

# Summary lecture IX

- The electron-light Hamilton operator reads in second quantization

$$H_{e-l}^{p \cdot A} = \frac{i\hbar e_0}{m_e} \sum_{l,l'} M_{l,l'} \cdot \mathbf{A}(\mathbf{r}_0, t) a_l^\dagger a_{l'}, \quad H_{e-l}^{r \cdot E} = \sum_{l,l'} d_{l,l'} \cdot \mathbf{E}(\mathbf{r}_0, t) a_l^\dagger a_{l'}$$

- Absorption coefficient  $\alpha(\omega)$  is given by the optical susceptibility  $\chi(\omega)$

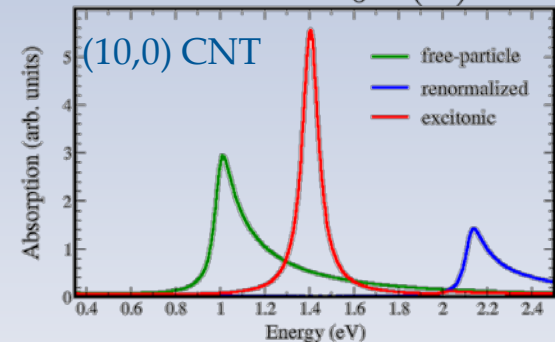
$$\alpha(\omega) = \frac{\omega}{n(\omega) c_0} \text{Im}\chi(\omega)$$

that is determined by  
microscopic polarization

$$\chi(\omega) = \frac{P(\omega)}{\varepsilon_0 E(\omega)}$$

- Bloch equation in the limit of linear optics

$$\dot{p}_{\mathbf{k}}(t) = \frac{i}{\hbar} \Delta \tilde{\varepsilon}_{\mathbf{k}}^{vc} p_{\mathbf{k}}(t) + i\tilde{\Omega}_{\mathbf{k}}(t) - \gamma p_{\mathbf{k}}(t)$$



# Chapter VI



## VI. Optical properties of solids

1. Electron-light interaction
2. Absorption spectra
3. Differential transmission spectra
4. Statistics of light



# Learning outcomes lecture X

- Recognize the importance of **pump-probe experiments** for revealing carrier dynamics
- Explain the **photon statistics** for different light sources



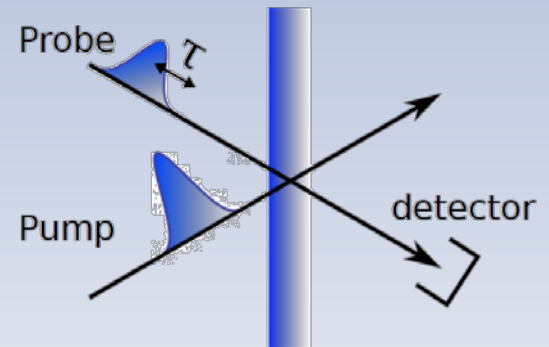
# Differential transmission spectra

## 3. Differential transmission spectra

- Bloch equations provide **microscopic access to carrier dynamics**, however it is **difficult to directly measure** the carrier occupation
- In **pump-probe** experiments, **differential transmission spectra (DTS)** are measured, where a **pump pulse** creates a **non-equilibrium distribution** and a weaker **probe pulse** measures the **dynamics** of excited carriers

$$\frac{T - T_0}{T_0}(\tau, \omega) \propto \left( \alpha^{(t)}(\omega) - \alpha^{(p+t)}(\tau, \omega) \right)$$

- Exploit the relation  $T = I/I_0$  with the intensity  $I = I_0 e^{-\alpha z}$  and assume that the absorption coefficient  $\alpha$  is relatively small



# Differential transmission spectra

## 3. Differential transmission spectra

- Assuming a **delta-shaped probe pulse** and exploiting the Bloch equations, we obtain for the differential transmission

$$\Delta T/T_0(\tau, \omega) \propto \int d\phi |M_{k_0, \phi}|^2 \Delta \rho_{k_0, \phi}(\tau) \approx (\rho_{k_0}^{(p)}(\tau) - \rho_{k_0}(-\infty))$$

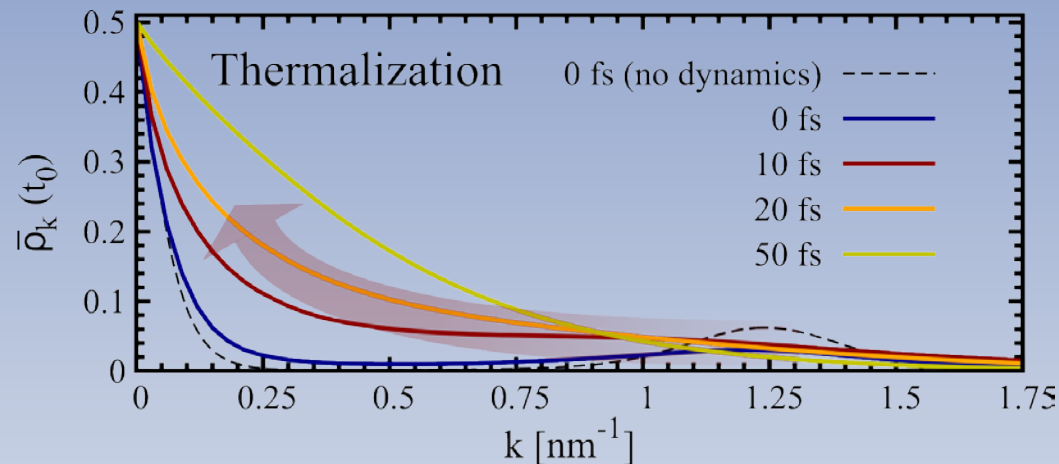
with the optical matrix element  $M_{k_t, \phi}$  in polar coordinates and with  $\Delta \rho_{k_t, \phi}(\tau) = \rho_{k_0, \phi}^{(p)}(\tau) - \rho_{k_0, \phi}(-\infty)$  where  $\rho_{k_0, \phi}(-\infty)$  is the **carrier occupation before the pump pulse** and  $\rho_{k_0, \phi}^{(p)}(\tau)$  the **pump-induced carrier occupation** (momentum  $k_0$  corresponds to the pumped state)

- The crucial quantity is the carrier occupation  $\rho_{\mathbf{k}}(t)$



# Carrier thermalization

## 3. Differential transmission spectra

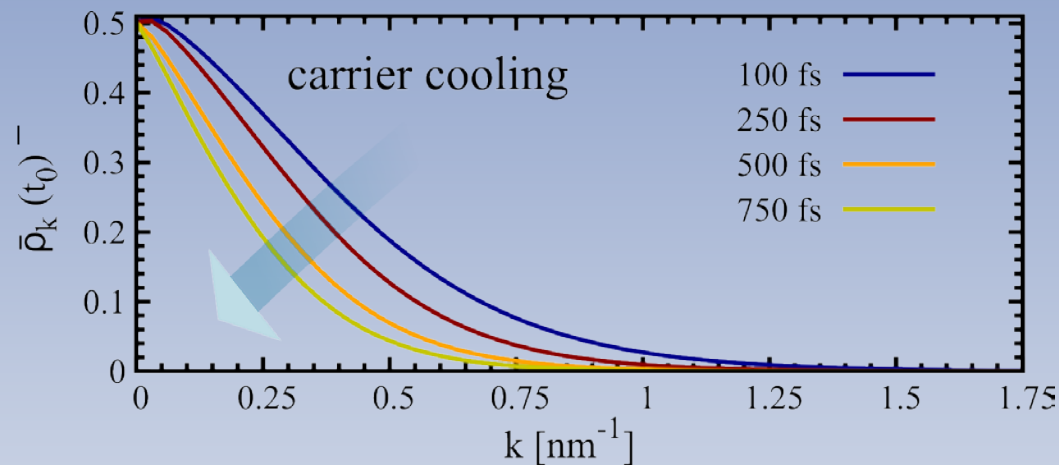


- Significant **relaxation** takes place already **during** the excitation **pulse**
- Coulomb-induced carrier-carrier scattering is the dominant channel
- **Thermalized Fermi distribution** reached within the first **50 fs**



# Carrier cooling

## 3. Differential transmission spectra



- Carrier cooling takes place on a picosecond time scale
- Optical phonons (in particular  $\Gamma$ LO,  $\Gamma$ TO and  $K$  phonons) are more efficient than acoustic phonons

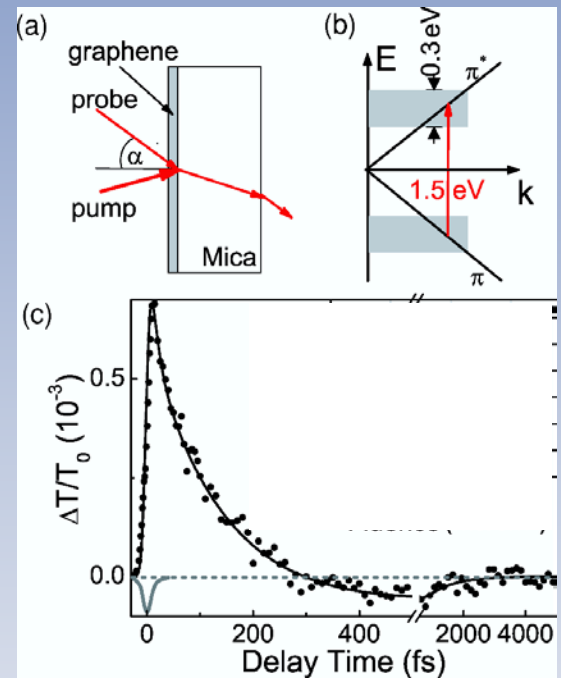


# Pump-probe experiment in the infrared

## 3. Differential transmission spectra

- Pump-probe-experiment measuring **differential transmission** in graphene
- Excitation energy is **1.5 eV**, temporal resolution is **10 fs**
- Initial increase of transmission is due to the **absorption bleaching**
- Following **decay** is characterized by **two time constants**:

