5 Optical Processes in Semiconductors:

- Optisch induzierte Polarisation Eines Moleküls
- Polarized Atomic Dipole in Optical Field
- Blue Silicon Carbide Light Emitting Diode LED
- Representation of band-to-band transitions in Semiconductors
Goals of the chapter:

Design of optical SC-devices (Laser, Photodetectors, optical amplifiers, etc.) depends critically on the calculation of the carrier transition rates $R$, the rate-equations of carriers and photons and the optical gain $g(\omega, n)$

- Nonclassical description of the motion of bound electrons in the static force fields of the atomic nucleus or crystal lattice and a oscillating light wave
- The equation of motion and polarization has to be described in a quantized 2-energy level material system by a quantum mechanical model based on the perturbed time dependent Schrödinger-equation
- The description of the interaction between light field and a 2-energy band Semiconductor needs an extension of the discrete 2-level concepts to continuum-to-continuum, resp. band-to-band optical transitions

Methods for the Solution:

- The classical model for electron motion $r(t)$ of “electrons-on-springs” will be replaced by the time-dependent Schrödinger-equation (TSE) for a harmonic oscillator providing a statistical expectation value $\langle r(t) \rangle$
- The quantum mechanical equation of motion of the expectation value $\langle r(t) \rangle$ of bound or quasi-free charges in atoms and SC will be obtained for weak optical fields.
- Perturbation-theory leads to the Transition-Rates $R$ and a realistic microscopic susceptibilities $\chi(\omega, n_2, n_1)$ depending on the of charge carriers densities $n_1, n_2$ in the lower and upper levels
- The quantum-mechanical analysis shows for carrier inversion $n_2 > n_1$ optical gain $g(\omega_{\text{opt}})$ occurs
5 Optical Processes in Semiconductors:

Introduction:
The classical dipole oscillator model „electrons on springs“ breaks down for
a) the quantized energy exchange between atom and light field,
b) the microscopic force constant and the relation to carrier state occupancy, that is:

- the „spring force constant“ $k_{DP}$ and the damping $\gamma_D$ of the dipole motion are not physically defined
- Realization of a positive $\chi'' > 0$, resp. $\gamma < 0$ to obtain optical gain is not obvious?
  ➔ Carrier motion in a atomic system with discrete quantized energy levels $E_2$ and $E_1$ and
  ➔ Distribution of carriers $n_2, n_1$ occupying these levels influence the optical gain $g$?
- Separation of transparent and absorbing spectral regions of SC

➢ Goal: Semi-classical QM-Theory of the atomic oscillator and a light field with
  - a classical optical field and
  - a quantum mechanical (QM) description of the microscopic, induced dipole motion
    by an optical field
Step 1: Einstein-Theory of optical transitions
- Phenomenological semi-classical description of optical processes in a quantized 2-level medium by the so-called Einstein-Rate-equation formalism of optical transitions (Einstein 1905)

Step 2: Quantum mechanical model of optical transitions
- Quantum mechanical model for the dipole-oscillator (perturbation theory) (~1930)
  - Relation between microscopic material parameters and the quantum mechanical susceptibility $\chi$
  - Condition for optical gain in atoms and SC and the concept of “pumping” and carrier inversion
  - Extension of the 2-level-interaction to band-to-band transitions in SCs
  - Calculation of optical gain / absorption spectrum $g(\omega,n)$ in SC as a function of carrier density $n$, $p$. 
What are the concepts for a solution from a QM viewpoint?:

A) Stationary Eigenstates:

Consider an electron moving in the attractive and repulsive static potential field \( V(r) \) of an individual atom or a crystal lattice without an optical field.

Quantization of motion defines static discrete energy eigenstates \( \Psi_i(r,t) \), with energy eigenvalues \( E_i \) (assumed dipole-free)

The matter wave functions \( \Psi_i(r,t) \) fulfill the
time-independent Schrödinger equation (SE):

\[
H \Psi(x,t) = \left( \frac{p^2}{2m} + qV(x) \right) \Psi(x,t) = E \Psi(x,t)
\]

Solving the Schrödinger Eigenvalue problem \( \rightarrow E_j \) (energy eigenvalue), \( \Psi_j \) (energy eigenfunction) with \( \omega_j = E_j/h \) and \( E_2 > E_1 \)

\( V(x) \) is the potential of the atomic electric force field
\( p \) is the momentum operator
\( m \) is the mass of the particle
\( H \) is the Hamilton operator

Generic stationary Solution:

\[
\psi_i(x,t) = u_i(x) e^{-j\omega_j t} = u_i(x) e^{-jE_i/h t}
\]

General solution:

\[
\psi(x,t) = \sum_i C_i \psi_i(x,t)
\]
with the normalizations:
\[ \langle \psi | \psi \rangle = \langle \psi_i | \psi_i \rangle = 1 \quad \rightarrow \quad \sum_i |C_i|^2 = 1 \]
\[ \langle \psi | \psi_i \rangle = C_i^* \]
\[ \langle \psi_i | \psi \rangle = C_i \]

Interpretation of the \( C_i \):

The coefficient \( |C_i|^2 = C_i C_i^* \) is proportional to the probability of finding the system in the state \( \psi_i(x,t) \) with the energy \( E_i \).

