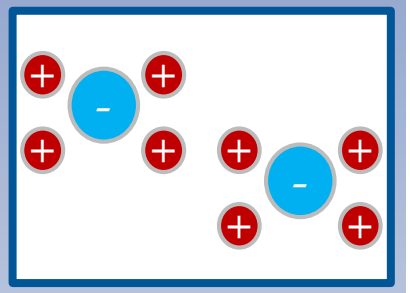
Summary lecture V

- **Lindhard equation** describes the screening of the Coulomb interaction due to the presence of many particles

$$W(\boldsymbol{q}) = \frac{V(\boldsymbol{q})}{\varepsilon(\boldsymbol{q})}, \qquad \varepsilon(\boldsymbol{q}) = 1 - V(\boldsymbol{q}) \sum_{\boldsymbol{k}} \frac{\rho_{\boldsymbol{k}+\boldsymbol{q}} - \rho_{\boldsymbol{k}}}{\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} - \hbar\omega}$$



- In the **static and long-wavelength limit** we find

$$W(\boldsymbol{q}) = \frac{e_0^2}{\varepsilon_0 V} \frac{1}{q^2 + \kappa^2}$$

- Besides a continuum of electron-hole excitations, there is a **collective oscillation** of the entire electron plasma with the characteristic **plasma frequency**

$$\omega_{pl} = \sqrt{\frac{n e_0^2}{\varepsilon_0 m_e}}$$

Learning outcomes lecture VI

- Describe the formation of excitons (bound-electron hole pairs) and calculate the **excitonic binding energy**
- Recognize the importance of the **statistical operator**
- Sketch the **derivation of Bloch equations** and discuss their contributions
- Explain the **many-particle hierarchy problem** and how it can be solved

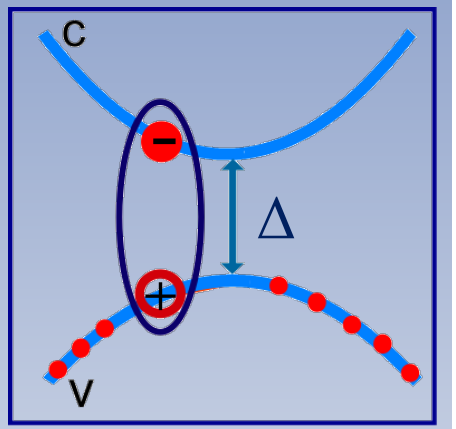
Chapter III

III. Electron-electron interaction

1. Coulomb interaction
2. Second quantization
3. Jellium & Hubbard models
4. Hartree-Fock approximation
5. Screening
6. Plasmons
7. Excitons

7. Excitons

- Coulomb-induced formation of **electron-hole pairs (excitons)** in semiconductors



- Assume a **2-band system** (λ = c, v) with a band gap $E_{gap} = \Delta$ focusing on **interband Coulomb interaction**

$$H = \sum_{\boldsymbol{k}} \left(\varepsilon_{v\boldsymbol{k}} a^{+}_{v\boldsymbol{k}} a_{v\boldsymbol{k}} + \varepsilon_{c\boldsymbol{k}} a^{+}_{c\boldsymbol{k}} a_{c\boldsymbol{k}} \right)$$

$$+ \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} V^{v\boldsymbol{k}_1,c\boldsymbol{k}_2}_{v\boldsymbol{k}_3,c\boldsymbol{k}_4} \; a^{+}_{v\boldsymbol{k}_1} a^{+}_{c\boldsymbol{k}_2} a^{v}_{\boldsymbol{k}_3} \, a_{c\boldsymbol{k}_4}$$

with the **effective mass energy** for the conduction and valence band

$$\varepsilon_{ck} = \frac{\hbar^2 k^2}{2m_c} + \Delta, \quad \varepsilon_{vk} = -\frac{\hbar^2 k^2}{2m_v}$$

Ground and excited state

7. Excitons

- In **ground state**, all valence band states are occupied, while the conduction band is empty

$$|\phi_0\rangle = \prod_{\boldsymbol{k}} a^{+}_{v\boldsymbol{k}} |0\rangle \quad \text{with the ground state energy} \quad E_0 = \sum_{\boldsymbol{k}} \varepsilon_{v\boldsymbol{k}}$$

- **Excited state** is build by a linear combination of all possibilities to generate an electron-hole pair

$$|\phi\rangle = \sum_{\boldsymbol{k}\boldsymbol{k}'} \alpha_{\boldsymbol{k}\boldsymbol{k}'}\, a^{+}_{c\boldsymbol{k}} a_{v\boldsymbol{k}'} |0\rangle$$

- Coefficients $\alpha_{\boldsymbol{k}\boldsymbol{k}'}$ are determined by solving the Schrödinger equation

$$\sum_{\boldsymbol{k}\boldsymbol{k}'} \left[\alpha_{\boldsymbol{k}\boldsymbol{k}'} \left(E_0 + \varepsilon_{c\boldsymbol{k}} - \varepsilon_{v\boldsymbol{k}'} - E \right) - \sum_{\boldsymbol{k}_1\boldsymbol{k}_4} \alpha_{\boldsymbol{k}_4\boldsymbol{k}_1} V^{v\boldsymbol{k}_1\, c\boldsymbol{k}}_{v\boldsymbol{k}'\, c\boldsymbol{k}_4} \right] a^{+}_{c\boldsymbol{k}} a_{v\boldsymbol{k}'} |0\rangle = 0$$