$$\tau_1 = 140 \text{ fs}; \quad \tau_2 = 0.8 \text{ ps}$$



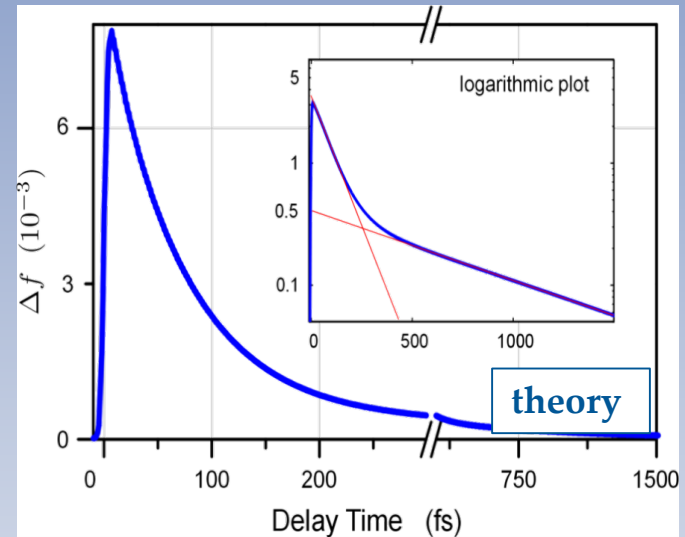
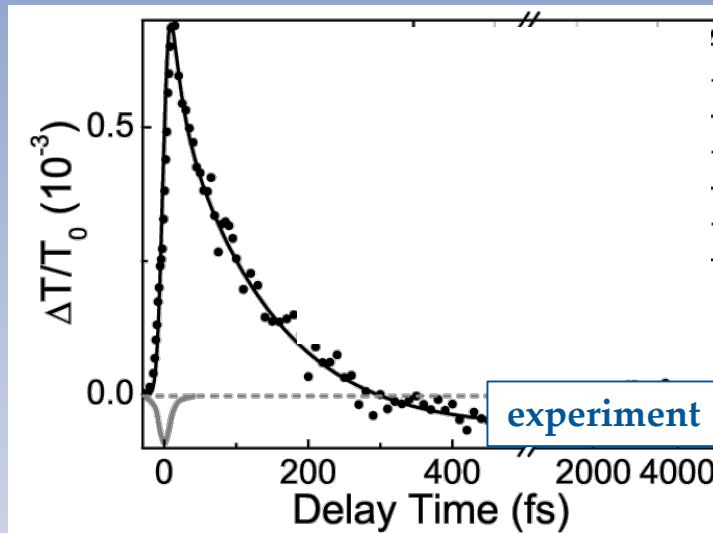
Experiments performed by **Thomas Elsaesser** (Max-Born Institut, Berlin)





# Experiment-theory comparison

## 3. Differential transmission spectra



$$\tau_1 = 140 \text{ fs}, \quad \tau_2 = 0.8 \text{ ps}$$

two decay times

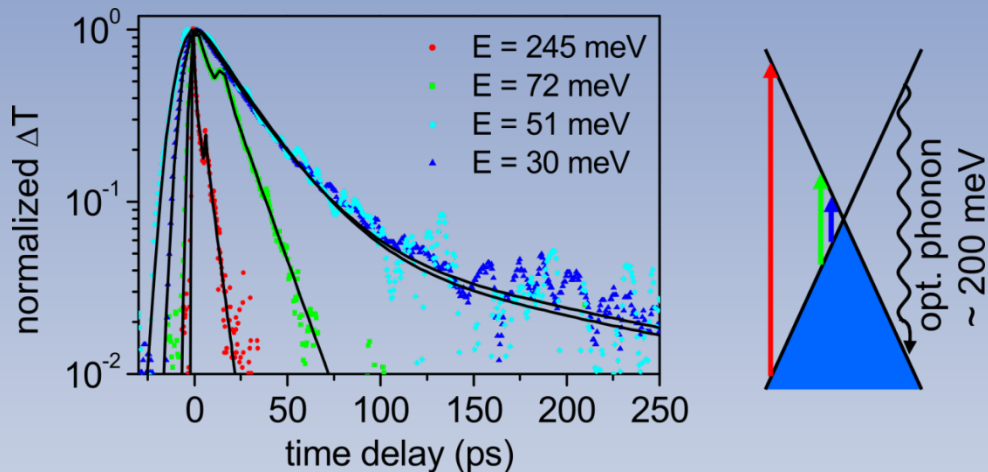
$$\tau_1 = 104 \text{ fs}, \quad \tau_2 = 0.7 \text{ ps}$$

- Theory is in **good agreement** with experiment:  $\tau_1$  corresponds to carrier **thermalization**,  $\tau_2$  describes **carrier cooling**



# Pump-probe experiment close to the Dirac point

## 3. Differential transmission spectra



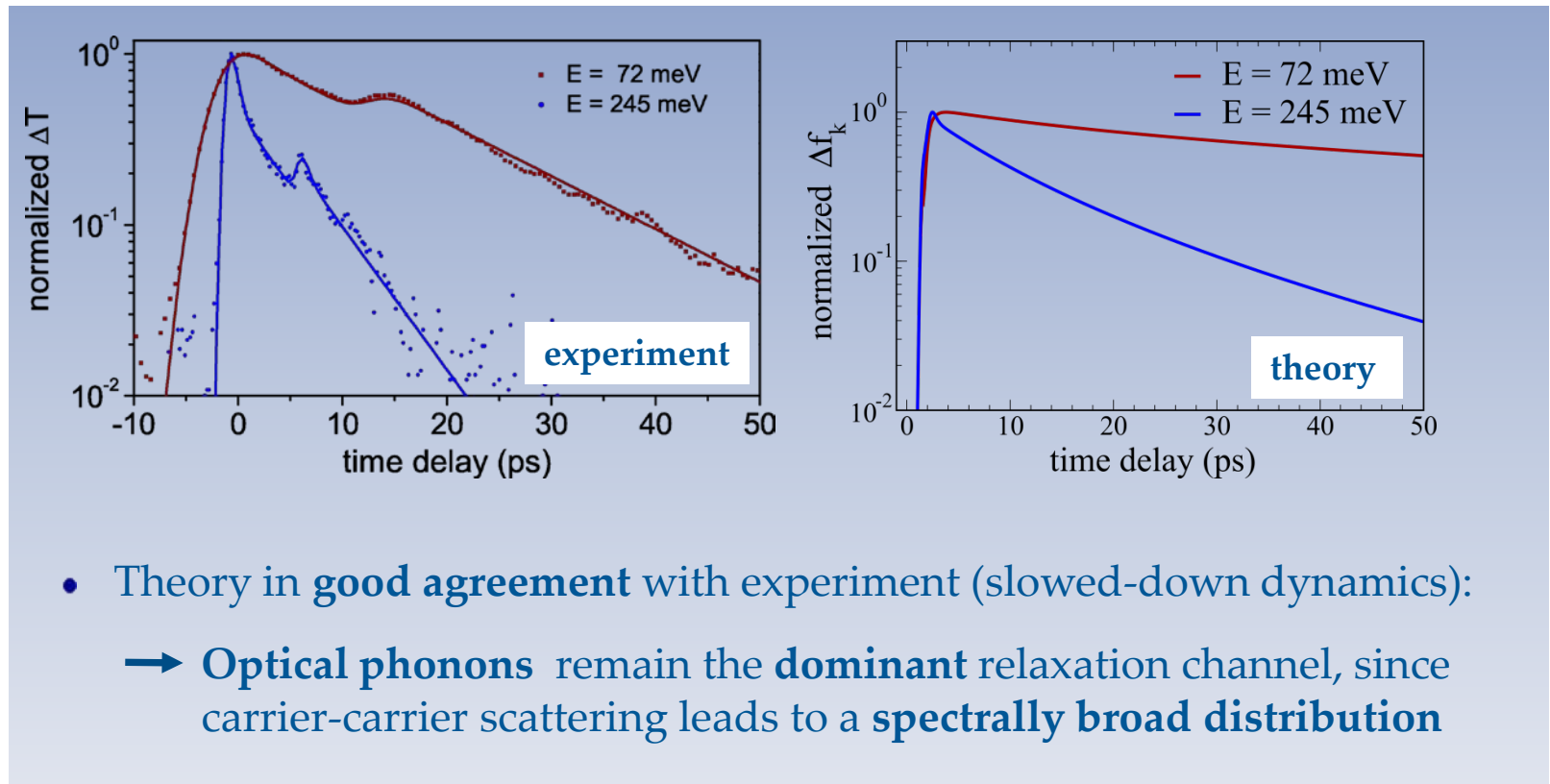
experiments performed by Manfred Helm (Helmholtz-Zentrum Dresden)

- Transmission in the vicinity of Dirac point and **below** the **energy** of **optical phonons** ( $\sim 200$  meV)  $\rightarrow$  acoustic phonons dominant?
- Relaxation **dynamics** is **slowed down** (5 ps at 245 meV, **25 ps** at 30 meV)