**B) Time dependence Eigenstate occupation**

**Perturbation of the static potential field \( V(r) \) by a superposed harmonic optical field \( (E, H, \omega) \) with its dynamic potential \( V_{opt}(r,t) \)**

Definition: **weak perturbation**  
the optical field is much weaker than the static atomic field, \( V_{atom} \gg V_{opt} \)

- **QM-interaction** between \( N \) quantized 2-level system \( (E_2, E_1) \) (level \( E_2 \) with \( N_2 \) electrons, level \( E_1 \) with \( N_1 \) electrons) and a classical, non-quantized optical harmonic EM-field \( (E, H) \) of **spectral energy-density** \( W(\omega) \), \( W(\omega) = \frac{\partial^2 E_{EM}}{\partial V \partial \omega} \)

- **The interaction** changes of the **occupation probabilities** \( (N_2(t)/N, N_1(t)/N) \) of the 2-level system by **photon absorption or emission**, resp. **transitions between levels** combined with an **energy exchange due to the EM-forces of the light field**
Quantum mechanical perturbation analysis: time-dependent SE

\[
H\Psi(x,t) = \left( \frac{p^2}{2m} + qV_{\text{atom}}(x) + qV_{\text{opt}}(x,t) \right)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)
\]

\text{static potential} \quad \text{oscillating potential of the EM-field} \ (\omega_{\text{opt}})

Assumed \textbf{dynamic solution} \ \Psi(x,t):

a superposition of static solutions \ \Psi_1(x,t) \ ; \ \Psi_2(x,t) \ \text{with time-dependent coefficients} \ C_i(t)

\[
\Psi(x,t) = C_1(t)\Psi_1(x,t) + C_2(t)\Psi_2(x,t) = C_1(t)u_1(x)e^{-j\omega t} + C_2(t)u_2(x)e^{-j\omega t}
\]

\(C_1(t), C_2(t)\) are now \textbf{time-functions}

\(\Psi(x,t)\) \textbf{describes the quantized system completely in its interaction with the optical field} !

Calculation of the \textbf{time dependent expectation values} of the variables of the atomic system relevant for optical properties:

\[
\langle x(t) \rangle; \langle P(t) \rangle; \langle \chi(\omega) \rangle; \langle N_2(t) \rangle; \langle N_1(t) \rangle \ \text{etc.}
\]
5.1 Quantum mechanical model of the dipole-oscillator

5.1.1 Semi-classical model for absorption and gain

**Optical Absorption and Amplification**

- The classical, mechanical model breaks down describing photon emission- and absorption properties and provides no clue for amplification and energy quantization.
- only the frequency dependence of the refractive index far away from the atomic resonance is well described (with phenomenological parameters)

The **classical, mechanical Lorentz-model** is based on:

1. classical description of optical fields with continuous E- und H-field variables and a spectral field-energy density

\[ W(\omega) = \frac{\partial^2 \text{Energy}}{\partial \omega \partial V} \]

2. it neglects the particle aspect of the optical field, the quantization \( E=\hbar \nu \) of the field and the particle concept of the photon

3. the atomic harmonic oscillator, described by the coordinate \( x(t) \) of the charge separation\(^\dagger\) of the dipole and its system energy \( E \) (potential and kinetic) as continuous observables of the Newton equation of motion.

The model does not describe:

1. Optical Gain and Absorption
2. Optical spontaneous emission

Extension to the **semi-classical quantum mechanical-model**:

\(^\dagger\) Specified by quantum mechanical model
5.1.2 Interaction of a EM-field with a discrete 2-level system

Introduction: (Lit. Loudon)

- The optical field is represented by a classical, not quantized field $H(r,t), E(r,t)$ → description by Maxwell's equations
- The medium response and its microscopic electrodynamics with respect to energy quantization $E_1, E_2$ under interaction with the optical field $E(t)$ (QM-description of the equation of motion for the electron position $x(t)$)
  → description of expectation value of $<x(t)>$ of the QM-dipole by the time-dependent Schrödinger equation

Atomic 2-level systems $(E_1, E_2, N_1, N_2)$ which interact with an optical EM-field $(\omega, E, H)$ exchange energy resulting in a change of the occupation probability of the of the electrons, resp. in a change of the electron numbers $N_1, N_2$.

