Seminar on the optical properties of semiconductors

Topic

Semiconductor Bloch equations

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Semiconductor Bloch equations

Contents

1. Introduction

So far:

- Interband transitions by Coulomb attraction between a cb electron and a vb hole
- Bound states (excitons)- time independent effects

Now:

- A number of excited electron-hole pairs and interaction between all of them (nonlinear regime)
- Time dependent effects (polarization, carrier densities)

2. Hamiltonian Equations

Starting with the Hamiltonian

$$\mathcal{H} = \mathcal{H}_{el} + \mathcal{H}_l$$

$$\mathcal{H}_{el} = \sum_{\mathbf{k}} \left(E_{c,k} a^\dagger_{c,\mathbf{k}} a_{c,\mathbf{k}} + E_{v,k} a^\dagger_{v,\mathbf{k}} a_{v,\mathbf{k}} \right)$$
$$+ \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}\neq\mathbf{0}} V_q \left(a^\dagger_{c,\mathbf{k}+\mathbf{q}} a^\dagger_{c,\mathbf{k}'-\mathbf{q}} a_{c,\mathbf{k}'} a_{c,\mathbf{k}} + a^\dagger_{v,\mathbf{k}+\mathbf{q}} a^\dagger_{v,\mathbf{k}'-\mathbf{q}} a_{v,\mathbf{k}'} a_{v,\mathbf{k}} \right.$$
$$\left. + 2 a^\dagger_{c,\mathbf{k}+\mathbf{q}} a^\dagger_{v,\mathbf{k}'-\mathbf{q}} a_{v,\mathbf{k}'} a_{c,\mathbf{k}} \right)$$

$$\mathcal{H}_I = -\sum_{\mathbf{k}} \mathcal{E}(t) (a^\dagger_{c,\mathbf{k}} a_{v,\mathbf{k}} d_{cv} + h.c.)$$

2. Hamiltonian Equations

Transformation to electron-hole representation

$$\beta^{\dagger}_{-\mathbf{k}} = a_{v,\mathbf{k}} \qquad \alpha^{\dagger}_{\mathbf{k}} = a^{\dagger}_{c,\mathbf{k}}$$

Electron-hole Hamiltonian

$$\begin{aligned}\mathcal{H} = &\sum_{\mathbf{k}} \left(E_{e,k} \alpha^{\dagger}_{\mathbf{k}} \alpha_{\mathbf{k}} + E_{h,k} \beta^{\dagger}_{-\mathbf{k}} \beta_{-\mathbf{k}} \right) \\ &+ \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}\neq 0} V_q \left(\alpha^{\dagger}_{\mathbf{k}+\mathbf{q}} \alpha^{\dagger}_{\mathbf{k}'-\mathbf{q}} \alpha_{\mathbf{k}'} \alpha_{\mathbf{k}} + \beta^{\dagger}_{\mathbf{k}+\mathbf{q}} \beta^{\dagger}_{\mathbf{k}'-\mathbf{q}} \beta_{\mathbf{k}'} \beta_{\mathbf{k}} - 2\alpha^{\dagger}_{\mathbf{k}+\mathbf{q}} \beta^{\dagger}_{\mathbf{k}'-\mathbf{q}} \beta_{\mathbf{k}'} \alpha_{\mathbf{k}} \right) \\ &- \sum_{\mathbf{k}} \mathcal{E}(t) \left(d_{cv} \alpha^{\dagger}_{\mathbf{k}} \beta^{\dagger}_{-\mathbf{k}} + \text{h.c.} \right) + \text{constant terms}\end{aligned}$$

single particle energies:

$$E_{e,k} = E_{c,k} = \hbar\epsilon_{e,k}$$

$$E_{h,k} = -E_{v,k} + \sum_{\mathbf{q}\neq 0} V_q = \hbar\epsilon_{h,k}$$

2. Hamiltonian Equations

Elements of the reduced density matrix

$$\begin{aligned}
\langle \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} \rangle &= n_{e,\mathbf{k}}(t) \\
\langle \beta^\dagger_{-\mathbf{k}} \beta_{-\mathbf{k}} \rangle &= n_{h,\mathbf{k}}(t) \\
\langle \beta_{-\mathbf{k}} \alpha_{\mathbf{k}} \rangle &= P_{he}(\mathbf{k}, t) \equiv P_{\mathbf{k}}(t)
\end{aligned}$$

