Derivation of quantum drift-diffusion equations for a spin-orbit 2D electron gas

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RECENT ADVANCES IN KINETIC EQUATIONS AND APPLICATIONS

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Outline

Physics

Mathematical modelling

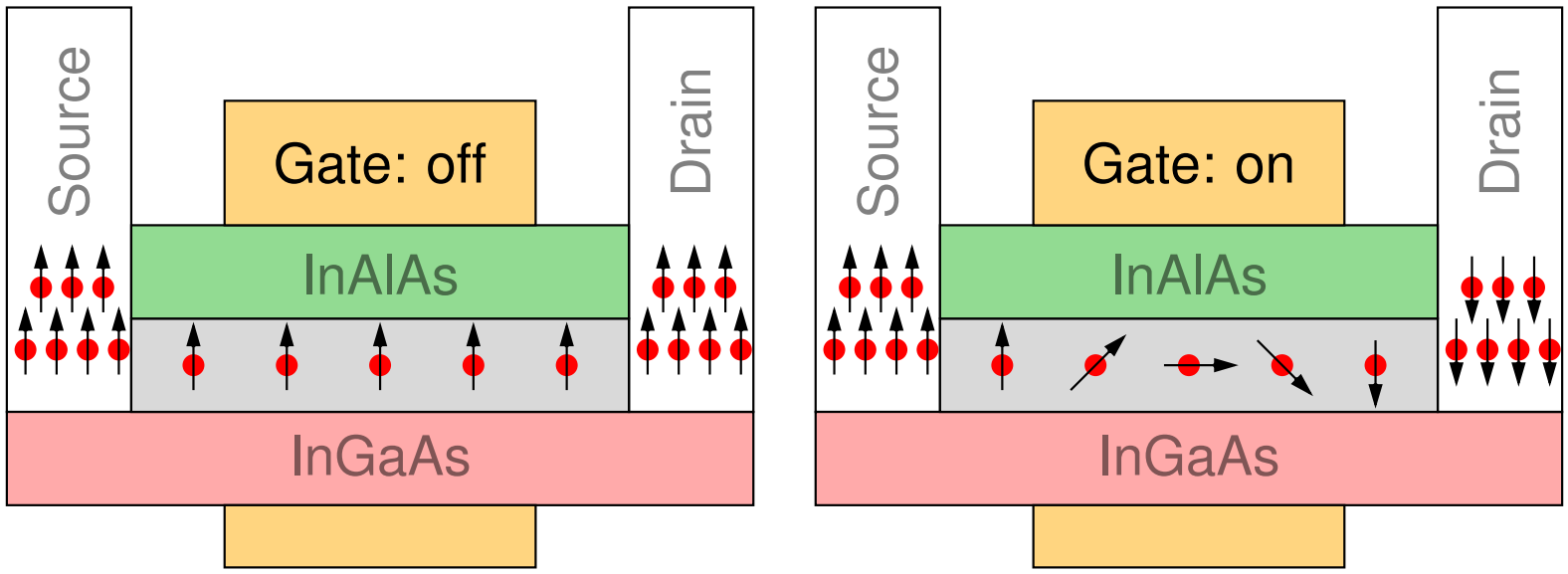
Transport picture

Quantum drift-diffusion equations

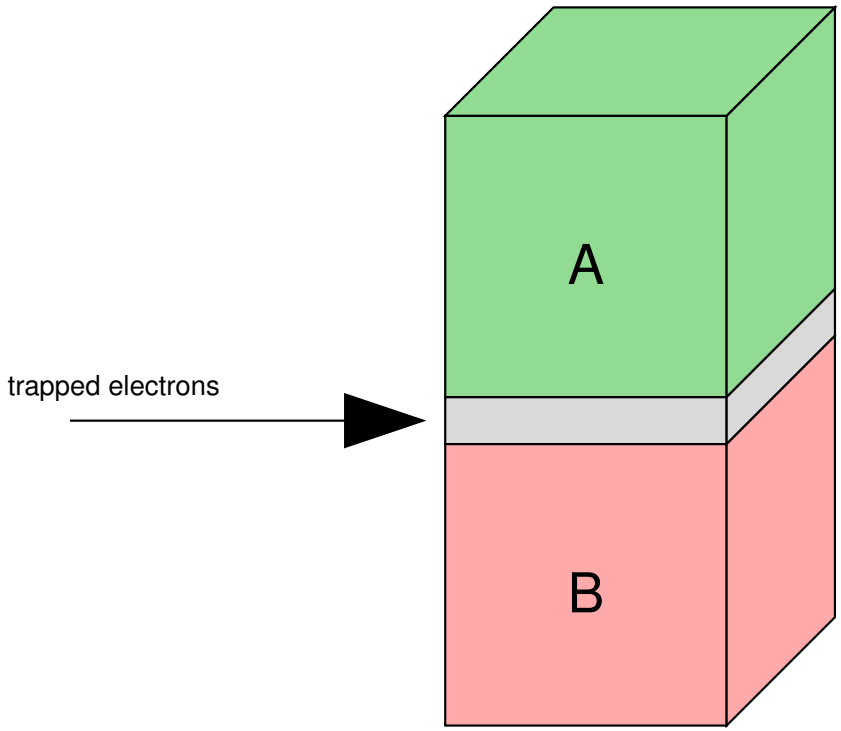
Semiclassical drift-dffusion equations

Conclusions

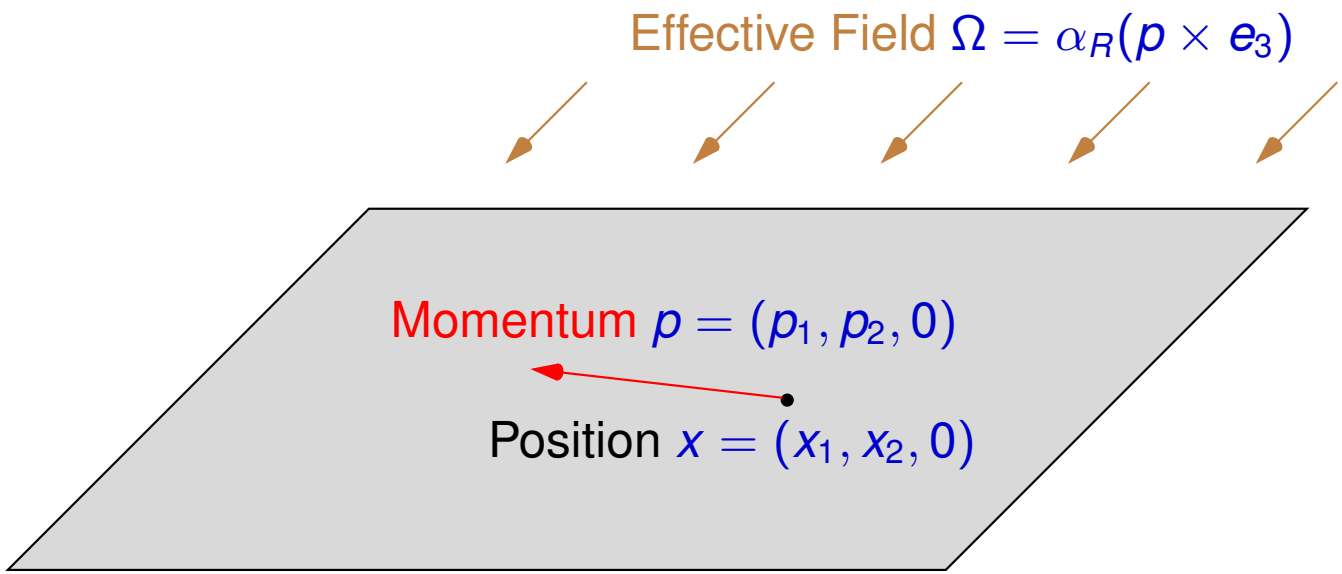
Spintronics (not to be confused with quantum computing)



