

A microscopic approach to spin dynamics: about the meaning of spin relaxation times

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- Motivation
- Spin relaxation in semiconductors
- The concept of Bloch equations
- The spin-dependent Bloch equations
 - An extension of the optical Bloch equations
 - Comparison with experimental observables
- Conclusion

- Reaching limits of conventional semiconductor technologies (e.g. transistors)
 - leakage currents
 - heat

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(not only electronic devices, also optical devices)

- Reaching limits of conventional semiconductor technologies (e.g. transistors)
 - leakage currents
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- Possible solution: **Spintronics**
 - ⇒ *Usage of the spin degree-of-freedom of carriers*
(not only electronic devices, also optical devices)
- Limits of spintronics:
 - spin injection
 - ⇒ **spin relaxation and spin dephasing**

D'yakonov Perel' (DP) mechanism

- Origin: spin-orbit (SO) interaction in systems without **inversion-symmetry**
→ band splitting: $E_{\uparrow}(\mathbf{k}) \neq E_{\downarrow}(\mathbf{k})$

Structure of SO interaction: $\mathcal{H}_{SO} \sim \sigma \cdot \mathbf{B}(\mathbf{k})$

→ splitting corresponds to an effective **k-dependent** magnetic field $\mathbf{B}(\mathbf{k})$

⇒ **precession** of the spins around $\mathbf{B}(\mathbf{k})$

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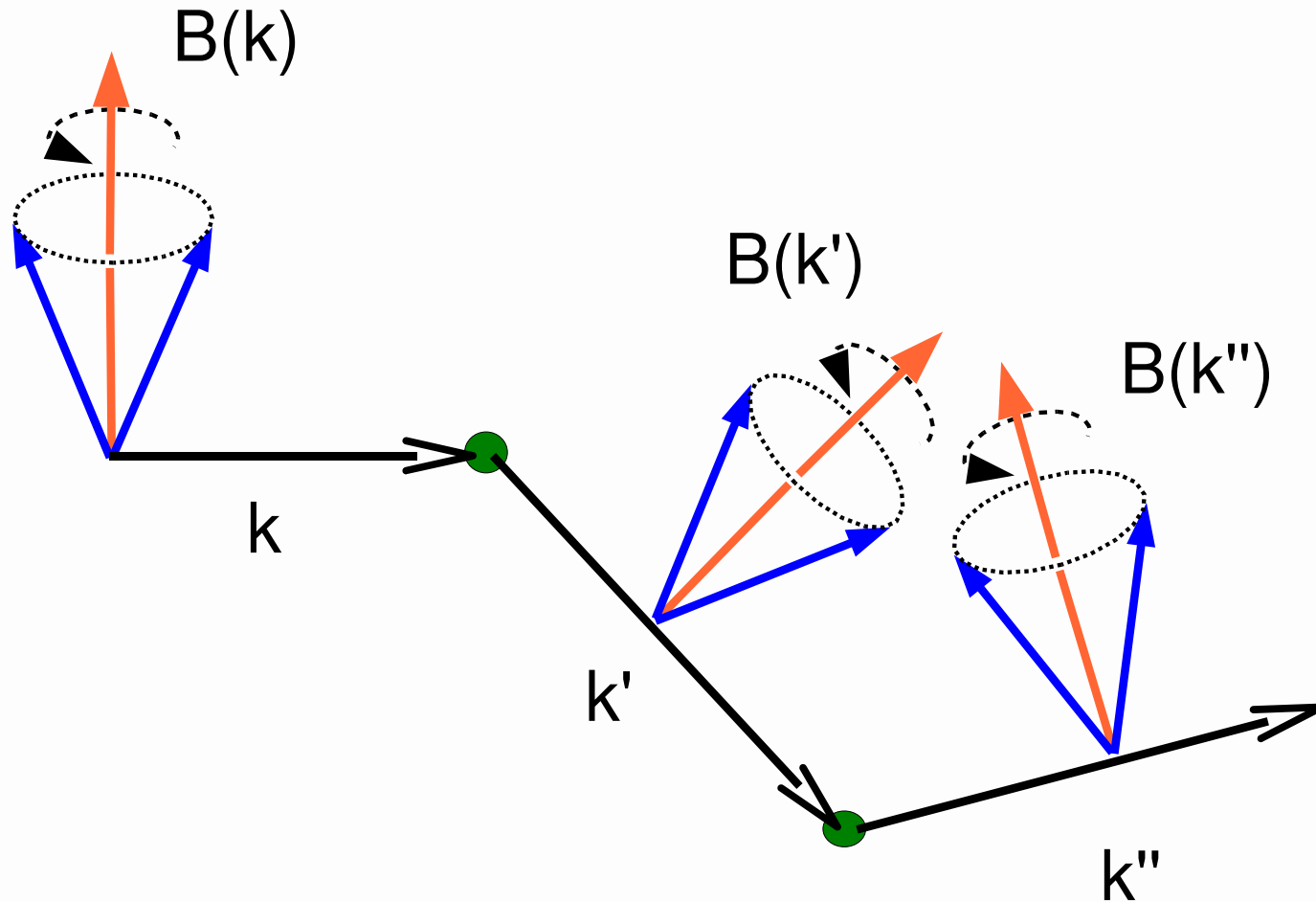
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- In addition: **scattering**
 - change of the $\mathbf{k}$ -vector of the electrons
 - change of the magnetic field $\mathbf{B}(\mathbf{k})$