Equations of motion $i\hbar \frac{\partial}{\partial t} \langle A \rangle = \langle [H, A] \rangle$

for polarization

$$\hbar \left[i \frac{d}{dt} - (\epsilon_{e,k} + \epsilon_{h,k}) \right] P_{\mathbf{k}} = (n_{e,\mathbf{k}} + n_{h,\mathbf{k}} - 1) d_{vc} \mathcal{E}(t)$$

$$+ \sum_{\mathbf{k}', \mathbf{q} \neq 0} V_q \Big(\langle \alpha^\dagger_{\mathbf{k}'+\mathbf{q}} \beta_{-\mathbf{k}+\mathbf{q}} \alpha_{\mathbf{k}'} \alpha_{\mathbf{k}} \rangle - \langle \beta^\dagger_{\mathbf{k}'+\mathbf{q}} \beta_{-\mathbf{k}+\mathbf{q}} \beta_{\mathbf{k}'} \alpha_{\mathbf{k}} \rangle$$

$$+ \langle \beta_{-\mathbf{k}} \alpha^\dagger_{\mathbf{k}'-\mathbf{q}} \alpha_{\mathbf{k}'} \alpha_{\mathbf{k}-\mathbf{q}} \rangle - \langle \beta_{-\mathbf{k}} \beta^\dagger_{\mathbf{k}'-\mathbf{q}} \beta_{\mathbf{k}'} \alpha_{\mathbf{k}-\mathbf{q}} \rangle \Big)$$

2. Hamiltonian Equations

Equations of motion for the electron population

$$\hbar \frac{\partial}{\partial t} n_{e,\mathbf{k}} = -2\,\mathrm{Im}\Big[d_{cv}\,\mathcal{E}(t)\,P^*_{\mathbf{k}}\Big]$$
$$+\, i \sum_{\mathbf{k}',\mathbf{q}\neq 0} V_q \Big(\langle \alpha^\dagger_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}'-\mathbf{q}} \alpha_{\mathbf{k}-\mathbf{q}} \alpha_{\mathbf{k}'} \rangle - \langle \alpha^\dagger_{\mathbf{k}+\mathbf{q}} \alpha^\dagger_{\mathbf{k}'-\mathbf{q}} \alpha_{\mathbf{k}} \alpha_{\mathbf{k}'} \rangle$$
$$+ \langle \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}-\mathbf{q}} \beta^\dagger_{\mathbf{k}'-\mathbf{q}} \beta_{\mathbf{k}'} \rangle - \langle \alpha^\dagger_{\mathbf{k}+\mathbf{q}} \alpha_{\mathbf{k}} \beta^\dagger_{\mathbf{k}'-\mathbf{q}} \beta_{\mathbf{k}'} \rangle \Big) \ ,$$

Equations of motion for the hole population

$$\hbar \frac{\partial}{\partial t} n_{h,\mathbf{k}} = -2\,\mathrm{Im}\Big[d_{cv}\,\mathcal{E}(t)\,P^*_{\mathbf{k}}\Big]$$
$$+\, i \sum_{\mathbf{k}',\mathbf{q}\neq 0} V_q \Big(\langle \beta^\dagger_{-\mathbf{k}} \beta^\dagger_{\mathbf{k}'-\mathbf{q}} \beta_{-\mathbf{k}-\mathbf{q}} \beta_{\mathbf{k}'} \rangle - \langle \beta^\dagger_{-\mathbf{k}+\mathbf{q}} \beta^\dagger_{\mathbf{k}'-\mathbf{q}} \beta_{-\mathbf{k}} \beta_{\mathbf{k}'} \rangle$$
$$+ \langle \alpha^\dagger_{\mathbf{k}'+\mathbf{q}} \alpha_{\mathbf{k}'} \beta^\dagger_{-\mathbf{k}} \beta_{-\mathbf{k}+\mathbf{q}} \rangle - \langle \alpha^\dagger_{\mathbf{k}'+\mathbf{q}} \alpha_{\mathbf{k}'} \beta^\dagger_{-\mathbf{k}-\mathbf{q}} \beta_{-\mathbf{k}} \rangle \Big) \ .$$

