 + \cdots \), with

\[ T_0 w = (p \cdot \nabla_x - \nabla V \cdot \nabla p) \begin{pmatrix} w_0 \\ \vec{w} \end{pmatrix} - 2 \begin{pmatrix} 0 \\ \vec{h}(p) \times \vec{w} \end{pmatrix} \]
Moreover, it can be shown that

\[ g^{\varepsilon} = g^{(0)} + \varepsilon g^{(1)} + \varepsilon^2 g^{(2)} + \ldots \]

where \( g^{(0)} \) is given by

\[ g^{(0)} = \frac{1}{2} \left( \begin{array}{c} \phi_+ + \phi_- \\ (\phi_+ - \phi_-) \vec{v} \end{array} \right) \]

with

\[ \phi_{\pm} = \phi_{\pm}(x, p, t) = (2\pi)^{-3/2} n_{\pm}(x, t) e^{-p^2/2} \]
Semiclassical diffusive model

Then, at order 0 in $\epsilon$ we can write

$$\partial_t n_{\pm} = \mathcal{N}_\pm T_0 T_0 g^{(0)}$$

which can be explicitly computed and yields the semiclassical diffusive model:

$$\left\{ \begin{aligned} \partial_t n_+ &= \Delta n_+ + \text{div}(\nabla V n_+) + \omega(V)(n_- - n_+) \\ \partial_t n_- &= \Delta n_- + \text{div}(\nabla V n_-) - \omega(V)(n_- - n_+) \end{aligned} \right.$$

where

$$\omega(V) = \frac{\gamma^2 (\alpha \cdot \nabla V)^2}{2(2\pi)^{3/2}} \int \frac{e^{-p^2/2}}{(\alpha \cdot p)^2 + \gamma^2} \, dp$$
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Numerical experiments

Parameter values

We performed some numerical experiments (in the one-dimensional case) with the following parameter values:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>reference length ( x_0 )</td>
<td>( 0.5 \times 10^{-7} ) m;</td>
</tr>
<tr>
<td>temperature ( T )</td>
<td>300 K</td>
</tr>
<tr>
<td>typical collision time ( \tau_c )</td>
<td>( 10^{-14} ) sec</td>
</tr>
<tr>
<td>reference time (computed) ( t_0 )</td>
<td>( 5.5 \times 10^{-11} ) sec</td>
</tr>
<tr>
<td>band gap ( E_g )</td>
<td>0.1 eV</td>
</tr>
<tr>
<td>effective mass ( m^* )</td>
<td>0.9</td>
</tr>
<tr>
<td>( \alpha ) (computed from ( E_g ) and ( m^* ))</td>
<td>( 3.1 \times 10^4 ) m/sec</td>
</tr>
</tbody>
</table>

In this case

\[ \tau = 0.014, \quad \epsilon = 0.034. \]
Simulations

In the following simulations we inject electrons from the left in the upper band.

In the “transient” case the input is switched on for a small amount of time while, in the “stationary” case, the input is stationary and the system reaches a steady state.
Numerical experiments

Constant field (transient)
Numerical experiments

Constant field (stationary)

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Quantum drift-diffusion modeling

SIMAI 2008 28 / 37
Constant field + step (transient)
Numerical experiments

Constant field + step (stationary)

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Quantum drift-diffusion modeling

SIMAI 2008 30 / 37
Constant field + well (transient)

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Numerical experiments

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Conclusions

- We have investigated the electron transport in a two-band semiconductor device.

- Starting at the kinetic from a kinetic Wigner-BGK equation, using the quantum maximum-entropy principle and the C-E method, we have first obtained a quantum diffusive model ($\tau \to 0, \epsilon \sim 1$).

- Then, the model has been semiclassically expanded ($\epsilon \to 0$) and we have obtained, at order 0, a drift-diffusion system with a (potential-dependent) generation/recombination-like coupling term.
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Conclusions

- We have investigated the electron transport in a two-band semiconductor device.

- Starting at the kinetic from a kinetic Wigner-BGK equation, using the quantum maximum-entropy principle and the C-E method, we have first obtained a quantum diffusive model \((\tau \to 0, \epsilon \sim 1)\).

- Then, the model has been semiclassically expanded \((\epsilon \to 0)\) and we have obtained, at order 0, a drift-diffusion system with a (potential-dependent) generation/recombination-like coupling term.
Future work

- We wish to do more serious numerical experiments, by nonlinearly coupling the drift-diffusion system with the Poisson equation for the potential $V$.

- We wish to perform a rigorous analysis of the diffusive and semiclassical limit by adapting the Mika-Banasiak theory.

- We wish to consider more terms in the semiclassical expansion (this should lead to $O(\hbar^2)$ Bohm-potential-like terms).
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Thank you!