Excited state

7. Excitons

- Neglecting the interaction, i.e. V=0, we obtain as solution

$$\Delta E = E - E_0 = \varepsilon_{c\boldsymbol{k}} - \varepsilon_{v\boldsymbol{k'}} = \Delta + \frac{\hbar^2 k^2}{2m_c} + \frac{\hbar^2 k'^2}{2m_v}$$

  i.e. the **lowest excited state lies Δ above the ground state energy E_0**

- Including the interaction V, the excited state lies lower

$$\Delta E\, \alpha_{\boldsymbol{k}\boldsymbol{k'}} = \left(\Delta + \frac{\hbar^2 k^2}{2m_c} + \frac{\hbar^2 k'^2}{2m_v}\right) \alpha_{\boldsymbol{k}\boldsymbol{k'}} - \sum_{\boldsymbol{q}} \frac{e_0}{\varepsilon_0 V q^2} \alpha_{\boldsymbol{k}-\boldsymbol{q},\boldsymbol{k'}-\boldsymbol{q}}$$

- This eigenvalue equation for the coefficients $\alpha_{\boldsymbol{k}\boldsymbol{k'}}$ corresponds to the **two-particle Schrödinger equation**

$$\left[-\frac{\hbar^2}{2m_c}\nabla^2_{\boldsymbol{r}_1} - \frac{\hbar^2}{2m_v}\nabla^2_{\boldsymbol{r}_2} - \frac{e_0^2}{4\pi\varepsilon_0|\boldsymbol{r}_1-\boldsymbol{r}_2|}\right] \Psi(\boldsymbol{r}_1,\boldsymbol{r}_2) = \hat{E}\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)$$

  i.e. electron-hole pairs behave like two free particles with effective masses

Excitonic binding energy

7. Excitons

- Schrödinger equation reads in **relative** and **center-of-mass** coordinates

$$\left[-\frac{\hbar^2}{2M}\nabla_{\boldsymbol{R}}^2 - \frac{\hbar^2}{2\mu}\nabla_{\boldsymbol{r}}^2 - \frac{e_0^2}{4\pi\varepsilon_0\, r}\right]\Psi(\boldsymbol{r},\boldsymbol{R}) = \hat{E}\Psi(\boldsymbol{r},\boldsymbol{R})$$

with $\boldsymbol{R} = \frac{m_c\boldsymbol{r}_1 + m_v\boldsymbol{r}_2}{M}$, $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, $M = m_c + m_v$, $\mu = \frac{m_c m_v}{M}$

- **Separation ansatz** (like in hydrogen problem)

$$\Psi(\boldsymbol{r},\boldsymbol{R}) = A(\boldsymbol{r})B(\boldsymbol{R}) = e^{i\boldsymbol{K}\cdot\boldsymbol{R}}\, f_n(\boldsymbol{r})$$

with $f_n(\mathbf{r})$ as **eigen functions** of an **effective hydrogen problem**

- **Eigen energies**

$$E_{K,n} = \frac{\hbar^2 K^2}{2M} - \frac{\mu e_0^4}{2\hbar^2\varepsilon_{bg}^2}\frac{1}{n^2}$$

Excitonic binding energy

7. Excitons

- Formation of Coulomb-bound **excitons** as new quasi-particle with **lower energy** compared to the ground state of free electron-hole excitations

$$E_{K,n} = \frac{\hbar^2 K^2}{2M} - E_b \frac{1}{n^2}$$

with the **excitonic binding energy**

$$E_b = \frac{\mu e_0^4}{2\hbar^2 \varepsilon_{bg}^2}$$ that is determined by the **effective mass μ** and the **dielectric screening constant ε_{bg}** describing the screening of the Coulomb potential through the surrounding medium

- **Wannier excitons**: spatially extended excitons with a **large Bohr radius**
- **Frenkel excitons**: spatially localized excitons with a **small Bohr radius**

Chapter IV

IV. Density matrix theory

1. Statistical operator
2. Semiconductor Bloch equations
3. Boltzmann scattering equation

Statistical operator

1. Statistical operator

- **Statistical operator (density matrix)** characterizes quantum systems in a **mixed state** (statistical ensemble of many quantum states)

$$\rho = \sum_n p_n |\Psi_n\rangle\langle\Psi_n|$$

with $0 \leq p_n \leq 1$ and $\sum_n p_n = 1$ corresponding to the probability to find the system in the state $|\Psi_n\rangle$

- In a **pure state**, the statistical operator reads $\rho = |\Psi_{n_0}\rangle\langle\Psi_{n_0}|$ since here $p_n = \delta_{n,n_0}$
- The statistic operator has been expressed in its **eigen basis** with $\rho\,|\Psi_n\rangle = p_n|\Psi_n\rangle$
- Statistical operator is **self-adjoint** $\rho = \rho^+$

Statistical operator

1. Statistical operator

- In a **pure state**, the **expectation value** of quantum mechanical observables is given by expressing **a quantum mechanical average**

$$\langle O \rangle = \langle \Psi_{n_0} | O | \Psi_{n_0} \rangle$$

- In a **mixed state**, there is **an additional statistic averaging** that is expressed by the statistical operator

$$\langle O \rangle = \sum_n p_n \langle \Psi_n | O | \Psi_n \rangle = tr\,(\rho\, O)$$