2. Hamiltonian Equations

For simplification: split the four-operator terms into two-operator terms of

Densities, interband polarization plus

unfactorized rest

$$\langle 4\,terms \rangle \;=\; \langle 2\,terms \rangle \langle 2\text{terms} \rangle \;+\; unfactorized$$

by seperating into Hartree-Fock and scatt. Parts

$$\frac{\partial}{\partial t}\langle A \rangle \;=\; \frac{\partial}{\partial t}\langle A \rangle_{HF} + \frac{\partial}{\partial t}\langle A \rangle\Big|_{scatt}$$

2. Hamiltonian Equations

Hartree-Fock Approximation for one term

$$\langle \alpha_i^\dagger \alpha_j^\dagger \alpha_k \alpha_l \rangle \simeq \langle \alpha_i^\dagger \alpha_l \rangle \langle \alpha_j^\dagger \alpha_k \rangle - \langle \alpha_i^\dagger \alpha_k \rangle \langle \alpha_j^\dagger \alpha_l \rangle$$

$$\langle \alpha_{k'+q}^\dagger \beta_{-k+q} \alpha_{k'} \alpha_k \rangle_{HF} \simeq \langle \alpha_{k'+q}^\dagger \alpha_k \rangle \langle \beta_{-k+q} \alpha_{k'} \rangle - \langle \alpha_{k'+q}^\dagger \alpha_{k'} \rangle \langle \beta_{-k+q} \alpha_k \rangle$$
$$= \delta_{k,k'+q} \langle \alpha_k^\dagger \alpha_k \rangle \langle \beta_{-k+q} \alpha_{k-q} \rangle - \delta_{q_0} \langle \alpha_{k'}^\dagger \alpha_{k'} \rangle \langle \beta_{-k} \alpha_k \rangle$$

with $\sum_{k',q\neq 0} V_q \delta_{q_0} \langle \alpha_{k'}^\dagger \alpha_{k'} \rangle \langle \beta_{-k} \alpha_k \rangle = 0$

$$\langle \alpha_{k'+q}^\dagger \beta_{-k+q} \alpha_{k'} \alpha_k \rangle_{HF} \simeq \delta_{k,k'+q} \langle \alpha_k^\dagger \alpha_k \rangle \langle \beta_{-k+q} \alpha_{k-q} \rangle = \delta_{k,k'+q} n_{e,k}(t) P_{k+q}(t)$$

[similar for all 4 operator terms]

2. Hamiltonian Equations

Equations of motion (with factorization)

$$\frac{\partial P_{\mathbf{k}}}{\partial t} = -i(e_{e,k} + e_{h,k})P_{\mathbf{k}}$$

$$-\frac{i}{\hbar}(n_{e,\mathbf{k}} + n_{h,\mathbf{k}} - 1)\left[d_{cv}\mathcal{E}(t) + \sum_{\mathbf{q}\neq\mathbf{k}} V_{|\mathbf{k}-\mathbf{q}|}P_{\mathbf{q}}\right] + \left.\frac{\partial P_{\mathbf{k}}}{\partial t}\right|_{scatt}$$

$$\frac{\partial n_{e,\mathbf{k}}}{\partial t} = -\frac{2}{\hbar}\mathrm{Im}\left\{\left[d_{cv}\mathcal{E}(t) + \sum_{\mathbf{q}\neq\mathbf{k}} V_{|\mathbf{k}-\mathbf{q}|}P_{\mathbf{q}}\right]P^*_{\mathbf{k}}\right\} + \left.\frac{\partial n_{e,\mathbf{k}}}{\partial t}\right|_{scatt}$$

$$\frac{\partial n_{h,\mathbf{k}}}{\partial t} = -\frac{2}{\hbar}\mathrm{Im}\left\{\left[d_{cv}\mathcal{E}(t) + \sum_{\mathbf{q}\neq\mathbf{k}} V_{|\mathbf{k}-\mathbf{q}|}P_{\mathbf{q}}\right]P^*_{\mathbf{k}}\right\} + \left.\frac{\partial n_{h,\mathbf{k}}}{\partial t}\right|_{scatt}$$

single particle energies $\hbar e_{i,k} = \hbar \epsilon_{i,k} - \sum_q V_{|k-q|} n_{i,q} \qquad i = e, h$