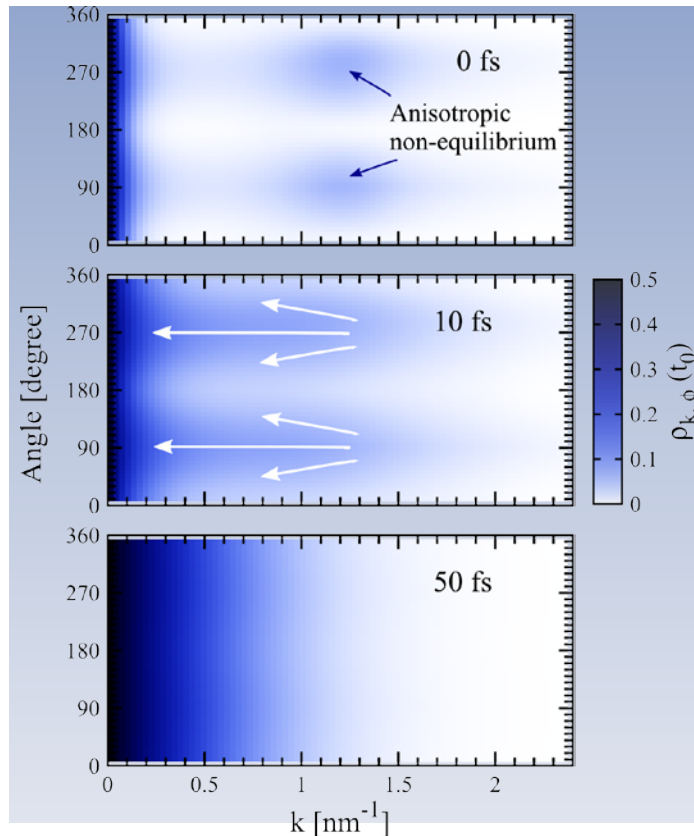
# Experiment-theory comparison

## 3. Differential transmission spectra



# Anisotropic carrier dynamics

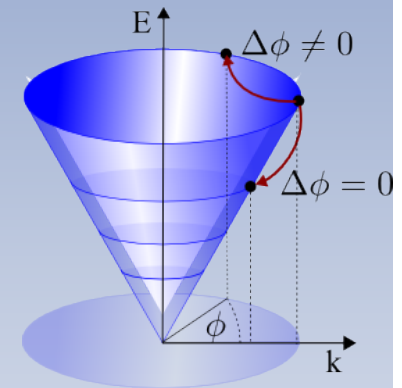
## 3. Differential transmission spectra



- Anisotropy of the carrier-light coupling element

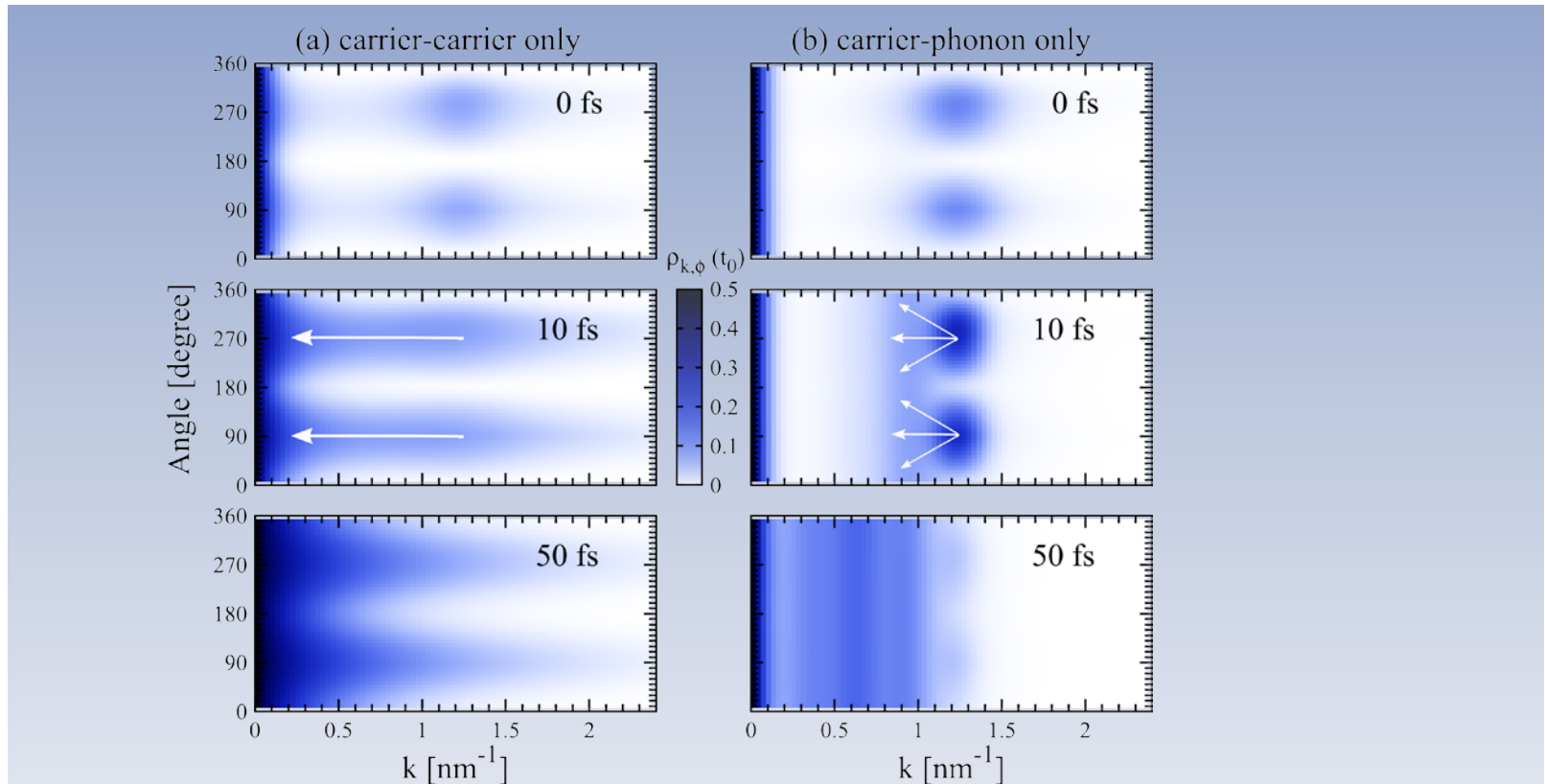
- Scattering across the Dirac cone reduces anisotropy

- Carrier distribution becomes entirely isotropic within the first 50 fs



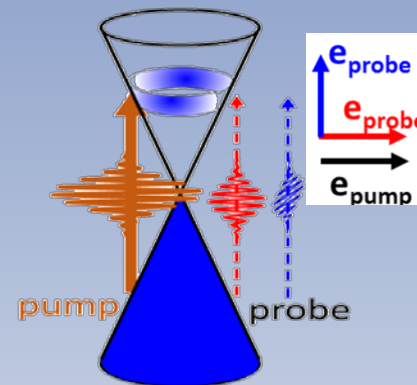
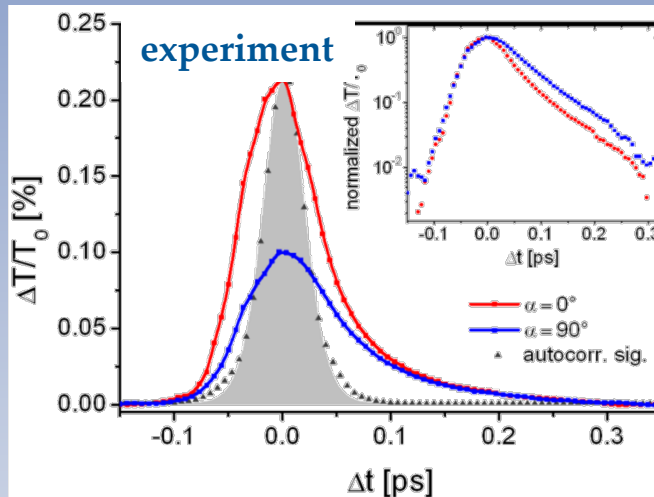
# Microscopic mechanism

## 3. Differential transmission spectra



# Polarization-dependent pump-probe experiment

## 3. Differential transmission spectra

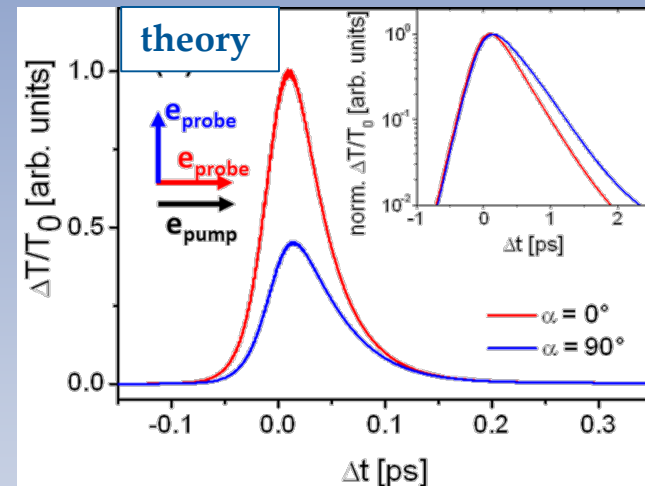
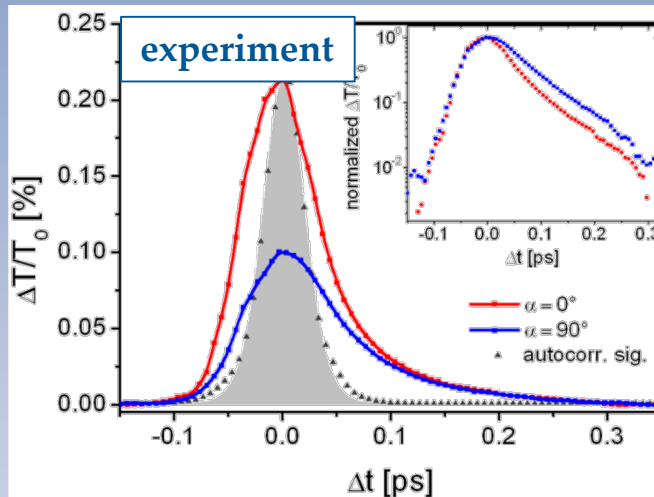


- **Polarization-dependent high-resolution pump-probe** experiments performed by Manfred Helm (Helmholtz-Zentrum Dresden)
- Variation of the **relative polarization** of the **pump** and the **probe** pulse



# Experiment-theory comparison

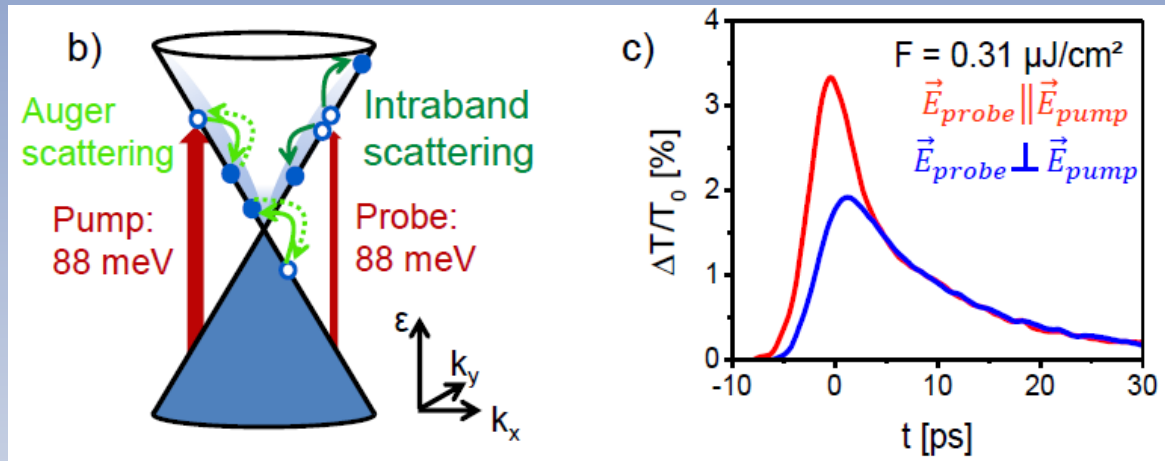
## 3. Differential transmission spectra



- Theoretical prediction is in **excellent agreement** with experiment:
  - **Anisotropic differential transmission** can be observed within the **first 100 fs**