- **Mixed and pure states** can be easily **distinguished:** while the trace of the statistical operator is 1, the trace of ρ^2 is different for pure and mixed states

$tr\,(\rho^2) = 1$ for **pure states** and $tr\,(\rho^2) < 1$ for **mixed states**

Density matrix elements

2. Semiconductor Bloch equations

- We have already introduced the **occupation number operator** $\hat{n}_\alpha = a_\alpha^+ a_\alpha$ that we now **statistically average** to describe a **mixed state**

$$\langle \hat{n}_\alpha \rangle = tr\left(\rho\, \hat{n}_\alpha\right) = tr\left(\rho\, a_\alpha^+ a_\alpha\right) = \rho_{\alpha\alpha}$$

- In the limiting case of one-particle systems, the **diagonal elements** of the **statistical operator** (density matrix) correspond to the **carrier occupation probability**

$$\langle \hat{n}_\alpha \rangle = \langle a_\alpha^+ a_\alpha \rangle = \rho_{\alpha\alpha} \quad \rightarrow \quad \rho_{\boldsymbol{k}}^{\lambda\lambda} = \rho_{\boldsymbol{k}}^{\lambda}$$

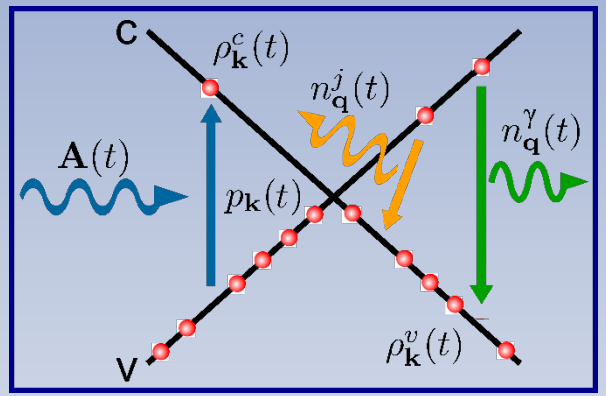
- **Non-diagonal elements** of the density matrix correspond to **microscopic polarization** being a measure for the **carrier transition probability**

$$\langle a_\alpha^+ a_\beta \rangle = \rho_{\alpha\beta} \quad \rightarrow \quad \rho_{\boldsymbol{k}}^{\lambda\lambda'} = p_{\boldsymbol{k}}^{vc}$$

Microscopic quantities

2. Semiconductor Bloch equations

- Semiconductor Bloch equations present a **coupled system of differential equations** for microscopic quantities:
  - **Microscopic polarization**
    $$p_{\boldsymbol{k}}(t) = \langle a^{+}_{c\boldsymbol{k}} a_{v\boldsymbol{k}} \rangle (t)$$
  - **Occupation probability**
    $$\rho^{\lambda}_{\boldsymbol{k}}(t) = \langle a^{+}_{\lambda\boldsymbol{k}} a_{\lambda\boldsymbol{k}} \rangle (t)$$
  - **Phonon occupation**
    $$n^{j}_{\boldsymbol{q}}(t) = \langle b^{+}_{j\boldsymbol{q}} b_{j\boldsymbol{q}} \rangle (t)$$
  - **Photon occupation**
    $$n^{\gamma}_{\boldsymbol{q}}(t) = \langle c^{+}_{\gamma\boldsymbol{q}} c_{\gamma\boldsymbol{q}} \rangle (t)$$



Temporal evolution is determined by **Heisenberg equation of motion**

$$i\hbar \frac{d}{dt} O(t) = [O(t), H]_{-}$$

Hamilton operator

2. Semiconductor Bloch equations

$$H = H_0 + H_{e-l} + H_{e-e}$$

free-particle **carrier-light interaction** **carrier-carrier interaction**

$$= \sum_l \varepsilon_l a_l^+ a_l + \frac{ie_0\hbar}{m_0} \sum_{l,l'} M_{l,l'} \cdot \boldsymbol{A}(t) a_l^+ a_{l'} + \frac{1}{2} \sum_{l_1,l_2,l_3,l_4} V_{l_3,l_4}^{l_1,l_2} a_{l_1}^+ a_{l_2}^+ a_{l_4} a_{l_3}$$

- The required **band structure** and **matrix elements** are calculated with nearest-neighbor **tight-binding wave functions**

$$\Psi_k^\lambda(\boldsymbol{r}) = C_{k,A}^\lambda \Phi_{k,A}(\boldsymbol{r}) + C_{k,B}^\lambda \Phi_{k,B}(\boldsymbol{r})$$

$$\Phi_{k,j}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}_n} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n} \phi_j(\boldsymbol{r} - \boldsymbol{R}_n)$$

with relevant atomic orbital functions $\phi_j(\boldsymbol{r} - \boldsymbol{R}_j)$