Spin relaxation DP II



⇒ Spin relaxation

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- Characteristics:
spin relaxation time $\leftrightarrow$ scattering time
(*motional narrowing*)

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- Sources of inversions-asymmetry:
bulk inversion-asymmetry (BIA/Dresselhaus)

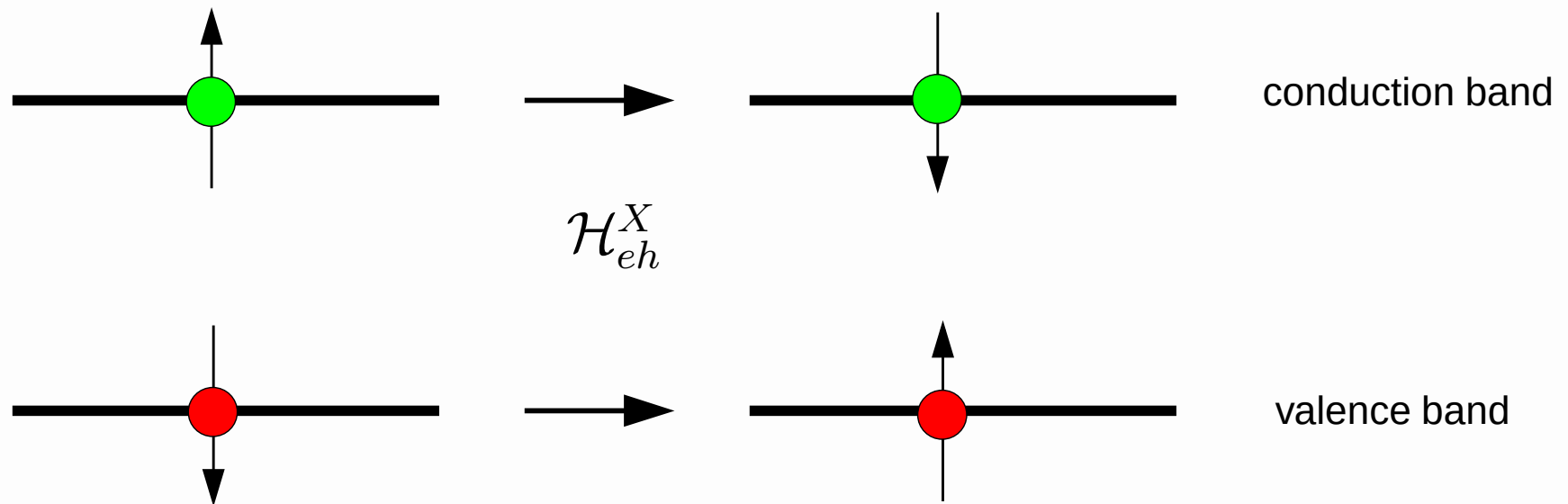
$$B(\mathbf{k}) \sim k^3$$

structure inversion-asymmetry (SIA/Rashba)

$$B(\mathbf{k}) \sim k$$

Bir Aronov Pikus (BAP) mechanism

- Scattering of electrons and holes due to **Coulomb-exchange interaction** possible
 - simultaneous spin-flip of electrons and holes
 - ⇒ restriction on electron system: spin relaxation