# Anisotropy close to the Dirac point

## 3. Differential transmission spectra



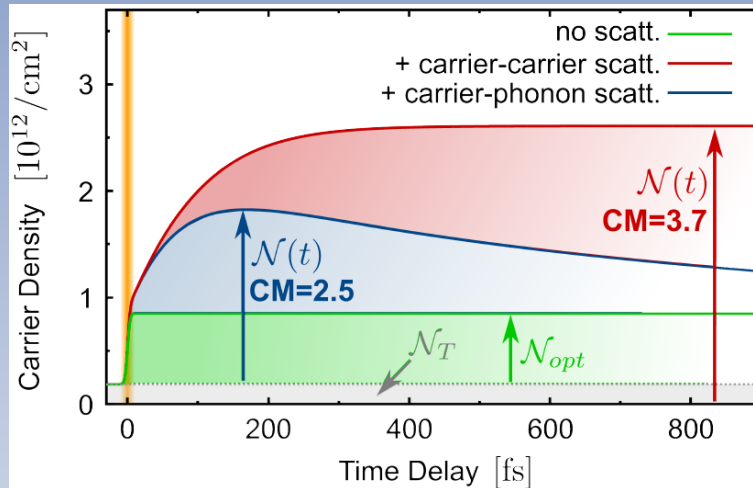
- Optical excitation below the optical phonon energy of 200 meV strongly suppress carrier-phonon scattering
  - Isotropic carrier distribution is reached via carrier-carrier scattering on a much smaller picosecond time scale





# Carrier multiplication

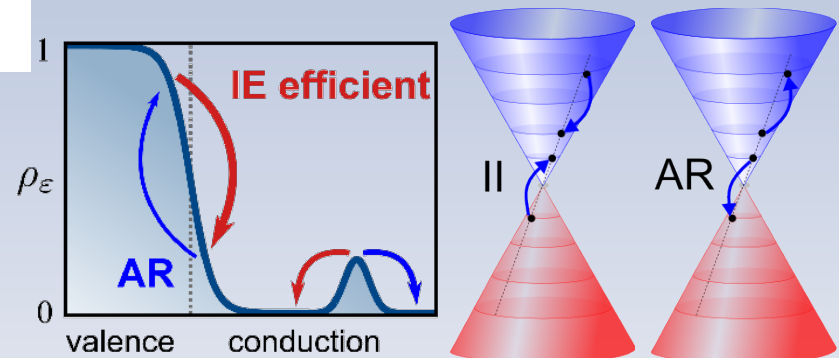
## 3. Differential transmission spectra



- Carrier density increases during the excitation pulse
- Auger scattering leads to **carrier multiplication (CM)**

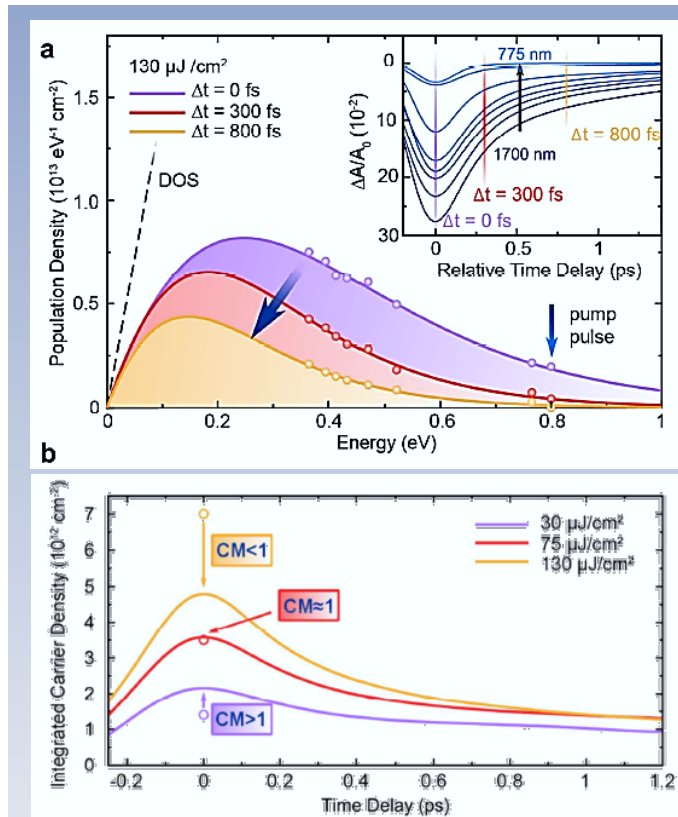
$$CM = \frac{\mathcal{N}(t) - \mathcal{N}_T}{\mathcal{N}_{opt}}$$

- **Carrier-phonon scattering reduces CM on a ps time scale**



# High-resolution multi-color pump-probe experiment

## 3. Differential transmission spectra



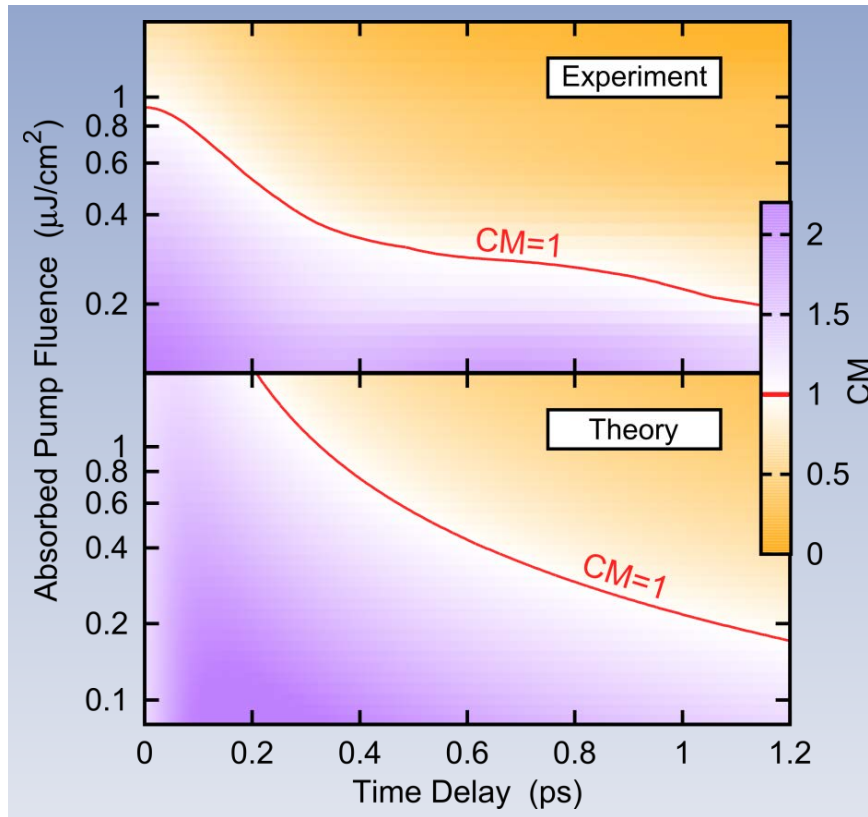
- Experiment performed by Daniel Neumaier and Heinrich Kurz, AMO Aachen
- Extract temporal evolution of the carrier density from **multi-color pump-probe** measurements and assume a **quick thermalization**
- Estimate the optically injected carrier density

→ **Carrier multiplication in dependence of pump fluence**



# Experiment-theory comparison

## 3. Differential transmission spectra



- Theoretical prediction is in **excellent agreement** with experiment:

Appearance of long-lived **CM** in the **weak excitation regime**

**Distinct fluence dependence** found both in theory and experiment



# Quantization of light

## 4. Statistics of light

- Light consists of **electromagnetic waves** with the energy

$$H = \frac{1}{2} \int \left( \varepsilon_0 E(r)^2 + \frac{1}{\mu_0} B(r)^2 \right) dr = \sum_j \left( \frac{1}{2} m_j \omega_j^2 q_j^2 + \frac{p_j^2}{2m_j} \right)$$

→ corresponds to the energy of **uncoupled harmonic oscillators**

- Quantization of light** through annihilation and creation operators

$$c_j = \frac{1}{\sqrt{2m_j \hbar \omega_j}} (m_j \omega_j \hat{q}_j + i \hat{p}_j), \quad c_j^+ = \frac{1}{\sqrt{2m_j \hbar \omega_j}} (m_j \omega_j \hat{q}_j - i \hat{p}_j)$$

- They fulfil the fundamental **commutation relations for bosons**

$$[\hat{q}_j, \hat{p}_{j'}] = i \hbar \delta_{j,j'}$$

$$[\hat{q}_j, \hat{q}_{j'}] = [\hat{p}_j, \hat{p}_{j'}] = 0$$



$$[c_j, c_{j'}^+] = \delta_{j,j'}$$

$$[c_j, c_{j'}] = [c_j^+, c_{j'}^+] = 0$$



# Photons

## 4. Statistics of light

- **Hamilton operator** for photons reads

$$H = \sum_j \hbar\omega_j \left( c_j^\dagger c_j + \frac{1}{2} \right)$$

- **Eigen states** are the **Fock states**

$$|n\rangle = \frac{1}{\sqrt{n!}} (c^\dagger)^n |0\rangle$$

- **Eigen energies** are **quantized**

$$E_n = \sum_j \hbar\omega_j \left( n + \frac{1}{2} \right)$$

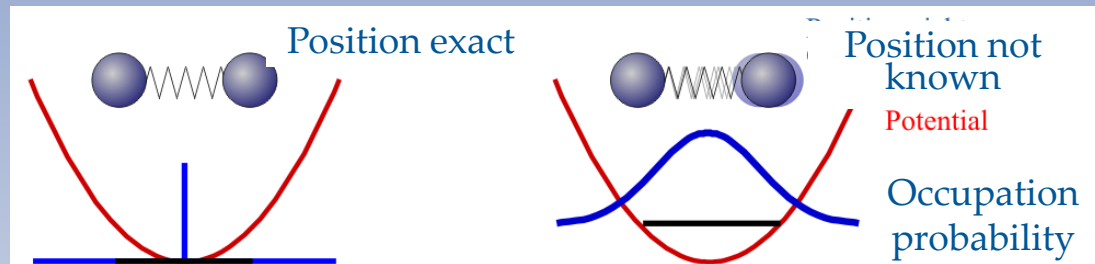
with the **photon number n** and the **zero-point energy**  $\frac{1}{2}\hbar\omega_j$