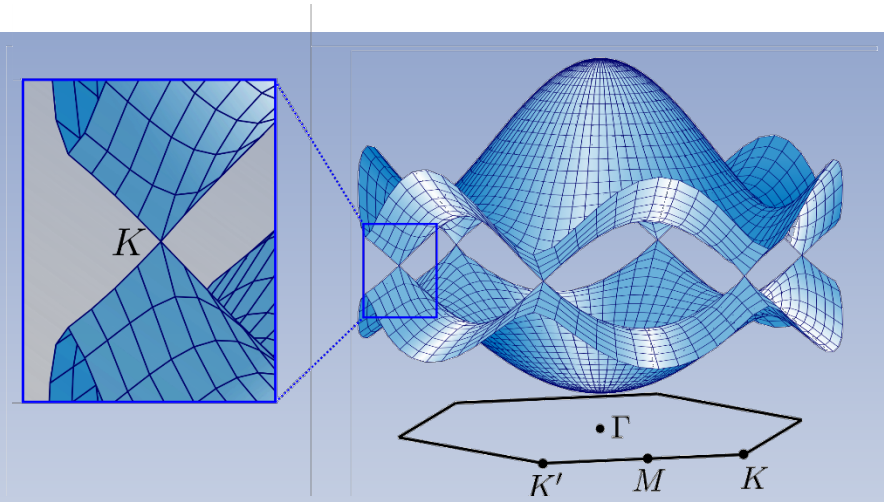
Band structure of graphene

2. Semiconductor Bloch equations

- Electronic band structure of graphene reads

$$E_\lambda(\boldsymbol{k}) = \frac{\sigma_\lambda \gamma_0 |e(\boldsymbol{k})|}{1 + \sigma_\lambda s_0 |e(\boldsymbol{k})|}$$

with $\sigma_c = -1$ and $\sigma_v = +1$



- Graphene has a **linear and gapless electronic band structure** around **Dirac points** (K, K′ points) in the Brillouine zone (semi-metal)

$$E_\lambda(\boldsymbol{k}) = \sigma_\lambda \hbar \nu_F |\boldsymbol{k}|$$

with the Fermi velocity υ_F

Optical matrix element of graphene

2. Semiconductor Bloch equations

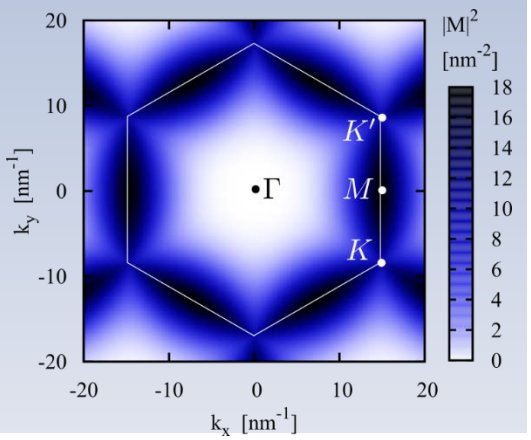
- Optical matrix element $\boldsymbol{M_{l,l'} = \langle \Psi_l(r) \,|\, \nabla \,|\, \Psi_{l'}(r) \rangle}$ determines the **strength** of **electron-light coupling** including **optical selection rules**

- Analytic expression obtained in **nearest- neighbor TB** approximation

$$\boldsymbol{M_k^{\lambda\lambda'} = M_0 \sum_{i=1}^{3} \frac{b_i}{|b_i|} \left(C_{A*}^{\lambda}(k) C_B^{\lambda'}(k) e^{ik\cdot b_i} - C_{B*}^{\lambda}(k) C_A^{\lambda'}(k) e^{-ik\cdot b_i} \right)}$$

- **Electron-light coupling** is strongly **anisotropic** around the Dirac points

- It shows **maxima** at **M points** and **vanishes** at the **Γ point** of the Brillouin zone (selection rule)



Coulomb matrix element

2. Semiconductor Bloch equations

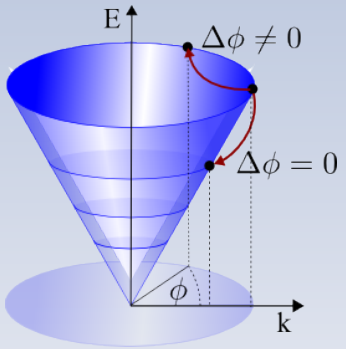
- The Coulomb matrix element $V^{l_1,l_2}_{l_3,l_4} = \langle \Psi^*_{l_1} \Psi^*_{l_2} | \, V(\boldsymbol{r}-\boldsymbol{r}') \, | \Psi_{l_4} \Psi_{l_3} \rangle$ reads in **nearest-neighbor TB** approximation

$$V^{l_1,l_2}_{l_3,l_4} = \frac{e_o^2}{2\varepsilon_0 A q}\left[\left(\frac{q\,a_B}{Z_{eff}}\right)^2 + 1\right]^{-6} \alpha^{l_1,l_2}_{l_3,l_4} \delta_{\boldsymbol{q},\boldsymbol{k}_3-\boldsymbol{k}_1}\,\delta_{\boldsymbol{q},\boldsymbol{k}_4-\boldsymbol{k}_2}$$

momentum conservation

with TB-coefficients $\alpha^{l_1,l_2}_{l_3,l_4} = \frac{1}{4}\left(1 + c_{\lambda_1\lambda_3}\frac{e^*(\boldsymbol{k}_1)e(\boldsymbol{k}_3)}{|e(\boldsymbol{k}_1)e(\boldsymbol{k}_3)|}\right)\left(1 + c_{\lambda_2\lambda_4}\frac{e^*(\boldsymbol{k}_2)e(\boldsymbol{k}_4)}{|e(\boldsymbol{k}_2)e(\boldsymbol{k}_4)|}\right)$