Elliott Yafet (EY) mechanism

- **SO interaction** leads to **admixture** of hole states in the valence band to electron states in the conduction band with opposite spin
 - no pure states
 - ⇒ **direct spin flip** scattering possible
- Characteristics:
spin relaxation time $\leftrightarrow$ scattering time

$$\tau_s \sim \tau_p$$

- What is one of the best methods to describe dynamics in optically excited semiconductors?

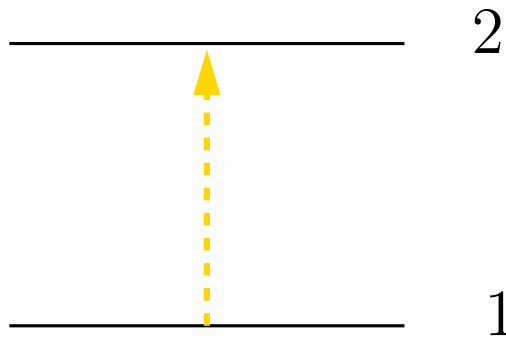
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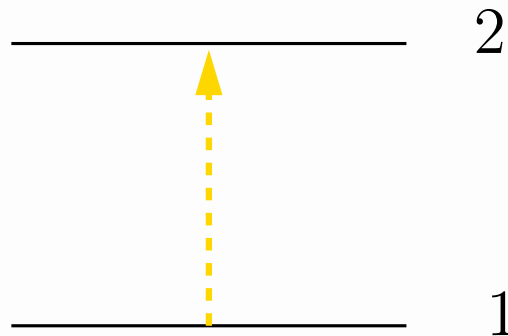
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Bloch equations

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Dynamical variables of the system:

occupation difference

coherence

- Description by 2×2 density matrix:

$$\varrho_{ij} := \langle c_i^\dagger c_j \rangle = \begin{cases} i = j & \text{occupation number} \\ i \neq j & \text{coherence} \end{cases}$$

- Equations of motion (EOM) given by *Liouville equation*

$$i \hbar \partial_t \varrho = [\mathcal{H}, \varrho]_-$$

- Decay of the components:
 - occupation number T_1 ($\rightarrow$ diagonal entries)
 - coherence T_2 ($\rightarrow$ offdiagonal entries)

- Possibility 1: classification of the spin states with respect to a **fixed quantization axis** (e.g. growth direction of a QW)

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- spin-up and spin-down electrons in the conduction band define two-level system (coupling via **SO interaction**)

$$\varrho(\mathbf{k}) := \begin{pmatrix} \varrho_{\uparrow\uparrow}(\mathbf{k}) & \varrho_{\uparrow\downarrow}(\mathbf{k}) \\ \varrho_{\downarrow\uparrow}(\mathbf{k}) & \varrho_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix}$$

Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{light} + \mathcal{H}_{scatt}$$

- Hamiltonian for a QW system with SO interaction

$$\mathcal{H}_0 = \sum_{\substack{\sigma \sigma' \\ \mathbf{k}'}} \left\{ \epsilon(\mathbf{k}') + \mathbf{h}(\mathbf{k}') \frac{\sigma_{\sigma \sigma'}}{2} \right\} c_{\sigma}^{\dagger}(\mathbf{k}') c_{\sigma'}(\mathbf{k}')$$

SO interaction: $\mathbf{h}(\mathbf{k}) = \left(h_x(\mathbf{k}), h_y(\mathbf{k}), 0 \right)$

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- EOM:

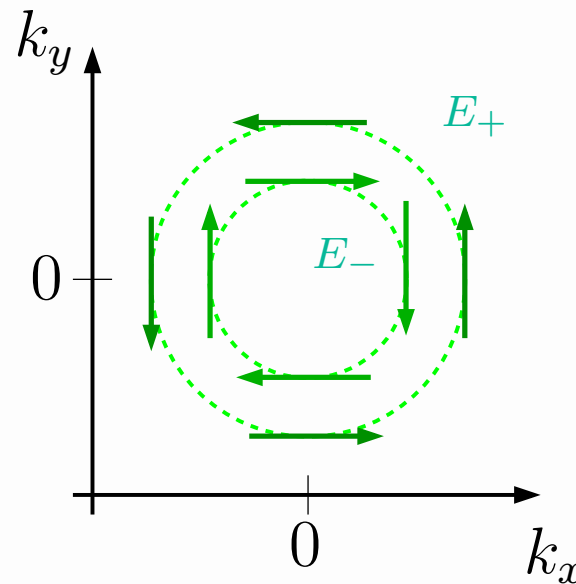
$$\partial_t \varrho_{\uparrow\uparrow}(\mathbf{k}) = -\frac{1}{\hbar} \left(h_x(\mathbf{k}) \Im\{\varrho_{\uparrow\downarrow}(\mathbf{k})\} - h_y(\mathbf{k}) \Re\{\varrho_{\uparrow\downarrow}(\mathbf{k})\} \right)$$

$$\partial_t \varrho_{\downarrow\downarrow}(\mathbf{k}) = \frac{1}{\hbar} \left(h_x(\mathbf{k}) \Im\{\varrho_{\uparrow\downarrow}(\mathbf{k})\} - h_y(\mathbf{k}) \Re\{\varrho_{\uparrow\downarrow}(\mathbf{k})\} \right)$$

$$\partial_t \varrho_{\uparrow\downarrow}(\mathbf{k}) = \frac{1}{2\hbar} \left(i h_x(\mathbf{k}) - h_y(\mathbf{k}) \right) \left(\varrho_{\uparrow\uparrow}(\mathbf{k}) - \varrho_{\downarrow\downarrow}(\mathbf{k}) \right)$$

Bloch equations with spin

- Aim: microscopic theory of spin relaxation based on the **Bloch equations**
- Formulation with **diagonal** kinetic part of Hamiltonian
 - Eigenstates
 - ⇒ Spin ($\pm \mathbf{m}_c$) depends on wavevector $\mathbf{k}$



- scattering described in the density matrix formalism
→ restriction on electron-phonon scattering

⇒ Extension of the *optical* Bloch equations

- Starting point: six-level system
- Spin polarization is controlled by excitation with circularly polarized light

Bloch equations with spin III

- Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{light} + \mathcal{H}_{phonon}$$

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- Kinetic contribution:

$$\mathcal{H}_0 = \sum_{\mathbf{k}' m'_c} \epsilon_{m'_c}(\mathbf{k}') c_{m'_c}^\dagger(\mathbf{k}') c_{m'_c}(\mathbf{k}') + \sum_{\mathbf{k}' m'_v} \epsilon_{m'_v}(\mathbf{k}') v_{m'_v}(\mathbf{k}') v_{m'_v}^\dagger(\mathbf{k}')$$

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- **Hamiltonian is diagonal**

→ spin precession contained in **eigenenergies** $\epsilon_{m_i}(\mathbf{k})$

[↻]

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- **Hamiltonian is diagonal**

→ spin precession contained in **eigenenergies** $\epsilon_{m_i}(\mathbf{k})$
[↻]

- Interaction with the light field:

$$\mathcal{H}_{light} = - \sum_{\substack{m'_c m'_v \\ \mathbf{k}'}} \left\{ \mathbf{E}(t) \cdot \mathbf{d}_{m'_c m'_v}^{cv}(\mathbf{k}') c_{m'_c}^\dagger(\mathbf{k}') v_{m'_v}^\dagger(\mathbf{k}') + \text{h.c.} \right\}$$