2. Hamiltonian Equations

Generalized Rabi frequency

$$\omega_{R,\mathbf{k}} = \frac{1}{\hbar}\left(d_{cv}\mathcal{E} + \sum_{\mathbf{q}\neq\mathbf{k}} V_{|\mathbf{k}-\mathbf{q}|}P_{\mathbf{q}}\right)$$

Semiconductor Bloch equations

$$\frac{\partial P_{\mathbf{k}}}{\partial t} = -i(e_{e,k} + e_{h,k})P_{\mathbf{k}} - i(n_{e,\mathbf{k}} + n_{h,\mathbf{k}} - 1)\omega_{R,\mathbf{k}} + \left.\frac{\partial P_{\mathbf{k}}}{\partial t}\right|_{scatt}$$

$$\frac{\partial n_{e,\mathbf{k}}}{\partial t} = -2\,\mathrm{Im}(\omega_{R,\mathbf{k}}P^*_{\mathbf{k}}) + \left.\frac{\partial n_{e,\mathbf{k}}}{\partial t}\right|_{scatt}$$

$$\frac{\partial n_{h,\mathbf{k}}}{\partial t} = -2\,\mathrm{Im}(\omega_{R,\mathbf{k}}P^*_{\mathbf{k}}) + \left.\frac{\partial n_{h,\mathbf{k}}}{\partial t}\right|_{scatt}$$

2. Hamiltonian Equations

Generalized Rabi frequency

$$\omega_{R,\mathbf{k}} = \frac{1}{\hbar}\left(d_{cv}\mathcal{E} + \sum_{\mathbf{q}\neq\mathbf{k}} V_{|\mathbf{k}-\mathbf{q}|} P_{\mathbf{q}}\right)$$

Semiconductor Bloch equations

$$\frac{\partial P_{\mathbf{k}}}{\partial t} = -i(e_{e,k} + e_{h,k})P_{\mathbf{k}} - i(n_{e,\mathbf{k}} + n_{h,\mathbf{k}} - 1)\omega_{R,\mathbf{k}} + \left.\frac{\partial P_{\mathbf{k}}}{\partial t}\right|_{scatt}$$

$$\frac{\partial n_{e,\mathbf{k}}}{\partial t} = -2\,\mathrm{Im}(\omega_{R,\mathbf{k}} P^*_{\mathbf{k}}) + \left.\frac{\partial n_{e,\mathbf{k}}}{\partial t}\right|_{scatt}$$

$$\frac{\partial n_{h,\mathbf{k}}}{\partial t} = -2\,\mathrm{Im}(\omega_{R,\mathbf{k}} P^*_{\mathbf{k}}) + \left.\frac{\partial n_{h,\mathbf{k}}}{\partial t}\right|_{scatt}$$

dephasing

relaxation

2. Hamiltonian Equations

Several relevant regimes:

- The low excitation regime (excitons dominate)
- The high excitation regime (e^--e^- dominates)
- The quasi-equilibrium regime ($n_e \approx f_e$, $n_h \approx f_h$)
- The ultrafast regime

3. Low Excitation Regime

Bloch Equations without non-linear terms describe excitation in semiconductors with low electron hole pair densities

→ nonlinear terms include terms for densities and/or Polarization (exchange terms) like $\sim n \cdot P$

Semiconductor Bloch Eq. with linear terms only:

$$\hbar\left[i\frac{\partial}{\partial t}-(\epsilon_{e,k}+\epsilon_{h,k})\right]P_k=(n_{e,k}+n_{h,k}-1)d_{cv}E(t)-\sum_{q\neq k}V_{|k-q|}P_q$$

$$\hbar\frac{\partial}{\partial t}n_{e,k}=i\left[d_{cv}E(t)P_k^{\dagger}-c.c.\right] \quad \text{and} \quad n_{h,k}=n_{e,k}$$