- Coulomb processes with **large momentum transfer** are **strongly suppressed** (decay scales with $1/q^{13}$)
- Coulomb interaction $V \propto 1 + e^{i\Delta\phi}$ **prefers parallel intraband scattering** along the Dirac cone



Equations of motion

2. Semiconductor Bloch equations

- Hamilton operator H is known → derivation of Bloch equations $\dot{\rho}^{\lambda}_{\boldsymbol{k}}$, $\dot{p}_{\boldsymbol{k}}$ applying the Heisenberg equation $i\hbar\dot{\rho}^{\lambda}_{\boldsymbol{k}} = [\rho^{\lambda}_{\boldsymbol{k}}, H]_-$

$$\dot{\rho}^{\lambda}_{\mathrm{k}}(t) = -2\mathrm{Im}\left(\Omega^{*}_{\mathrm{k}}(\mathrm{t})\,\mathrm{p}_{\mathrm{k}}(\mathrm{t})\right) - \frac{i}{\hbar}\sum_{ABC}\left(V^{c\boldsymbol{k}\,A}_{BC}\langle a^{+}_{v\,\boldsymbol{k}}a^{+}_{A}a_{C}a_{B}\rangle - V^{AB}_{v\boldsymbol{k}\,C}\langle a^{+}_{A}a^{+}_{B}a_{C}a_{c\,\boldsymbol{k}}\rangle\right)$$

$$\dot{p}_{\mathbf{k}}(t) = \frac{i}{\hbar}(\varepsilon^{v}_{\boldsymbol{k}} - \varepsilon^{c}_{\boldsymbol{k}})\,p_{\boldsymbol{k}}(t) - i\Omega_{\boldsymbol{k}}(t)\left(\rho^{c}_{\boldsymbol{k}}(t) - \rho^{v}_{\boldsymbol{k}}(t)\right) + \frac{2}{\hbar}\sum_{ABC}\mathrm{Im}\left(\mathrm{V}^{\mathrm{vk\,A}}_{\mathrm{BC}}\langle \mathrm{a}^{+}_{\mathrm{v\,k}}\mathrm{a}^{+}_{\mathrm{A}}\mathrm{a}_{\mathrm{C}}\mathrm{a}_{\mathrm{B}}\rangle\right)$$

$$H = H_0 + H_{e-l} + H_{e-e}$$

- **Single-particle quantities** $p_{\boldsymbol{k}}(t) = \langle a^{+}_{c\boldsymbol{k}}a_{v\boldsymbol{k}}\rangle$, $\rho^{\lambda}_{\boldsymbol{k}}(t) = \langle a^{+}_{\lambda\boldsymbol{k}}a_{\lambda\boldsymbol{k}}\rangle$ couple to **two-particle quantities** $C^{AB}_{CD} = \langle a^{+}_{A}a^{+}_{B}a_{C}a_{D}\rangle$ through **Coulomb interaction** → system of **coupled equations** is **not closed**

Correlation expansion

2. Semiconductor Bloch equations

- Many-particle interaction leads to a **hierarchy problem** (system of equations is not closed)

$$\frac{d}{dt}\langle a_1^+ a_2 \rangle \propto \langle a_A^+ a_B^+ a_C a_D \rangle$$

$$\frac{d}{dt}\langle a_A^+ a_B^+ a_C a_D \rangle \propto \langle a_1^+ a_2^+ a_3^+ a_4\, a_5\, a_6 \rangle \quad \ldots$$

- Solution by applying the **correlation expansion** and systematic truncation
  Example: **Hartree-Fock** factorization (single-particle quantities only)

$$\langle a_A^+ a_B^+ a_C a_D \rangle = \langle a_A^+ a_D \rangle \langle a_B^+ a_C \rangle - \langle a_A^+ a_C \rangle \langle a_B^+ a_D \rangle + \cancel{\langle a_A^+ a_B^+ a_C a_D \rangle^c}$$

closed system of equations (already sufficient for description of **excitons**)

Graphene Bloch equations

2. Semiconductor Bloch equations

- **Coupled system of differential equations on Hartree-Fock level**

$$\dot{\rho}^{\lambda}_{\mathbf{k}}(t) = -2\mathrm{Im}\left(\Omega^{*}_{\mathrm{k}}(t)\,\mathrm{p_k}(t)\right) + \frac{2}{\hbar}\sum_{\boldsymbol{k}'} V^{\boldsymbol{k}\ v,\boldsymbol{k}'c}_{\boldsymbol{k}'v,\boldsymbol{k}\ c}\, p_{\boldsymbol{k}'}(t)\, p^{*}_{\boldsymbol{k}}(t)$$

$$\dot{p}_{\mathbf{k}}(t) = \frac{i}{\hbar}\left(\varepsilon^{v}_{\boldsymbol{k}} - \varepsilon^{c}_{\boldsymbol{k}}\right) p_{\boldsymbol{k}}(t) - i\Omega_{\boldsymbol{k}}(t)\left(\rho^{c}_{\boldsymbol{k}}(t) - \rho^{v}_{\boldsymbol{k}}(t)\right) - \gamma_{\boldsymbol{k}}(t)\, p_{\boldsymbol{k}}(t)$$