Bloch equations with spin VI

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$$+ \sum_{\mathbf{k}' \mathbf{q}} \left\{ \sum_{m'_c m''_c} \left(g_{m'_c m''_c}^e(\mathbf{q}) c_{m''_c}^\dagger(\mathbf{k}' + \mathbf{q}) b(\mathbf{q}) c_{m'_c}(\mathbf{k}') \right. \right.$$

$$\left. \left. + \text{h.c.} \right) \right\}$$

- Electron-phonon interaction $\mathcal{H}_{phonon}$:

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 \mathcal{H}_{phonon} = & \sum_{\mathbf{q}} \hbar \omega(\mathbf{q}) b^\dagger(\mathbf{q}) b(\mathbf{q}) \\
 & + \sum_{\mathbf{k}' \mathbf{q}} \left\{ \sum_{m'_c m''_c} \left(g_{m'_c m''_c}^e(\mathbf{q}) c_{m''_c}^\dagger(\mathbf{k}' + \mathbf{q}) b(\mathbf{q}) c_{m'_c}(\mathbf{k}') \right. \right. \\
 & \quad \left. \left. + \text{h.c.} \right) \right. \\
 & \quad \left. + \sum_{m'_v m''_v} \left(g_{m'_v m''_v}^h(\mathbf{q}) v_{m''_v}^\dagger(\mathbf{k}' + \mathbf{q}) b(\mathbf{q}) v_{m'_v}(\mathbf{k}') \right) \right. \\
 & \quad \left. + \text{h.c.} \right)
 \end{aligned}$$

- Restriction to conduction band
→ 2×2 density matrix:

$$\varrho^{(m_c \bar{m}_c)}(\mathbf{k}) = \begin{pmatrix} \varrho_{m_c m_c}(\mathbf{k}) & \varrho_{m_c -m_c}(\mathbf{k}) \\ \varrho_{-m_c m_c}(\mathbf{k}) & \varrho_{-m_c -m_c}(\mathbf{k}) \end{pmatrix}$$

- Scattering treated in 2nd order Born approximation

- EOM of $\varrho_{m_c m_c}(\mathbf{k})$:

$$\begin{aligned}
 i\hbar\partial_t \varrho_{m_c m_c}(\mathbf{k}) &= \sum_{m_v} \left\{ \mathbf{E}(t) \cdot \mathbf{d}_{m_c m_v}^{cv}(\mathbf{k}) P_{m_c m_v}(\mathbf{k}) - \text{h.c.} \right\} \\
 &+ \sum_{\mathbf{q} m'_c} \left\{ g_{m'_c m_c}^e(\mathbf{q}) \langle c_{m'_c}^\dagger(\mathbf{k} + \mathbf{q}) b(\mathbf{q}) c_{m_c}(\mathbf{k}) \rangle \right. \\
 &\quad - g_{m_c m'_c}^e(\mathbf{q}) \langle c_{m_c}^\dagger(\mathbf{k}) b(\mathbf{q}) c_{m'_c}(\mathbf{k} - \mathbf{q}) \rangle \\
 &\quad + g_{m_c m'_c}^{e*}(\mathbf{q}) \langle c_{m'_c}^\dagger(\mathbf{k} - \mathbf{q}) b^\dagger(\mathbf{q}) c_{m_c}(\mathbf{k}) \rangle \\
 &\quad \left. - g_{m'_c m_c}^{e*}(\mathbf{q}) \langle c_{m_c}^\dagger(\mathbf{k}) b^\dagger(\mathbf{q}) c_{m'_c}(\mathbf{k} + \mathbf{q}) \rangle \right\}
 \end{aligned}$$

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 \end{aligned}$$

- **Hierarchy problem** due to *phonon-assisted* density matrices

Solution: **truncation of the hierarchy**

1. Derive EOM of the phonon-assisted density matrices
2. Factorize the expectation values into their macroscopic parts
3. Take only those which lead to a absolute squared value of the interaction matrix element
4. Integrate and apply the *Markov* and *adiabatic* approximation
5. Insert result into initial EOM

→ Boltzmann limit

- Diagonal entry:

$$\begin{aligned} \partial_t \varrho_{m_c m_c}(\mathbf{k})|_{\text{phonon}} = & -\Gamma_{m_c m_c}^{\text{out}}(\mathbf{k}) \varrho_{m_c m_c}(\mathbf{k}) \\ & +\Gamma_{m_c m_c}^{\text{in}}(\mathbf{k})(1 - \varrho_{m_c m_c}(\mathbf{k})) \end{aligned}$$