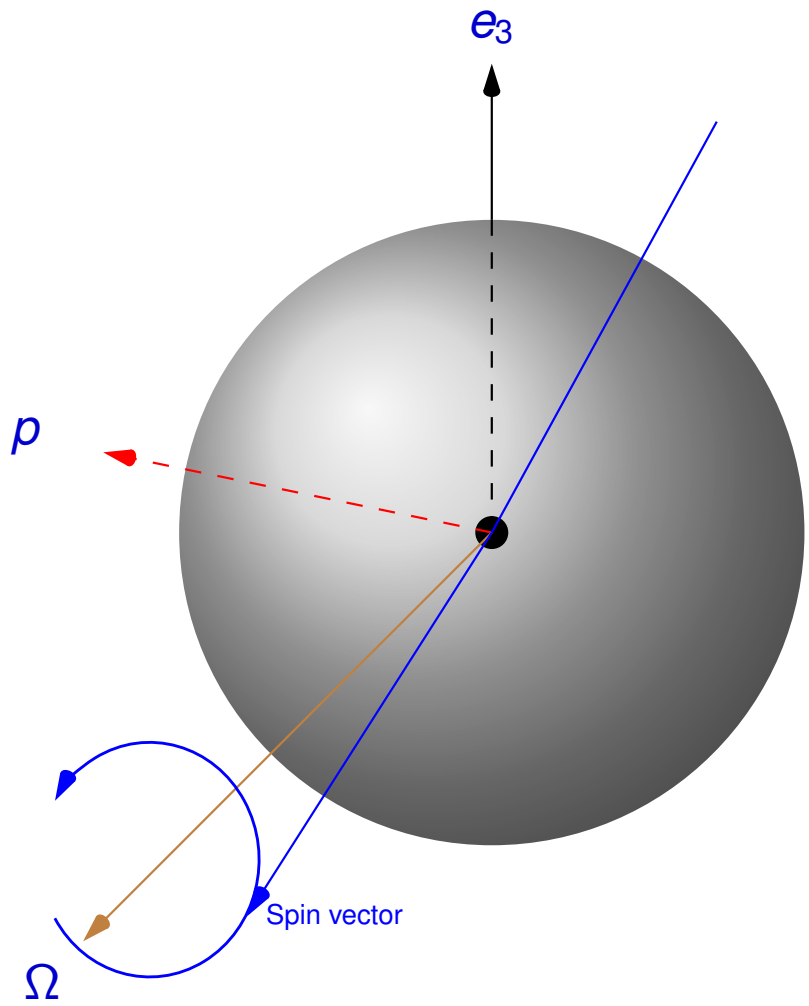
The Rashba effect



The Rashba effect



The Rashba effect



The Rashba Hamiltonian

$$H_R = \left(-\frac{\hbar^2}{2m}\Delta + V\right) I - i\hbar\alpha \begin{pmatrix} 0 & i\partial_2 - \partial_1 \\ i\partial_2 + \partial_1 & 0 \end{pmatrix}$$

α = Rashba constant.

V = external (e.g. gate) potential

$\partial_1 \equiv \frac{\partial}{\partial x_1}$, $\partial_2 \equiv \frac{\partial}{\partial x_2}$

Diffusive models of spin-orbit transport

	Spin structure	Dynamics	Collisions
El Hajj (2008) - CMS (2014)	BIPOLAR/FULL	CLASSICAL	BGK
Barletti-Méhats JMP (2010)	BIPOLAR	QUANTUM	(Q)BGK
Negulescu-Possanner, KRM (2011)	FULL	CLASSICAL	DETAILED
This work	FULL	QUANTUM	(Q)BGK

Fundamental tool: the Wigner transform

$$a(x,p) = \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} \rho_A\left(x + \frac{\xi}{2}, x - \frac{\xi}{2}\right) \mathrm{e}^{-i\xi\cdot p/\hbar}\, d\xi.$$

Provides a 1-1 correspondence $\mathcal{W}$ between a QM operator A (with formal kernel $\rho_A(x,y)$) and a phase-space function $a(x,p)$

$$a = \mathcal{W}(A)$$

Moyal product - definition

The operator algebra is transferred to phase-space functions, which defines the *Moyal product:*

$$a\#b = \mathcal{W}(AB)$$

(where $a = \mathcal{W}(A)$ and $b = \mathcal{W}(B)$).

Moyal product - semiclassical expansion

The Moyal product can be semiclassically expanded as follows:

$$a\#b = \sum_{k=0}^{\infty} \hbar^k \, a\#_k b,$$

$$a\#_k b = \frac{1}{(2i)^k} \sum_{|\alpha|+|\beta|=k} \frac{(-1)^{|\alpha|}}{\alpha!\,\beta!} \left(\nabla_x^\alpha \nabla_p^\beta a\right) \left(\nabla_p^\alpha \nabla_x^\beta b\right).$$

In particular,

$$a\#_0 b = ab, \qquad a\#_1 b = \frac{i}{2}\{a, b\}.$$

Wigner equation - 1

By applying the Wigner transform to the Schrödinger equation

$$i\hbar\partial_t\psi = H_R\psi$$

we obtain the Wigner equation for our system

$$\begin{cases} \partial_t w_0 + p\cdot\nabla w_0 + \alpha\nabla^\perp\cdot\vec{w} - \Theta[V]w_0 = 0 \\ \partial_t\vec{w} + p\cdot\nabla\vec{w} + \alpha\nabla^\perp w_0 + -\Theta[V]\vec{w} - \dfrac{2\alpha}{\hbar}\,p^\perp\times\vec{w} = 0 \end{cases}$$

where w_0 and $\vec{w} = (w_1, w_2, w_3)$ are the Pauli components of the Wigner matrix w

$$w = w_0 I + \vec{w}\cdot\vec{\sigma} = \mathcal{W}(\psi\psi^*)$$

Wigner equation - 2

We have used the following notations:

$$p^{\perp} := p \times e_3 = (p_2, -p_1, 0)$$

$$\nabla^{\perp} := \nabla \times e_3 = (\partial_2, -\partial_1, 0),$$

$$\Theta[V] := \frac{1}{i\hbar}\left[V\left(x + \frac{i\hbar}{2}\nabla_p\right) - V\left(x - \frac{i\hbar}{2}\nabla_p\right)\right]$$