3. Low Excitation Regime

Transformation to realspace

initial conditions: $n_{h,k} = n_{e,k} = P_{cv,k} = 0$

with $H_{eh} = E_g - \frac{\hbar^2 \nabla^2}{2\mathrm{m}_r} - V(r)$

$$i\hbar \frac{\partial}{\partial t} P(r) = H_{eh} P(r) + d_{cv} E(t) [2\mathrm{n}(r) - \delta(r)]$$

$$\hbar \frac{\partial}{\partial t} n(r) = i \left[d_{cv} E(t) P_k^* - c.c. \right]$$

Equations yield local charge neutrality $n_e(r) = n_h(-r) \equiv n(r)$

3. Low Excitation Regime

multiply equations by $\psi_\lambda(r)$ and integrate of r:

$$i\hbar\frac{\partial}{\partial t}P_\lambda=\hbar\epsilon_\lambda P_\lambda+d_{cv}E(t)[2\mathrm{n}_\lambda-\psi_\lambda(r=0)]$$

$$\hbar\frac{\partial}{\partial t}n_\lambda=i\,d_{cv}E(t)P_\lambda^*+i\,d_{cv}^*E(t)P_\lambda$$

introducing the following definitions:

$$\int d^3r\,\psi_\lambda(r)P(r)=P_\lambda$$

$$\int d^3r\,\psi_\lambda(r)n(r)=n_\lambda$$

$$P_\lambda=\psi_\lambda(r=0)\tilde{P}_\lambda,\quad n_\lambda=\psi_\lambda(r=0)\tilde{n}_\lambda$$

3. Low Excitation Regime

We obtain the simplified equation of motion:

$$i\hbar\frac{\partial}{\partial t}\tilde{P}_\lambda=\hbar\epsilon_\lambda\tilde{P}_\lambda+d_{cv}E(t)[2\tilde{n}_\lambda-1]$$
$$\hbar\frac{\partial}{\partial t}\tilde{n}_\lambda=i\,d_{cv}E(t)\tilde{P}^*_\lambda+i\,d^*_{cv}E(t)\tilde{P}_\lambda$$

equivalent to Optical Bloch Equations (but dynamics described by excitons)

3. Low Excitation Regime

Polarization is described by

$$P(t) = \sum_k P_k(t) d_{vc} + c.c. = d_{cv} P(r=0) + c.c.$$

with $P(r) = \sum_\lambda P_\lambda \psi_\lambda^*(r)$ we get:

$$P(t) = d_{cv} P(r=0) + c.c. = d_{cv} \sum_\lambda P_\lambda \psi^*(r=0) + c.c.$$

Inserting $P_\lambda = \psi_\lambda(r=0)\tilde{P}_\lambda$ for r=0 we get the optical Polarization as

$$P(t) = d_{cv} \sum_\lambda \left[\psi_\lambda(r=0)\right]^2 \tilde{P}_\lambda + c.c.$$

(describes inhomogeneously broadened two-level system)

4. Scattering Terms

All interaction effects beyond the mean field approximation are contained in the scatt terms.

The scattering terms describe:

- Dephasing for interband polarization

  = decay of quantum coherence in coherently excited system

- Relaxation of electron and hole distributions

4. Scattering Terms

Dissipation kinetics of intraband relaxation in low excitation regime dominated by:

- Impurity scattering
- Scattering of excited carriers with phonons

    fastest dynamics by longitudinal optical phonon scattering

high excitation regime:

- Dissipation procces dominated by carrier carrier collision (dense electron-hole plasma)

4.1 Phenomenological description

a simple relaxation model needs at least two relaxation times T'_1 and T_1 for densities:

$$\frac{dn_{e,k}}{dt}\bigg|_{scatt} = \frac{f_{e,k} - n_{e,k}(t)}{T'_1} - \frac{n_{e,k}(t)}{T_1}$$