- with:

$$\begin{aligned} \Gamma_{m_c m_c}^{\text{out}}(\mathbf{k}) = & \frac{\pi}{\hbar} \sum_{\mathbf{q}, m'_c} |g_{m'_c m_c}(\mathbf{q})|^2 \times \\ & \left\{ \delta(\epsilon_{m'_c}(\mathbf{k} + \mathbf{q}) - \epsilon_{m_c}(\mathbf{k}) - \hbar\omega(\mathbf{q})) (1 - \varrho_{m'_c m'_c}(\mathbf{k} + \mathbf{q})) \beta(\mathbf{q}) + \right. \\ & \delta(\epsilon_{m'_c}(\mathbf{k} - \mathbf{q}) - \epsilon_{m_c}(\mathbf{k}) + \hbar\omega(\mathbf{q})) (1 - \varrho_{m'_c m'_c}(\mathbf{k} - \mathbf{q})) \times \\ & \left. (1 + \beta(\mathbf{q})) \right\} \end{aligned}$$

- Offdiagonal entry:

$$\partial_t \varrho_{m_c - m_c}(\mathbf{k})|_{phonon} = \frac{1}{i\hbar} \Sigma_{m_c - m_c}^{e-p}(\mathbf{k}) \varrho_{m_c - m_c}(\mathbf{k})$$

- Self-energy

$$\Sigma_{m_c - m_c}^{e-p}(\mathbf{k}) = \hbar \left(\Omega_{m_c - m_c}^{e-p}(\mathbf{k}) - i \Gamma_{m_c - m_c}^{e-p}(\mathbf{k}) \right)$$

- real and imaginary part are connected via
Kramers-Kronig relation

Imaginary part of the self-energy

$$\begin{aligned}
 \Gamma_{m_c - m_c}^{e-p}(\mathbf{k}) = & \frac{\pi}{\hbar} \sum_{\mathbf{q} m'_c} \left\{ |g_{m'_c m_c}^e(\mathbf{q})|^2 \delta(\epsilon_{m'_c}(\mathbf{k} + \mathbf{q}) - \epsilon_{-m_c}(\mathbf{k}) - \hbar\omega(\mathbf{q})) \times \right. \\
 & \left[(1 - \varrho_{m'_c m'_c}(\mathbf{k} + \mathbf{q})) \beta(\mathbf{q}) + \varrho_{m'_c m'_c}(\mathbf{k} + \mathbf{q}) (1 + \beta(\mathbf{q})) \right] \\
 & + |g_{m'_c m_c}^e(\mathbf{q})|^2 \delta(\epsilon_{m'_c}(\mathbf{k} - \mathbf{q}) - \epsilon_{-m_c}(\mathbf{k}) + \hbar\omega(\mathbf{q})) \times \\
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 & \left. \left[(1 - \varrho_{m'_c m'_c}(\mathbf{k} + \mathbf{q})) \beta(\mathbf{q}) + \varrho_{m'_c m'_c}(\mathbf{k} + \mathbf{q}) (1 + \beta(\mathbf{q})) \right] \right\}
 \end{aligned}$$

Result IV

- Offdiagonal-entry: scattering contributions *beyond* the Boltzmann limit
(different truncation rules, but still 2nd order Born approximation)

$$\partial_t \varrho_{m_c - m_c}(\mathbf{k}) = -\frac{1}{i\hbar} \sum_{\mathbf{q} m'_c} \bar{\Sigma}_{m'_c - m'_c}^{e-p}(\mathbf{q}) \varrho_{m'_c - m'_c}(\mathbf{k} + \mathbf{q})$$

- self-energy

$$\bar{\Sigma}_{m'_c - m'_c}^{e-p}(\mathbf{q}) = \hbar \left(\bar{\Omega}_{m'_c - m'_c}^{e-p}(\mathbf{q}) - i \bar{\Gamma}_{m'_c - m'_c}^{e-p}(\mathbf{q}) \right)$$