(Scaled) Wigner-BGK equation

Add a BGK-like collisional term and rescale variables:

$$\begin{cases} \partial_t w_0 + p \cdot \nabla w_0 + \epsilon\alpha \nabla^\perp \cdot \vec{w} - \Theta[V] w_0 = \dfrac{g_0 - w_0}{\tau} \\ \partial_t \vec{w} + p \cdot \nabla \vec{w} + \epsilon\alpha \nabla^\perp w_0 - \Theta[V] \vec{w} - 2\alpha\, p^\perp \times \vec{w} = \dfrac{\vec{g} - \vec{w}}{\tau} \end{cases}$$

ϵ = scaled Planck constant
τ = scaled collision time

Quantum equilibrium

"Quantum Maxwellian":

$$g = \mathcal{E}xp(-h_R + a) = \mathcal{W}\left[\exp(-H_R + A)\right]$$

a = matrix of Lagrange multipliers

Constraint of assigned density:

$$\langle g \rangle := \int g(x,p)\, dp = n$$

Assumption of *small polarization regime*:

$$n = n_0 I + \epsilon \vec{n} \cdot \vec{\sigma}$$

Chapman-Enskog expansion

In this part we consider the diffusive limit

$$\tau \ll 1$$

in the fully-quantum regime

$$\epsilon \sim 1$$

We rewrite the Wigner-BGK equation in the concise form

$$\tau \partial_t w + \tau T_\epsilon w = g - w$$

Note that this is *not* a diffusive scaling.

Chapman-Enskog expansion: standard case

Usually the C-E expansion works as follows:

$$\tau^2 \partial_t w + \tau T w = g - w, \qquad w = w^{(0)} + \tau w^{(1)} + \tau^2 w^{(2)} + \dots$$

Then:

$$w^{(0)} = g, \qquad w^{(1)} = -Tg, \quad \dots$$

and, by integration w.r.t. p,

$$\tau \partial_t n = -\langle Tg \rangle + \tau \langle TTg \rangle$$

which is only compatible with $\langle Tg \rangle = 0$ (the equilibrium carries no current).

Chapman-Enskog expansion: quantum case

Theorem

Let g be the quantum Maxwellian (depending on the Lagrange multipliers a and subject to the density constraint $\langle g \rangle = n$). Then

$$\langle Tg \rangle = -i\,[a, n] = 2\vec{a} \times \vec{n} \cdot \vec{\sigma}$$

Then, in the non-commutative case, the equilibrium state *does* carry a nonvanishing current.

That is why a change of the scaling is required.

Quantum DD equations

Our modified C-E method leads to

$$\partial_t n = -\langle T_\epsilon g\rangle + \tau\langle T_\epsilon T_\epsilon g\rangle - \tau\langle T_\epsilon \frac{\delta g}{\delta n}\,\partial_t^{(0)} n\rangle$$

Explicitly yields the quantum DD equations (QDDE):

$$\partial_t n_0 = \tau\partial_j\left[n_0\partial_j(a_0+V) + \epsilon^2\vec{n}\cdot\partial_j\vec{a}\right] - 2\tau\epsilon^2\alpha\nabla^\perp\cdot(\vec{a}\times\vec{n})$$

$$\begin{aligned}\partial_t\vec{n} = {} & 2\epsilon\,\vec{a}\times\vec{n} + \tau\epsilon\,\partial_j\left[\vec{n}\,\partial_j(a_0+V) + n_0\partial_j\vec{a} - 2\vec{a}\times\langle p_j\vec{g}\rangle\right] \\ & - 2\tau\epsilon\alpha\nabla^\perp(a_0+V)\times\vec{n} - 2\tau\epsilon\alpha(\nabla^\perp\times\vec{a})n_0 \\ & + 2\tau\alpha\langle p^\perp\cdot\vec{g}\rangle\vec{a} - 2\tau\alpha\langle(\vec{a}\cdot p^\perp)\vec{g}\rangle\end{aligned}$$

Drawbacks

Remember that a depend on n through the constraint

$$\langle \mathcal{E}xp(-h_R + a) \rangle = n$$

- very implicit
- very non-local
- few numerical methods available [Gallego-Méhats (2005), B.-Méhats-Negulescu-Possanner (2015)]

Expansion of equilibrium state: method

We now assume $\epsilon \ll 1$ and perform a semiclassical expansion of the quantum Maxwellian $g = \mathcal{E}xp(-h_R + a)$.