T_1 : *recombination time of carriers*

T'_1 : *intraband relaxation*

and a dephasing time T_2 for polarization:

$$\frac{dP_k}{dt}\bigg|_{scatt} = -\frac{P_k}{T_2}$$

4.2 Beyond HF approximation

Show general treatment for adding scatt. and dephasing rates to the Semicond. Bloch Eq. and look at the final results

- Equation of motion for electron population

$$\hbar\,\frac{\partial}{\partial t}n_{e,\mathbf{k}} = -2\,\mathrm{Im}\Big[d_{cv}\,\mathcal{E}(t)\,P^*_{\mathbf{k}}\Big]$$
$$+\,i\sum_{\mathbf{k}',\mathbf{q}\neq 0} V_q\Big(\langle\alpha^\dagger_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}'-\mathbf{q}}\alpha_{\mathbf{k}-\mathbf{q}}\alpha_{\mathbf{k}'}\rangle - \langle\alpha^\dagger_{\mathbf{k}+\mathbf{q}}\alpha^\dagger_{\mathbf{k}'-\mathbf{q}}\alpha_{\mathbf{k}}\alpha_{\mathbf{k}'}\rangle$$
$$+\,\langle\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}-\mathbf{q}}\beta^\dagger_{\mathbf{k}'-\mathbf{q}}\beta_{\mathbf{k}'}\rangle - \langle\alpha^\dagger_{\mathbf{k}+\mathbf{q}}\alpha_{\mathbf{k}}\beta^\dagger_{\mathbf{k}'-\mathbf{q}}\beta_{\mathbf{k}'}\rangle\Big)\;,$$

4.2 Beyond HF approximation

Treatment for $\langle \alpha_k^\dagger \alpha_{k'-q}^\dagger \alpha_{k-q} \alpha_{k'} \rangle$

scattering term is (based on the reduced four operator term)
difference between this term and the Hartree-Fock approximation

$$\delta \langle \alpha_k^\dagger \alpha_{k'-q}^\dagger \alpha_{k-q} \alpha_{k'} \rangle = \langle \alpha_k^\dagger \alpha_{k'-q}^\dagger \alpha_{k-q} \alpha_{k'} \rangle - \langle \alpha_k^\dagger \alpha_k \rangle \langle \alpha_{k-q}^\dagger \alpha_{k-q} \rangle \delta k, k'$$

calculate equation of motion for this term

$$\frac{\partial}{\partial t} \delta \langle \alpha_k^\dagger \alpha_{k'-q}^\dagger \alpha_{k-q} \alpha_{k'} \rangle = \langle \frac{\partial}{\partial t} (\alpha_k^\dagger \alpha_{k'-q}^\dagger \alpha_{k-q} \alpha_{k'}) \rangle$$
$$- \left[\langle \frac{\partial}{\partial t} (\alpha_k^\dagger \alpha_k) \rangle \langle \alpha_{k-q}^\dagger \alpha_{k-q} \rangle + \langle \alpha_k^\dagger \alpha_k \rangle \langle \frac{\partial}{\partial t} (\alpha_{k-q}^\dagger \alpha_{k-q}) \rangle \right] \delta_{k,k'}$$

Using the Heisenberg Eq. with the full electron-hole Hamiltonian for time derivatives

4.2 Beyond HF approximation

Coulomb Term → lenghty expression

general expression:

$$\frac{\partial}{\partial t}\delta\langle \alpha_k^\dagger \alpha_{k'-q}^\dagger \alpha_{k-q} \alpha_{k'}\rangle = \frac{i}{\hbar}\delta\langle \alpha_k^\dagger \alpha_{k'-q}^\dagger \alpha_{k-q} \alpha_{k'}\rangle \Delta\epsilon_{e,k,k',q} \quad \text{kinetic energy term}$$

$$+ \frac{\partial}{\partial t}\delta\langle \alpha_k^\dagger \alpha_{k'-q}^\dagger \alpha_{k-q} \alpha_{k'}\rangle\Big|_{Coulomb} \quad \text{with 6 operator terms}$$

$$\text{with } \Delta\epsilon_{e,k,k',q} = \epsilon_{e,k} + \epsilon_{e,k'-q} - \epsilon_{e,k-q} - \epsilon_{e,k'}$$