$$+\frac{i}{\hbar}\sum_{\boldsymbol{k}'}\left[V^{\boldsymbol{k}\boldsymbol{k}'}_{\mathrm{ren}}\left(\rho^{v}_{\boldsymbol{k}'}(t) - \rho^{c}_{\boldsymbol{k}'}(t)\right)p_{\boldsymbol{k}}(t) - V^{\boldsymbol{k}\boldsymbol{k}'}_{\mathrm{exc}}\left(\rho^{c}_{\boldsymbol{k}}(t) - \rho^{v}_{\boldsymbol{k}}(t)\right)p_{\boldsymbol{k}'}(t)\right]$$

$$H = H_0 + H_{e-l} + H_{e-e}$$

- **Interaction-free contribution** (kinetic energy) leads to an **oscillation** of the **microscopic polarization $p_k(t)$**

Graphene Bloch equations

2. Semiconductor Bloch equations

- **Coupled system of differential equations on Hartree-Fock level**

$$\dot{\rho}^{\lambda}_{\mathbf{k}}(t) = -2\mathrm{Im}\left(\Omega^{*}_{\mathrm{k}}(t)\,\mathrm{p_k}(t)\right) + \frac{2}{\hbar}\sum_{\boldsymbol{k}'} V^{\boldsymbol{k}\ v,\boldsymbol{k}'c}_{\boldsymbol{k}'v,\boldsymbol{k}\ c}\, p_{\boldsymbol{k}'}(t)\, p^{*}_{\boldsymbol{k}}(t)$$

$$\dot{p}_{\mathbf{k}}(t) = \frac{i}{\hbar}\left(\varepsilon^{v}_{\boldsymbol{k}} - \varepsilon^{c}_{\boldsymbol{k}}\right) p_{\boldsymbol{k}}(t) - i\Omega_{\boldsymbol{k}}(t)\left(\rho^{c}_{\boldsymbol{k}}(t) - \rho^{v}_{\boldsymbol{k}}(t)\right) - \gamma_{\boldsymbol{k}}(t)\, p_{\boldsymbol{k}}(t)$$

$$+\frac{i}{\hbar}\sum_{\boldsymbol{k}'}\left[V^{\boldsymbol{k}\boldsymbol{k}'}_{\mathrm{ren}}\left(\rho^{v}_{\boldsymbol{k}'}(t) - \rho^{c}_{\boldsymbol{k}'}(t)\right)p_{\boldsymbol{k}}(t) - V^{\boldsymbol{k}\boldsymbol{k}'}_{\mathrm{exc}}\left(\rho^{c}_{\boldsymbol{k}}(t) - \rho^{v}_{\boldsymbol{k}}(t)\right)p_{\boldsymbol{k}'}(t)\right]$$

$$H = H_0 + H_{e-l} + H_{e-e}$$

- **Electron-light coupling** is determined by the **Rabi frequency** $\Omega_{\boldsymbol{k}}(t) = i\frac{e_0}{m_0}\boldsymbol{M}^{vc}_{\boldsymbol{k}} \cdot \boldsymbol{A}(t)$ giving rise to a **non-equilibrium distribution** of electrons after optical excitation

Graphene Bloch equations

2. Semiconductor Bloch equations

- **Coupled system of differential equations on Hartree-Fock level**

$$\dot{\rho}^{\lambda}_{\mathbf{k}}(t) = -2\mathrm{Im}\left(\Omega^{*}_{\mathrm{k}}(t)\,\mathrm{p_k}(t)\right) + \frac{2}{\hbar}\sum_{\boldsymbol{k}'} V^{\boldsymbol{k}\ v,\boldsymbol{k}'c}_{\boldsymbol{k}'v,\boldsymbol{k}\ c}\, p_{\boldsymbol{k}'}(t)\, p^{*}_{\boldsymbol{k}}(t)$$

$$\dot{p}_{\mathbf{k}}(t) = \frac{i}{\hbar}\left(\varepsilon^{v}_{\boldsymbol{k}} - \varepsilon^{c}_{\boldsymbol{k}}\right) p_{\boldsymbol{k}}(t) - i\Omega_{\boldsymbol{k}}(t)\left(\rho^{c}_{\boldsymbol{k}}(t) - \rho^{v}_{\boldsymbol{k}}(t)\right) - \gamma_{\boldsymbol{k}}(t)\, p_{\boldsymbol{k}}(t)$$

$$+\frac{i}{\hbar}\sum_{\boldsymbol{k}'}\left[V^{\boldsymbol{k}\boldsymbol{k}'}_{\mathrm{ren}}\left(\rho^{v}_{\boldsymbol{k}'}(t) - \rho^{c}_{\boldsymbol{k}'}(t)\right)p_{\boldsymbol{k}}(t) - V^{\boldsymbol{k}\boldsymbol{k}'}_{\mathrm{exc}}\left(\rho^{c}_{\boldsymbol{k}}(t) - \rho^{v}_{\boldsymbol{k}}(t)\right)p_{\boldsymbol{k}'}(t)\right]$$