This can be computed by using

$$g(\beta) := \mathcal{E}xp\left(-\beta(h_R + a)\right)$$

so that

$$\partial_\beta g(\beta) = -(h_R - a)\#g(\beta), \qquad g(0) = I$$

or, for the Laplace transform $\hat{g}(z)$,

$$\hat{g}(z) - I = -(h_R - a)\#\hat{g}(z)$$

Expansion of equilibrium state: method

Now we expand

$$h_R = h_0 + \epsilon h_1$$

(where $h_0 = \frac{|p|^2}{2} + V$ and $h_1 = \alpha p^\perp \times \vec{\sigma}$)

$$\# = \#_0 + \epsilon \#_1 + \epsilon^2 \#_2 + \cdots$$

$$g = g^{(0)} + \epsilon g^{(1)} + \epsilon^2 g^{(2)} + \cdots$$

and substitute into the equation for $\hat{g}(z)$.

Expansion of equilibrium state: method

We obtain in this way

$$\hat{g}^{(0)}(z) = R(z) := \frac{1}{z + \frac{|p|^2}{2} + V - a_0}$$

and (omitting z)

$$\hat{g}^{(1)} = R\, h_1\, R + R\, h_0 \#_1 R$$

$$\hat{g}^{(2)} = R\left[R^2 h_1^2 + h_1 \#_1 R + h_0 \#_1 (R^2 h_1) + h_0 \#_2 R\right]$$

Expansion of equilibrium state: result

Computations yield:

$$g_0^{(0)} = \mathrm{e}^{-\frac{p^2}{2}-V+a_0}$$

$$\vec{g}^{(0)} = \vec{0}$$

$$g_0^{(1)} = 0$$

$$\vec{g}^{(1)} = \mathrm{e}^{-\frac{p^2}{2}-V+a_0}(\vec{a} - \alpha p^{\perp})$$

$$g_0^{(2)} = \frac{\mathrm{e}^{-\frac{p^2}{2}-V+a_0}}{2}\left[|\vec{a} - \alpha p^{\perp}|^2 - \frac{1}{2}\left(p_i p_j \partial_i \partial_j a_0 - |\nabla a_0|^2 - 3\Delta a_0\right)\right]$$

$$\vec{g}^{(2)} = 0$$

Expansion of the Lagrange multipliers

$$a_0^{(0)} = \log\left(\frac{n_0}{c}\right)$$

$$\vec{a}^{(0)} = \frac{\vec{n}}{n_0}$$

$$a_0^{(1)} = 0$$

$$\vec{a}^{(1)} = 0$$

$$a_0^{(2)} = -\left(\alpha^2 + \frac{1}{2}\frac{|\vec{n}|^2}{n_0^2} + \frac{1}{6}\frac{\Delta\sqrt{n_0}}{\sqrt{n_0}}\right)$$

($\vec{a}^{(2)}$ is not needed)

Substituting into the QDDE yields the following

$\mathcal{O}(\epsilon^2)$ DD equations

$$\begin{cases} \partial_t n_0 = \tau \partial_j \left(\partial_j n_0 + n_0 \partial_j V \right) - \tau \epsilon^2 \dfrac{1}{6} n_0 \partial_j \dfrac{\Delta \sqrt{n_0}}{\sqrt{n_0}} \\ \partial_t \vec{n} = \tau \epsilon \partial_j \left(\partial_j \vec{n} + \vec{n} \partial_j V \right) - 2\tau\epsilon\alpha^2 \vec{n} \\ \qquad\qquad - 2\tau\epsilon\alpha \left(2\nabla^\perp + \nabla^\perp V - \dfrac{\nabla^\perp n_0}{n_0} \right) \times \vec{n} \end{cases}$$

- drift-diffusion
- Bohm potential
- D'yakonov–Perel' spin decoherence
- spin-orbit coupling and gate control

Summary

- QDD equation for spin-orbit electrons
- $\mathcal{O}(\epsilon^2)$-DD approximation
- assumption of small polarization regime
- previous models arising as particular cases

Future work

- drop the small polarization assumption
- proceed with HD
- extend to other spin-orbit Hamiltonians

Thank you!