factorized into 2 operator terms

→ leads to carrier Boltzmann scattering rates

4.2 Beyond HF approximation

Carrier Boltzmann scattering rates

for the electron population (e-e and e-h-scatt)

$$\frac{\partial n_{e,k}}{\partial t}\Big|_{scatt.} = -\sum_{k',q\neq 0}\frac{2\pi}{\hbar}V_q^2\,\delta(\epsilon_{e,k}+\epsilon_{e,k'}-\epsilon_{e,k+q}-\epsilon_{e,k'-q})$$

$$\times\left[n_{e,k}n_{e,k'}(1-n_{e,k+q})(1-n_{e,k'-q})-n_{e,k'-q}n_{e,k+q}(1-n_{e,k'})(1-n_{e,k})\right]$$

$$-\sum_{k',q\neq 0}\frac{2\pi}{\hbar}V_q^2\,\delta(\epsilon_{e,k}+\epsilon_{h,k'}-\epsilon_{e,k-q}-\epsilon_{h,k'})$$

$$\times\left[n_{e,k}n_{h,k'}(1-n_{e,k+q})(1-n_{h,k'-q})-n_{h,k'-q}n_{e,k+q}(1-n_{e,k})(1-n_{h,k'})\right]$$

$$=-n_{e,k}\Gamma_{e,k}^{\text{out}}(n)+(1-n_{e,k})\Gamma_{e,k}^{\text{in}}(n)$$

$n_{h,k}$: change everywhere $e\leftrightarrow h$

4.2 Beyond HF approximation

Scatt. Term for Polarization in form of

$$\frac{\partial P_k}{\partial t}\Big|_{scatt.} = -A_k P_k + \sum_{q\neq 0} B_{k,q} P_{k+q}$$

with complex functions A and B

- realpart of A yields decay rate of polarization

$$\Gamma_k = \Re(A_k) = \frac{1}{2}\left(\Gamma^{\text{out}}_{e,k}(n) + \Gamma^{\text{in}}_{e,k}(n) + \Gamma^{\text{out}}_{h,k}(n) + \Gamma^{\text{in}}_{h,k}(n)\right)$$

- $Re(B_{k,q})$ describes rate of polarization transfer between state k and q caused by carrier-carrier collisions.

4.2 Beyond HF approximation

Decay time:

$$\Gamma_k = \Re(A_k) = \frac{1}{2}\left(\Gamma^{\text{out}}_{e,k}(n) + \Gamma^{\text{in}}_{e,k}(n) + \Gamma^{\text{out}}_{h,k}(n) + \Gamma^{\text{in}}_{h,k}(n)\right) = \frac{1}{T_2}$$

T_2 is the decay time of the polarization

$$T_2 = 2 \cdot T_1$$

T_1 describes the decay time of carrier population

→ lifetime determined by time an electron/hole spends in its state k rather than recombination time

4.3 LO-phonon scattering

Optical phonons have little dispersion

- discribed by energy $\hbar\omega_0$
- heterogen semiconductor $\hbar\omega_0$ between 20 to 40meV
- absorption/emission of LO-phonons lead to intraband scattering of carriers

- Intraband scattering Hamiltonian (Fröhlich H.):

$$H_{e-LO} = \sum_{i,k,q} \hbar g_q \alpha^{\dagger}_{i,k+q} \alpha_{i,k} (b_q + b^{\dagger}_{-q})$$

With the bosonic phonon annihilation and creation operators b_q and $b^{\dagger}_{-q}$

4.3 LO-phonon scattering

Fröhlich Hamiltonian

$$H_{e-LO} = \sum_{i,k,q} \hbar g_q \alpha^\dagger_{i,k+q} \alpha_{i,k} (b_q + b^\dagger_{-q})$$

Interaction matrix:

$$|g_q|^2 = \frac{\omega_0 V_q}{2\hbar} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right)$$

V_q: Coulomb matrix element

ϵ_∞: high frequency dielectric constant

ϵ_0: low frequency dielectric constant

V_q shows coulombic nature in exchange of optical phonons in carrier-carrier interaction