# Vacuum fluctuations

## 4. Statistics of light

### Classical oscillator    quantum mechanical oscillator

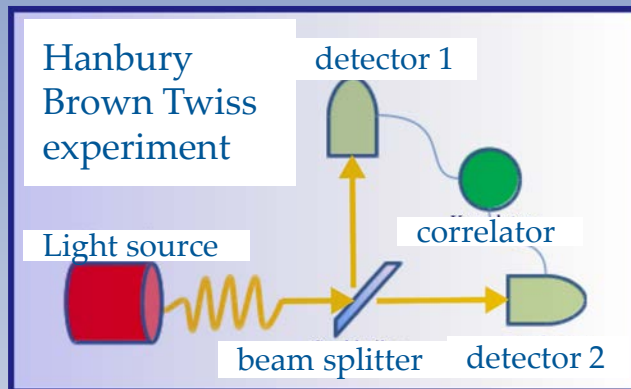


- Zero-point energy corresponds  $\frac{1}{2}\hbar\omega_j$  to vacuum fluctuations and results from the Heisenberg uncertainty principle  $\Delta q\Delta p \geq \frac{\hbar}{2}$
- Vacuum fluctuations give rise to non-classical phenomena
  - **spontaneous emission (light emission without excitation)**
  - **Lamb-Shift** (Energy shift in hydrogen atom)



# Hanbury Brown – Twiss Experiment

## 4. Statistics of light



R. Hanbury Brown and R. Twiss,  
Nature 178, 1046 (1956)

- **1956: Hanbury Brown and Twiss** measure correlations between starlight intensities with two separate detectors (star radius determination)
- The signal is proportional to  $\langle I_1(t)I_2(t) \rangle$  where  $I_1(t)$  is the intensity measured at detector 1
  - **characteristic photon statistics** for different light sources



# Poisson distribution

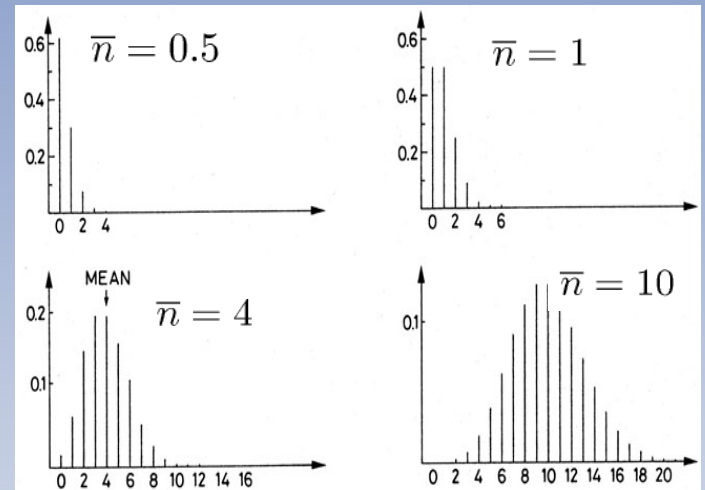
## 4. Statistics of light

- For **coherent light** with constant frequency, phase, and amplitude, the **signal** at both detectors is **uncorrelated**
- Photon statistics corresponds to the **Poisson distribution**

$$\mathcal{P}(n) = \frac{\bar{n}^n}{n!} e^{-\bar{n}} \quad (n = 0, 1, 2, 3, \dots)$$

probability to measure  $n$  photons at an averaged photon number  $\bar{n}$

- For large  $\bar{n}$  goes into a **Gaussian distribution**
- **Standard deviation** is  $\Delta n = \sqrt{\bar{n}}$



M. Fox, Quantum Optics, Oxford University Press (2006)





# Super-Poisson distribution

## 4. Statistics of light

- Thermal light shows **intensity fluctuations**

→ **Super-Poisson** distribution

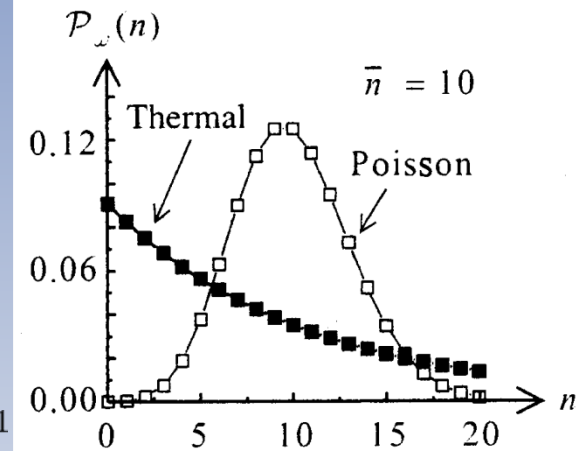
$$\Delta n > \sqrt{\bar{n}}$$

- Thermal light corresponds to **Bose-Einstein** distribution

$$\mathcal{P}(n) = \frac{\bar{n}^n}{(\bar{n} + 1)^{n+1}} \quad \text{with } \bar{n} = (e^{\hbar\omega/k_B T} - 1)^{-1}$$

- **Thermal light** is characterized by a **broader distribution** compared to coherent light (Poisson distribution)

- Bose-Einstein distribution has a **standard deviation** of  $\Delta n = \sqrt{\bar{n}^2 + \bar{n}}$



M. Fox, Quantum Optics



# Sub-Poisson distribution

## 4. Statistics of light

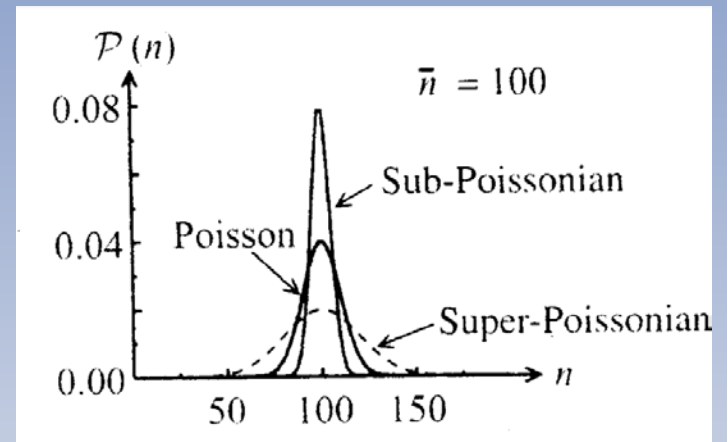
- Sub-Poisson distribution with

$$\Delta n < \sqrt{\bar{n}}$$

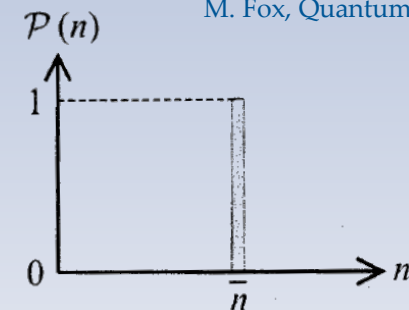
is **narrower** compared to Poisson  
(**less fluctuations** than coherent light)

→ **non-classical light**

- **Fock states** with  $\Delta n = 0$  correspond to purest non-classical light
- Detection of such light is a proof of **quantum nature of light**, but difficult to measure, since all losses destroy the Poisson statistics

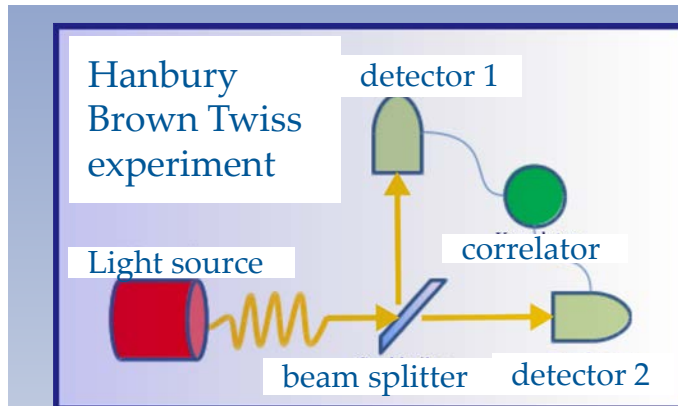


M. Fox, Quantum Optics



# Second-order correlation function $g^{(2)}$

## 4. Statistics of light



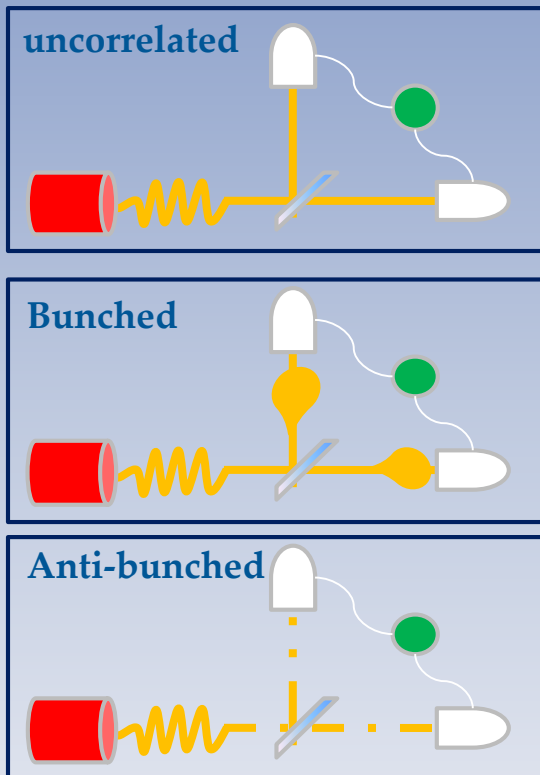
$$g^{(2)}(\tau) = \frac{\langle I_1(t)I_2(t + \tau) \rangle}{\langle I_1(t) \rangle \langle I_2(t + \tau) \rangle}$$

with intensities  $I_1(t)$  and  $I_2(t + \tau)$  measured at detectors 1 and 2 with a time delay  $\tau$