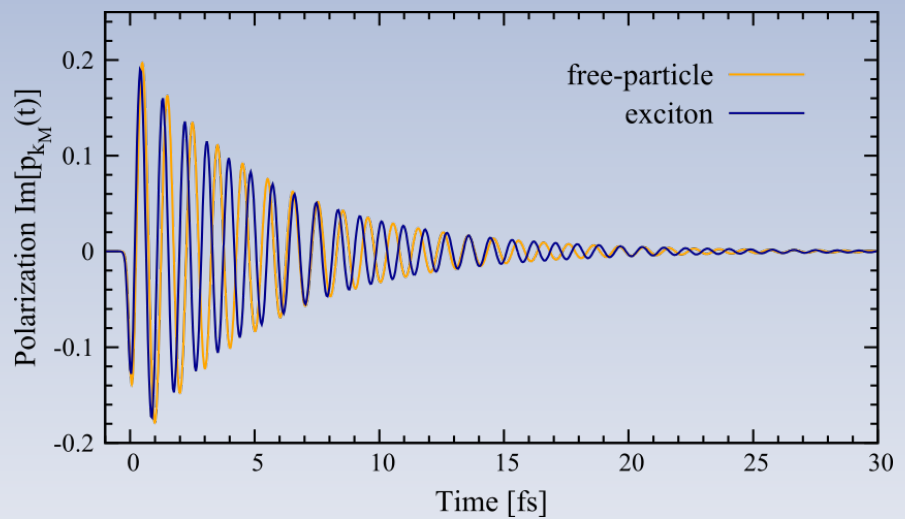
$$H = H_0 + H_{e-l} + H_{e-e}$$

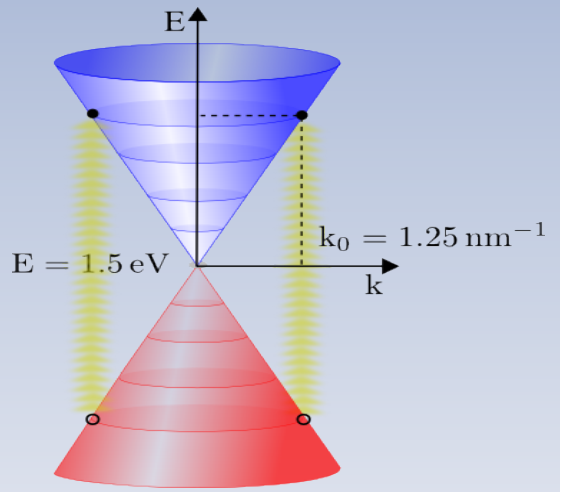
- **Electron-electron interaction** leads to **renormalization** of **energy** ($V^{\boldsymbol{k}\boldsymbol{k}'}_{\mathrm{ren}} = V^{\boldsymbol{k}\ c,\boldsymbol{k}'v}_{\boldsymbol{k}'v,\boldsymbol{k}\ c} - V^{\boldsymbol{k}'v,\boldsymbol{k}\ v}_{\boldsymbol{k}\ v,\boldsymbol{k}'v}$) and **Rabi frequency (excitons!)** ($V^{\boldsymbol{k}\boldsymbol{k}'}_{\mathrm{exc}} = V^{\boldsymbol{k}\ c,\boldsymbol{k}'v}_{\boldsymbol{k}'c,\boldsymbol{k}\ v}$) as well as to **dephasing** of the polarization γ_{k}

Microscopic polarization

2. Semiconductor Bloch equations

- **Optical excitation** with a laser pulse with an excitation energy of 1.5 eV
- Frequency of the **oscillation** of the **microscopic polarization changes** due to the Coulomb interaction