- contributions are **not** connected via *Kramers-Kronig relation*

Summary of results

- Typical form of EOM in 2nd order Born approximation
(compared with carrier dynamics)

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- **But:** Explicit inclusion of spin degree-of-freedom

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⇒ Decay times

- Formal definition of decay times:

$$\frac{1}{T_{1,\mathbf{k}}} = \sum_{m'_c} \left(\Gamma_{m'_c m'_c}^{in}(\mathbf{k}) + \Gamma_{m'_c m'_c}^{out}(\mathbf{k}) \right)$$

$$\frac{1}{T_{2,\mathbf{k}}} = \Gamma_{m_c - m_c}^{e-p}(\mathbf{k})$$

- Result for **small spin splitting**:

$$T_{1,\mathbf{k}} \simeq T_{2,\mathbf{k}}$$

- Result for **spin degenerate**:

$$T_{1,\mathbf{k}} = T_{2,\mathbf{k}}$$

⇒ Experimental observables

- Experimental observables:

Spin polarization S ($\rightarrow$ spin relaxation):

$$S = \sum_{\mathbf{k}} (\varrho_{\uparrow\uparrow}(\mathbf{k}) - \varrho_{\downarrow\downarrow}(\mathbf{k}))$$

Spin coherence C ($\rightarrow$ spin dephasing):

$$C = \sum_{\mathbf{k}} |\varrho_{\uparrow\downarrow}(\mathbf{k})|$$

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$\Rightarrow$ **Unitary transformation**

- Transformed density matrix (*Rashba SO interaction*)

$$\varrho^{(\uparrow\downarrow)}(\mathbf{k})|_{\text{Rashba}} = \frac{1}{2} \begin{pmatrix} d_+ + 2\Im \{ \varrho_{m_c - m_c}(\mathbf{k}) \mathbf{e}^{i\varphi} \} & d_- + 2i \Re \{ \varrho_{m_c - m_c}(\mathbf{k}) \mathbf{e}^{i\varphi} \} \\ d_- - 2i \Re \{ \varrho_{m_c - m_c}(\mathbf{k}) \mathbf{e}^{i\varphi} \} & d_+ - 2\Im \{ \varrho_{m_c - m_c}(\mathbf{k}) \mathbf{e}^{i\varphi} \} \end{pmatrix}$$

with

$$d_{\pm} = \varrho_{m_c m_c}(\mathbf{k}) \pm \varrho_{-m_c - m_c}(\mathbf{k})$$

and

$$\varphi = \angle(k_x, k_y)$$

- Observables:

$$S = \sum_{\mathbf{k}} 4\Re \left\{ -i \mathbf{e}^{-i\varphi} \varrho_{m_c - m_c}(\mathbf{k}) \right\}$$

$$C = \sum_{\mathbf{k}} \sqrt{d_-^2 + 4\Im \left\{ -i \mathbf{e}^{-i\varphi} \varrho_{m_c - m_c}(\mathbf{k}) \right\}}$$

- **Spin relaxation** is ruled by $T_{2,\mathbf{k}}$ of the Bloch equations
- **Spin dephasing** is ruled by a *combination* of $T_{1,\mathbf{k}}$ and $T_{2,\mathbf{k}}$ of the Bloch equations
- Connection discussed by M.E. Flatté et al. in *Semiconductor Spintronics and Quantum Computation* but here: **microscopic theory**

- Concept of Bloch equations:

Extension towards spin dynamics

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- Microscopic description of spin dynamics:
optical Bloch equations with spin
→ electron-phonon scattering

Conclusion

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- Formal definition of T_1 and T_2 times

Conclusion

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- Microscopic description of spin dynamics:
optical Bloch equations with spin
→ electron-phonon scattering
- Formal definition of T_1 and T_2 times
- Connection between decay times of Bloch equations and spin relaxation/dephasing times

- Extension of semiconductor Bloch equations
→ inclusion of many-particle effects (**already done**)
- Numerical evaluation of equations (**work in progress**)
- **More information: [cond-mat/0412370](#)**

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THANK YOU FOR YOUR
ATTENTION!