4.3 LO-phonon scattering

Collision term of LO-phonon scattering:

$$\frac{\partial \rho_{i,j}(k)}{\partial t}\Big|_{scatt} = \frac{i}{\hbar}\langle([H_{e-LO}, \alpha^{\dagger}_{j,k}]\alpha_{i,k} + \alpha^{\dagger}_{j,k}[H_{e-LO}, \alpha_{i,k}])\rangle$$

$$= i\sum_q g_q\left(\langle \alpha^{\dagger}_{j,k+q}\alpha_{i,k}(b_q + b^{\dagger}_{-q})\rangle - \langle \alpha^{\dagger}_{j,k}\alpha_{i,k-q}(b_q + b^{\dagger}_{-q})\rangle\right)$$

$$= i\sum_q g_q\left(F^{-}_{ij,k,q} + F^{+}_{ij,k,q} - G^{-}_{ij,k,q} - G^{+}_{ij,k,q}\right)$$

term couples expectation values of two electron and one phonon operator.

phonon assisted density matrices

$$F^{-}_{ij,k,q} = \langle \alpha^{\dagger}_{j,k+q}\alpha_{i,k} b_q\rangle \qquad F^{+}_{ij,k,q} = \langle \alpha^{\dagger}_{j,k+q}\alpha_{i,k} b^{\dagger}_{-q}\rangle$$

$$G^{-}_{ij,k,q} = \langle \alpha^{\dagger}_{j,k}\alpha_{i,k-q} b_q\rangle \qquad G^{+}_{ij,k,q} = \langle \alpha^{\dagger}_{j,k}\alpha_{i,k-q} b^{\dagger}_{-q}\rangle$$

4.3 LO-phonon scattering

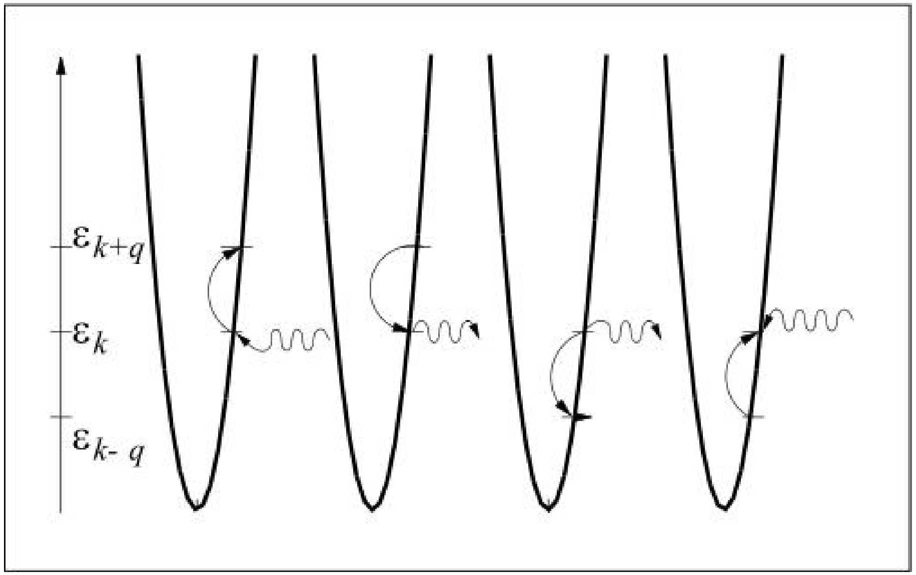

Fig. 1: Sketch of electron phonon scattering proceses (solid lines: electron scattering between states. Curled lines: phonon absorption / emission)

Equation of motion for phonon assisted density matrices is:

$$\frac{\partial F^{-}_{ij,k,q}}{\partial t} = \frac{i}{\hbar}\langle[H_{e-LO} + H_{HF} + H_{LO}, \alpha^{\dagger}_{j,k+q}\alpha_{i,k}b_q]\rangle$$

Conclusion

Semiconductor Bloch Equations:

- Set of coupled equations to describe polarization and population dynamics
- Levels of approximation
  - Low excitation: independant excitons
  - Scattering:
    - Decay rates
    - 4-operator density matrices
    - Phonon assisted processes

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