- $g^{(2)}$  is a measure for the probability to detect a photon at the detector 2, after a photon has already been measured at the detector 1
- The **correlation vanishes** for  $\tau \gg \tau_c$  with the **coherence time**  $\tau_c$ , since on this time scale the intensity fluctuations become small

# Photon statistics

## 4. Statistics of light



- Measurements at detectors are uncorrelated



coherent light

- **Positive correlation** between the measurements (**bunching**)



thermal light

- **Negative correlation** between the measurements (**anti-bunching**)



non-classical light



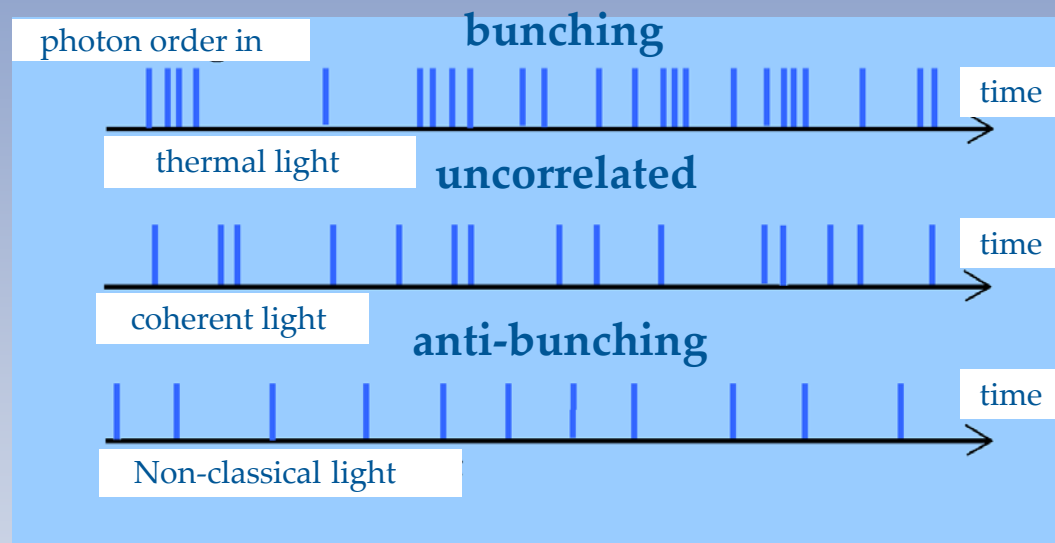
**CHALMERS**

UNIVERSITY OF TECHNOLOGY

A. Carmele (TU Berlin)

# Photon statistics

## 4. Statistics of light



forphys.de

- Classification of light via  $g^{(2)}$  – **function** (quantitative determination of photon correlation in different light sources)
- Evaluation at  $\tau = 0$  sufficient, since here the **correlation the strongest**



# Photon statistics via $g^{(2)}$

## 4. Statistics of light

$$g^{(2)}(0) = \frac{\langle c^+ c^+ c c \rangle}{\langle c^+ c \rangle \langle c^+ c \rangle} = \frac{\langle (\Delta n)^2 \rangle - \bar{n}}{\bar{n}^2} + 1 \quad \bar{n} = \langle c^+ c \rangle$$
$$\langle (\Delta n)^2 \rangle = \langle c^+ c c c^+ c \rangle - \langle c^+ c \rangle^2$$

⇒ **Coherent light**

Poisson distribution  $\Delta n = \sqrt{\bar{n}}$

Example: **laser**

$$g^{(2)} = 1$$

**uncorrelated**

⇒ **Thermal light**

Super-Poisson distribution  $\Delta n > \sqrt{\bar{n}}$

Example: **sun light**  $\Delta n = \sqrt{\bar{n}^2 + \bar{n}} \rightarrow g^{(2)} = 2$

$$g^{(2)} > 1$$

**bunching**

⇒ **Non-classical light**

Sub-Poisson distribution  $\Delta n < \sqrt{\bar{n}}$

Example: **Fock state**  $\Delta n = 0 \rightarrow g^{(2)} = 1 - \frac{1}{\bar{n}}$

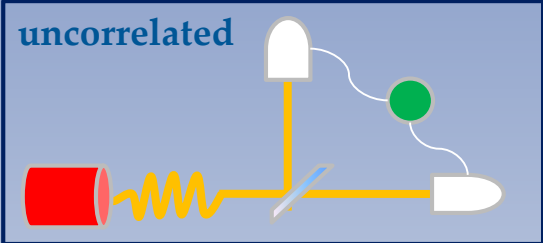
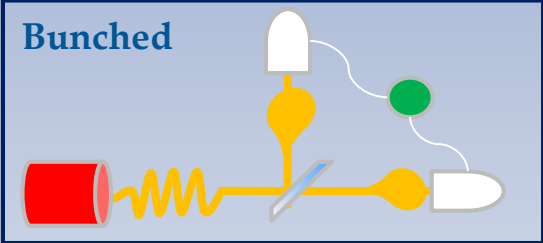
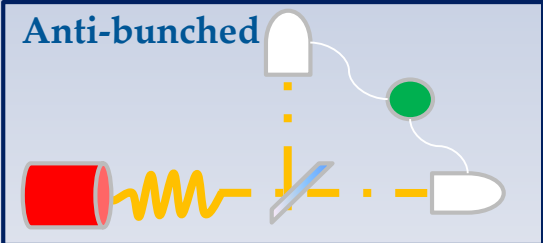
$$g^{(2)} < 1$$

**anti-bunching**



# Photon statistics at one sight

## 4. Statistics of light

$g^{(2)} = 1$	<p>uncorrelated</p> 	<p>Poisson</p> <p>Coherent light (e.g. laser light)</p>
$g^{(2)} > 1$	<p>Bunched</p> 	<p>Super-Poisson</p> <p>thermal light (e.g. sun light)</p>
$g^{(2)} < 1$	<p>Anti-bunched</p> 	<p>Sub-Poisson</p> <p>Non-classical light (e.g. Fock states)</p>



# Learning outcomes lecture X

- Recognize the importance of **pump-probe experiments** for revealing carrier dynamics
- Explain the **photon statistics** for different light sources





# Contents: FKA091 Part I



## I. Introduction

1. Main concepts
2. Theoretical approaches
3. Born-Oppenheimer approximation



## II. Electronic properties of solids

1. Bloch theorem
2. Electronic band structure
3. Density of states



## III. Electron-electron interaction

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



# Contents: FKA091 Part I

- IV. Density matrix theory
  1. Statistic operator
  2. Bloch equations
  3. Boltzmann equation
- V. Density functional theory (guest lecture by Paul Erhart)
- VI. Optical properties of solids
  1. Electron-light interaction
  2. Absorption spectra
  3. Differential transmission spectra
  4. Statistics of light



# Learning Outcomes

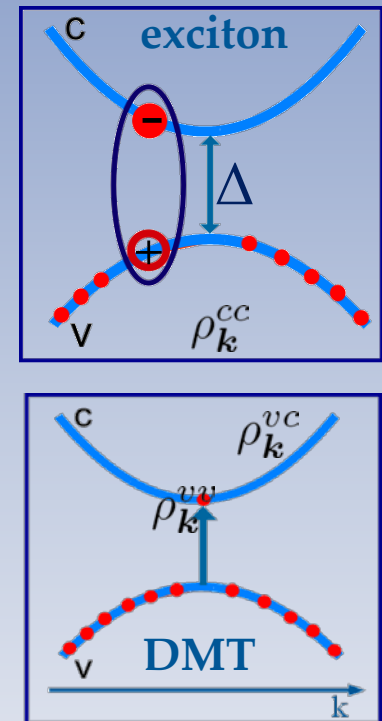
- Recognize the **main concepts** of condensed matter physics including introduction of **quasi-particles** (such as excitons, plasmons)
- Realize the importance of **Born-Oppenheimer, Hartree-Fock, and Markov approximations**
- Explain the **Bloch theorem** and calculate the **electronic band structure**
- Define **Hamilton operator** in the formalism of **second quantization**
- Realize the potential of **density matrix** and **density functional theory**
- Explain the semiconductor **Bloch** and **Boltzmann equations**
- Recognize the **optical finger print** of nanomaterials



# Recap chapter I

## Born-Oppenheimer approximation

- Introduction of **non-interacting quasi-particles** (eg excitons) is an important concept of condensed matter physics to deal with many-particle systems
- Main theoretical approaches include **density matrix theory** (DMT) with **semiconductor Bloch** and **Boltzmann scattering equations** and **density functional theory** (DFT) with the central Hohenberg-Kohn theorem
- In **Born-Oppenheimer approximation**, **electron and ion dynamics** is **separated** based on the much larger mass and slower motion of ions



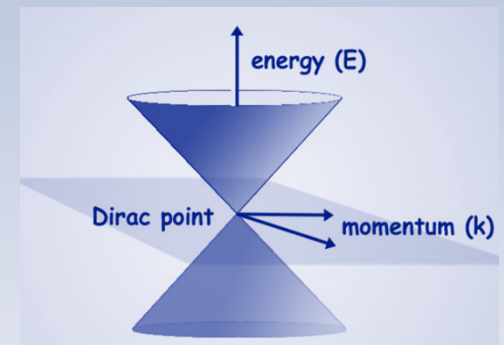
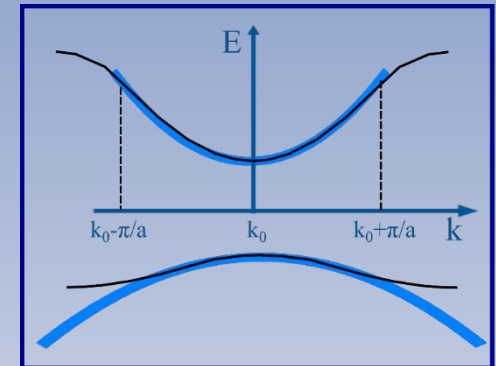
# Recap chapter II

## Bloch theorem

- **Bloch theorem: eigen functions** of an electron in a periodic potential have the shape of **plane waves modulated with a periodic Bloch factor**