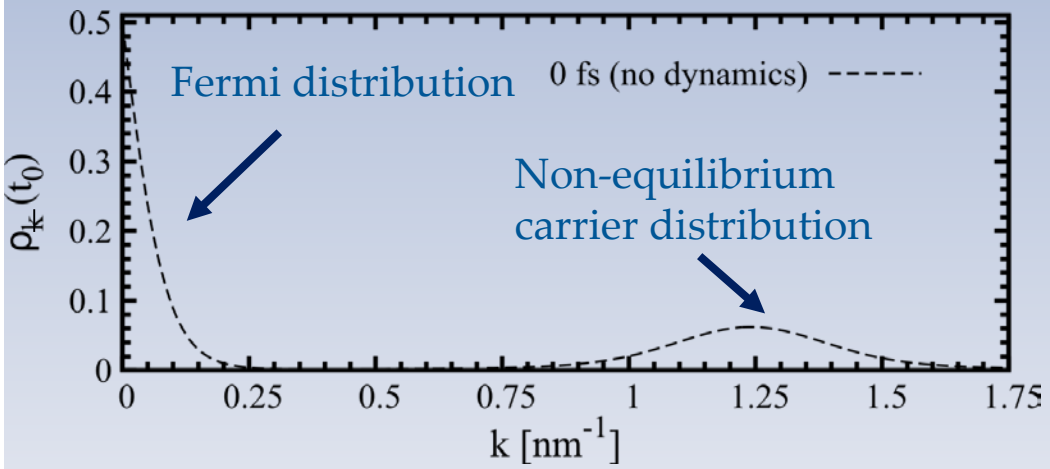


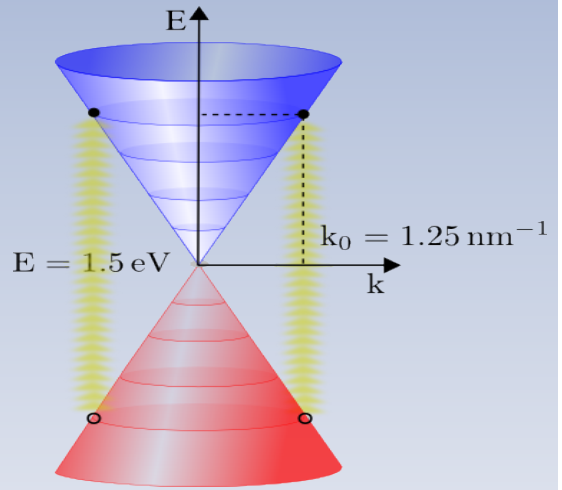


Optical excitation

2. Semiconductor Bloch equations

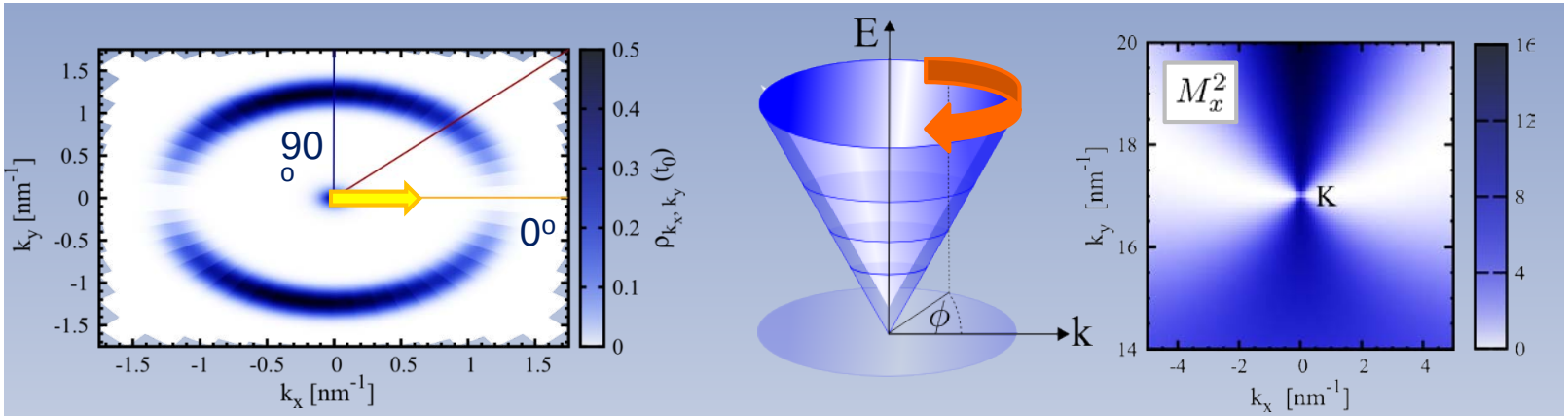
- **Optical excitation** with a laser pulse with an excitation energy of 1.5 eV
- We generate **a non-equilibrium carrier distribution** around the excitation energy (corresponding momentum $k_0 = 1.25\ nm^{-1}$)





Anisotropic carrier distribution

2. Semiconductor Bloch equations



- Generation of an **anisotropic non-equilibrium** carrier distribution
- **Maximal occupation perpendicular to polarization** of excitation pulse (90°) due to the **anisotropy** of the **optical matrix element**
- **Carrier dynamics** needs to be modelled by extending Bloch equations beyond the Hartree-Fock approximation (Boltzmann equation)

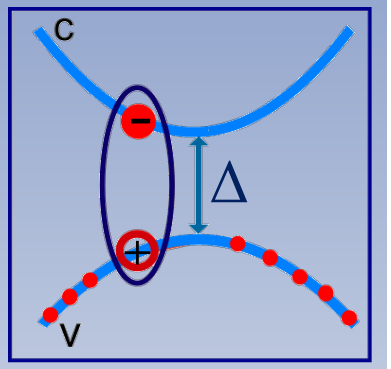
Summary lecture VI

- **Excitonic binding energy reads**

$$E_b = \frac{\mu e_0^4}{2\hbar^2 \varepsilon_{bg}^2}$$

with the reduced mass $\mu = \frac{m_c m_v}{M}$

and the dielectric background constant



- **Statistical operator** (density matrix) characterizes quantum systems in a **mixed state**

$$\rho = \sum_n p_n |\Psi_n\rangle\langle\Psi_n|$$

and builds the **expectation value of observables**

$$\langle O \rangle = tr\,(\rho\, O)$$

- To tackle the many-particle-induced hierarchy problem, we perform the correlation expansion followed by a **systematic truncation** resulting in **semiconductor Bloch equations** on Hartree-Fock level

Learning outcomes lecture VI

- Describe the formation of excitons (bound-electron hole pairs) and calculate the **excitonic binding energy**
- Recognize the importance of the **statistical operator**
- Sketch the **derivation of Bloch equations** and discuss their contributions
- Explain the **many-particle hierarchy problem** and how it can be solved