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

- **Eigen energies** are expressed in material-specific **electronic band structure** that can be calculated in **effective mass** or **tight-binding approximation**
- **Graphene** exhibits a remarkable **linear and gapless** electronic band structure  $E_{\lambda}(\mathbf{k}) = \sigma_{\lambda} \hbar v_F |\mathbf{k}|$



# Recap chapter III

## Second quantization

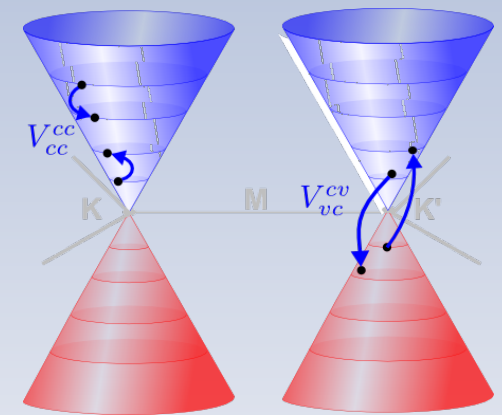
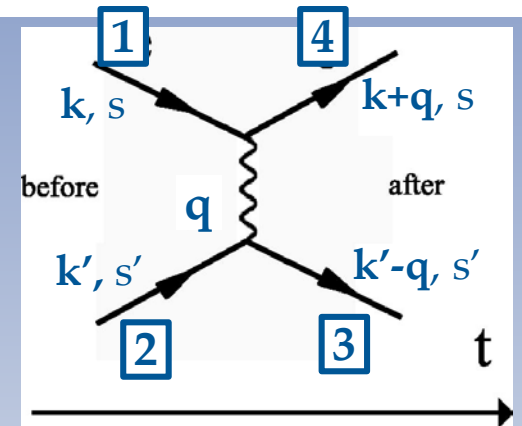
- **Electron-electron interaction** is driven by the repulsive **Coulomb potential**

$$V_q^{3D} = \frac{e_0^2}{\epsilon_0 L^3} \frac{1}{q^2} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \delta_{s_1, s_4} \delta_{s_2, s_3}$$

- Second quantization **avoids (anti-)symmetrisation** of many-particle states and mirrors the physics in **fundamental commutation relations**

$$[a_\alpha, a_\beta^\dagger]_\pm = a_\alpha a_\beta^\dagger \pm a_\beta^\dagger a_\alpha = \delta_{\alpha\beta}$$

$$[a_\alpha^\dagger, a_\beta^\dagger]_\pm = [a_\alpha, a_\beta]_\pm = 0$$



# Recap chapter III

## Jellium/Hubbard model

- **Jellium** model assumes **interacting electrons** in a **smearred potential** of ions (no lattice structure considered)

$$H_J = \sum_{\mathbf{k}s} \varepsilon_{\mathbf{k}s} a_{\mathbf{k}s}^+ a_{\mathbf{k}s} + \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \sum_{ss'}^{q \neq 0} V_q a_{\mathbf{k}+\mathbf{q}s}^+ a_{\mathbf{k}'-\mathbf{q}s'}^+ a_{\mathbf{k}'s'} a_{\mathbf{k}s}$$

- **Hubbard** model assumes **strong lattice potential** and **tightly bound electrons**

$$H_H = \sum_{ijs} T_{ijs} a_{is}^+ a_{js} + \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1)$$



# Recap chapter III

## Hartree-Fock approximation

- **Hartree-Fock approximation** introduces an **effective one-particle problem** by considering a single particle in a **mean-field potential** generated by all other particles

$$H_{\text{eff}} = \sum_{l_1} \left[ \varepsilon_{l_1} + \sum_{l_2} \left( V_{l_2 l_1}^{l_1 l_2} - V_{l_1 l_2}^{l_1 l_2} \right) \langle a_{l_2}^+ a_{l_2} \rangle_{\text{eff}} \right] a_{l_1}^+ a_{l_1}$$

Hartree term (direct term)    Fock term (exchange term)

- Most important approximation is the **factorization of 2-particle into single-particle** expectation values

$$\langle a_A^+ a_B^+ a_C a_D \rangle = \langle a_A^+ a_D \rangle \langle a_B^+ a_C \rangle \delta_{A,D} \delta_{B,C} - \langle a_A^+ a_C \rangle \langle a_B^+ a_D \rangle \delta_{A,C} \delta_{B,D}$$



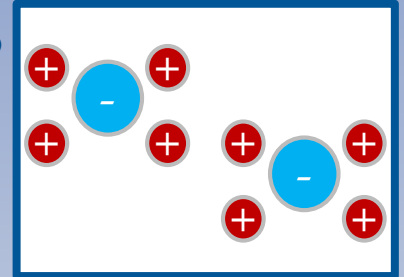


# Recap chapter III

## Screening

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

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



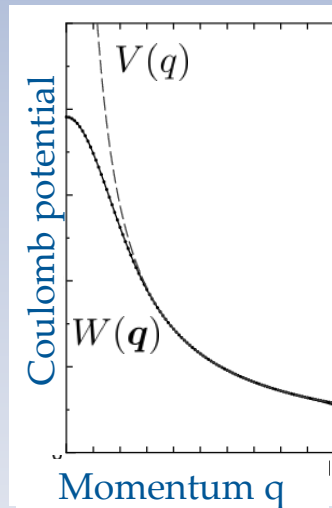
- In the **static and long-wavelength limit** we find

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

with the screening length

$$\kappa = \sqrt{\frac{e_0^2}{\varepsilon_0} \partial_{\mu} n}$$

- Screening **removes** the **divergence** of Coulomb potential for  $q \rightarrow 0$

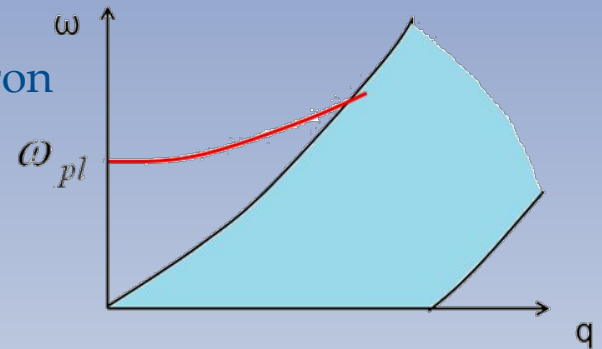


# Recap chapter III

## Plasmons and excitons

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

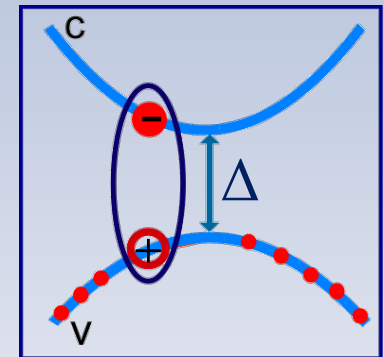
$$\omega_{pl} = \sqrt{\frac{ne_0^2}{\epsilon_0 m_e}}$$



- Excitonic binding energy** reads

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

with the reduced mass  $\mu = \frac{m_c m_v}{M}$   
and the dielectric background constant



# Recap chapter IV

## Statistical operator (density matrix)

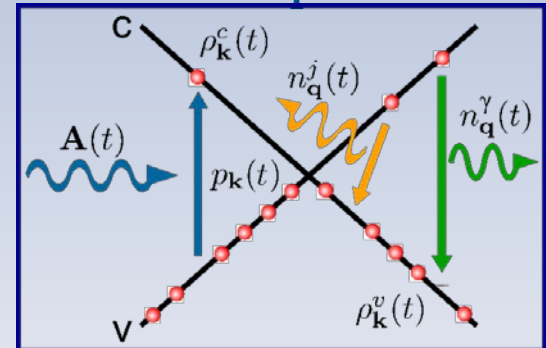
- **Statistical operator** (density matrix) characterizes quantum systems in a **mixed state**

$$\rho = \sum_n p_n |\Psi_n\rangle \langle \Psi_n| \quad \text{and builds the expectation value of observables}$$
$$\langle O \rangle = \text{tr}(\rho O)$$

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

- **Carrier occupation**  $\rho_{\mathbf{k}}^{\lambda}(t) = \langle a_{\lambda\mathbf{k}}^+ a_{\lambda\mathbf{k}} \rangle(t)$

- **Microscopic polarization**  $p_{\mathbf{k}}(t) = \langle a_{c\mathbf{k}}^+ a_{v\mathbf{k}} \rangle(t)$



# Recap chapter IV

## Semiconductor Bloch equations

- 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

$$\begin{aligned}\dot{\rho}_{\mathbf{k}}^{\lambda}(t) &= -2\text{Im}(\Omega_{\mathbf{k}}^*(t) p_{\mathbf{k}}(t)) + \frac{2}{\hbar} \sum_{\mathbf{k}'} V_{\mathbf{k}'v,\mathbf{k}c}^{\mathbf{k}v,\mathbf{k}'c} p_{\mathbf{k}'}(t) p_{\mathbf{k}}^*(t) \\ \dot{p}_{\mathbf{k}}(t) &= \frac{i}{\hbar} (\varepsilon_{\mathbf{k}}^v - \varepsilon_{\mathbf{k}}^c) p_{\mathbf{k}}(t) - i\Omega_{\mathbf{k}}(t) (\rho_{\mathbf{k}}^c(t) - \rho_{\mathbf{k}}^v(t)) - \gamma_{\mathbf{k}}(t) p_{\mathbf{k}}(t) \\ &\quad + \frac{i}{\hbar} \sum_{\mathbf{k}'} \left[ V_{\text{ren}}^{\mathbf{k}\mathbf{k}'} (\rho_{\mathbf{k}'}^v(t) - \rho_{\mathbf{k}'}^c(t)) p_{\mathbf{k}}(t) - V_{\text{exc}}^{\mathbf{k}\mathbf{k}'} (\rho_{\mathbf{k}}^c(t) - \rho_{\mathbf{k}}^v(t)) p_{\mathbf{k}'}(t) \right]\end{aligned}$$

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



# Recap chapter IV

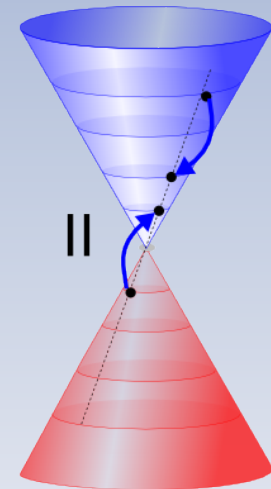
## Boltzmann scattering equation

- Boltzmann scattering equation reads in second-order Born-Markov approximation

$$\dot{\rho}_{\mathbf{k}}^{\lambda}(t) = \Gamma_{\mathbf{k},\lambda}^{in}(t) (1 - \rho_{\mathbf{k}}^{\lambda}(t)) - \Gamma_{\mathbf{k},\lambda}^{out}(t) \rho_{\mathbf{k}}^{\lambda}(t)$$

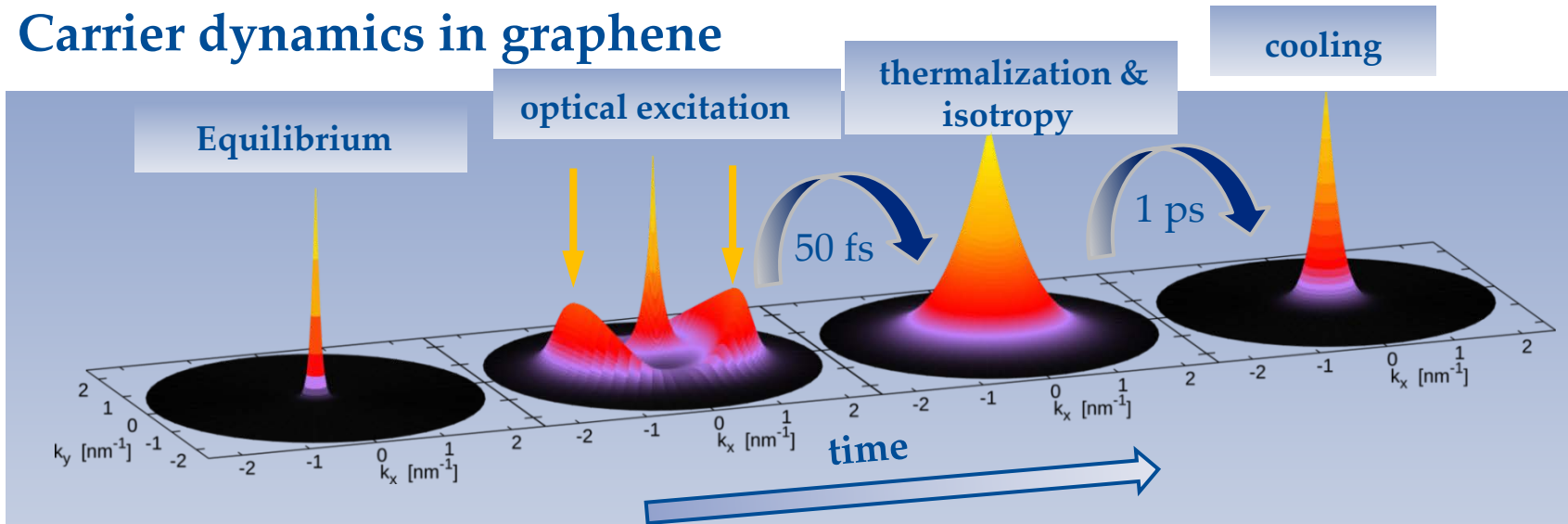
and describes **time- and momentum-resolved electron scattering** dynamics in non-equilibrium

- Markov approximation neglects **quantum-mechanical memory effects** stemming from energy-time uncertainty
- In graphene, **carrier multiplication** can take place due to efficient Auger scattering channels



# Recap chapter IV

## Carrier dynamics in graphene



- Optically generated **anisotropic non-equilibrium** carrier distribution
- **Carrier-phonon** scattering accounts for **isotropy**, while **carrier-carrier** scattering leads to a spectrally broad **thermalized** distribution in the first 50 fs
- **Carrier-phonon** scattering gives rise to carrier **cooling** on **ps time scale**



# Recap chapter V

## Density functional theory

- **Density functional theory** aims at the calculation of the quantum mechanic **ground state**  $\Psi_0(x_1, x_2, \dots, x_N)$  of a many-particle system
- Ground state can be unambiguously determined from the **electron density**  $n_0(\mathbf{r}) = \sum_i |\Psi_i(\mathbf{r})|^2$  (**Hohenberg-Kohn Theorem**)
  - full Schrödinger equation with  $N^3$  degrees of freedom does not need to be solved
- Electron density is solved through **Kohn-Sham equations** assuming an effective one-particle Hamilton operator



# Recap chapter VI

## Electron-light interaction

- The electron-light Hamilton operator reads in second quantization

$$H_{e-l}^{p \cdot A} = \frac{i\hbar e_0}{m_e} \sum_{l,l'} M_{l,l'} \cdot A(\mathbf{r}_0, t) a_l^\dagger a_{l'}, \quad H_{e-l}^{r \cdot E} = \sum_{l,l'} d_{l,l'} \cdot E(\mathbf{r}_0, t) a_l^\dagger a_{l'}$$

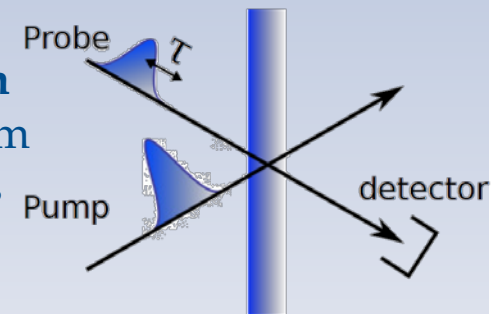
- Absorption coefficient  $\alpha(\omega)$  is given by the optical susceptibility  $\chi(\omega)$

$$\alpha(\omega) = \frac{\omega}{n(\omega) c_0} \text{Im}\chi(\omega)$$

that is determined by microscopic polarization

- In pump-probe experiments, differential transmission is measured, where pump pulse creates non-equilibrium and weaker probe pulse measures the carrier dynamics

$$\Delta T/T_0(\tau, \omega) \propto (\rho_{k_0}^{(p)}(\tau) - \rho_{k_0}(-\infty))$$





# Recap chapter VI

## Semiconductor Bloch equation (linear optics)

- Graphene Bloch equation in the limit of linear optics

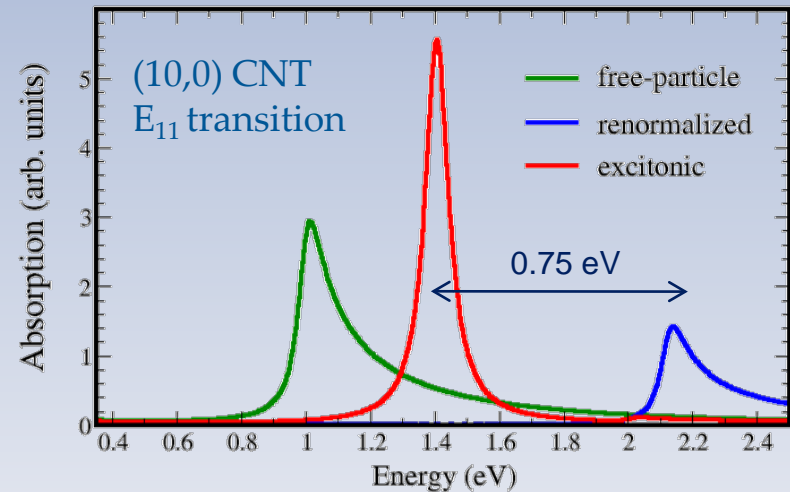
$$\dot{p}_{\mathbf{k}}(t) = \frac{i}{\hbar} \Delta \tilde{\varepsilon}_{\mathbf{k}}^{vc} p_{\mathbf{k}}(t) + i \tilde{\Omega}_{\mathbf{k}}(t) - \gamma p_{\mathbf{k}}(t)$$

- Electron-electron interaction leads to a **renormalization of the energy**

$$\Delta \tilde{\varepsilon}_{\mathbf{k}}^{vc} = (\varepsilon_{\mathbf{k}}^v - \varepsilon_{\mathbf{k}}^c) + \frac{i}{\hbar} \sum_{\mathbf{k}'} V_{\text{ren}}^{\mathbf{k}\mathbf{k}'}$$

and to a **renormalization of the Rabi frequency (excitons)**

$$\tilde{\Omega}_{\mathbf{k}}(t) = \Omega_{\mathbf{k}}(t) + \frac{i}{\hbar} \sum_{\mathbf{k}'} V_{\text{exc}}^{\mathbf{k}\mathbf{k}'} p_{\mathbf{k}'}(t)$$

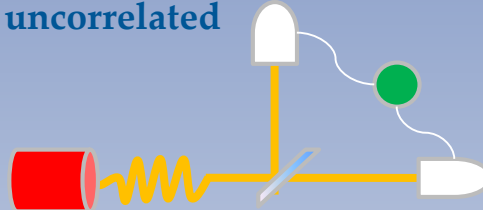


# Recap chapter VI

## Photon statistics

$$g^{(2)} = 1$$

uncorrelated

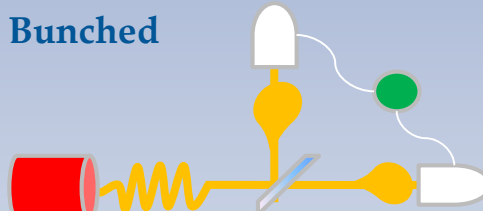


Poisson

Coherent light  
(e.g. laser light)

$$g^{(2)} > 1$$

Bunched

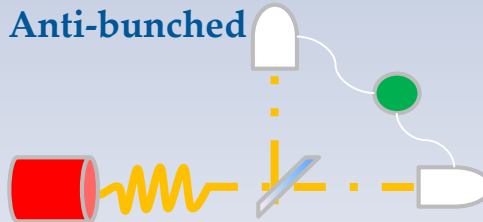


Super-Poisson

thermal light  
(e.g. sun light)

$$g^{(2)} < 1$$

Anti-bunched



Sub-Poisson

non-classical light  
(e.g. Fock states)



# Learning Outcomes

- Recognize the **main concepts** of condensed matter physics including introduction of **quasi-particles** (such as excitons, plasmons)
- Realize the importance of **Born-Oppenheimer, Hartree-Fock, and Markov approximations**
- Explain the **Bloch theorem** and calculate the **electronic band structure**
- Define **Hamilton operator** in the formalism of **second quantization**
- Realize the potential of **density matrix** and **density functional theory**
- Explain the semiconductor **Bloch** and **Boltzmann equations**
- Recognize the **optical finger print** of nanomaterials