The goal is to calculate the time evolution of $N_1(t)$ and $N_2(t)$ for an idealized “2-level atom” and the formation of an atomic dipole $p(t)$ under the influence of the harmonic optical field $\tilde{E}(\tilde{r},t), \tilde{H}(\tilde{r},t)$.

Strong interaction only close to the atomic transition frequency $\omega_{21} = (E_2 - E_1)/\hbar$

Quantum mechanical 2-Level-System

as a model: (quantitative description, QM >1930)

- 1-electron-atom-model with
  (no collision processes → infinite state-lifetime)
  2 discrete „sharp“ energy-levels $E_1$ and $E_2$ ($E_1 < E_2$)

- The 2 energy levels are Eigenvalues $E_1$ und $E_2$ of the 1-D time independent Schrödinger-equation
  for the electron in the stationary, parabolic potential $V(x)$ of the nucleus:

Energy-Levels of a harmonic Oscillator (electron in a parabolic potential $V(x) = -kx^2$, no light field)
**Stationary state without optical field: Time independent Schrödinger-Equation**

The matter wave \( \psi(x,t) \) representing the probabilistic motion of a particle of constant total energy \( E = E_{\text{tot}} \) (kinetic and potential) in a stationary electrostatic potential \( V(x) \) is a solution (eigenfunction) with the energy eigenvalue \( E \) of:

\[
H \psi(x,t) = (H_{\text{kin}} + H_{\text{pot}}) \psi(x,t) = \left( \frac{p^2}{2m} + qV(x) \right) \psi(x,t) = E \psi(x,t)
\]

\( H = \) Hamilton (Energy)-Operator

**Stationary Schrödinger equation with time-invariant potential \( V(x) \)**

\[
H = \left( \frac{p^2}{2m} + qV(x) \right) = \text{Hamilton – Operator} \quad \text{(of the time-independent potential } V(x) \text{ of the positive nucleus)}
\]

\( p = -j\hbar \frac{\partial}{\partial x} = \) impulse operator ; \( p^2 = -\hbar^2 \frac{\partial^2}{\partial x^2} \)

\( E = \) total energy = potential and kinetic energy

\( V(x) = \) time-independent potential of the nucleus

\( q = \) charge of the particle (-e)

\( \psi(x,t) = \) Eigenfunction of the matter wave

with the time-space-dependent **Eigenfunctions** \( \psi(x,t) = u(x)e^{-j\omega t} = u(x)e^{-jE/\hbar t} \), resp. spatial term \( u(x) \) and **Energy Eigenvalues** \( E \) as solutions:

\[
H u_i(x) = \left( \frac{p^2}{2m} + qV(x) \right) u_i(x) = E_i u_i(x) \quad \text{with} \quad u_i(x) = \text{spatial Eigenfunction and Eigenvalue } E_i
\]
Eigenfunction are a complete orthonormal set $\mu_i$ (= orthogonal and normalized):

$$\langle u_i | u_j \rangle = \int_{-\infty}^{+\infty} u_i^* u_j \, dx = \delta_{ij} \quad \text{with} \quad \delta_{ii} = 1, \quad \delta_{ij} = 0 \text{ if } i \neq j$$

(without proof)

$E_1$:
$$\Psi_1(x,t) = u_1(x) e^{-jE_1/h \, t} \quad \text{Standing wave with the oscillation frequency } \omega_1 = E_1/h$$

$E_2$:
$$\Psi_2(x,t) = u_2(x) e^{-jE_2/h \, t} \quad \text{Standing wave with the oscillation frequency } \omega_2 = E_2/h$$

**General solution:**
$$\psi(x,t) = C_1 \psi_1(x,t) + C_2 \psi_2(x,t) \quad C_1, C_2 = \text{constant}$$

$|C_1|^2$ and $|C_1|^2$ are the probabilities of finding the system at $E_1$ or $E_2$; $|C_1|^2 + |C_1|^2 = 1$

- $\Psi(x,t)$ describes the statistical behaviour of the electron in the potential field $V(x)$ with constant total Energy $E$.

- $\Psi\Psi^* = |\Psi|^2$ is interpreted as probability density of finding the electron at the position $x$, if normalized to: $\int \psi\psi^* \, dx = 1$.

- The statistical expectation value $<x>$ for the space variable $x$ of the particle is (probability of finding the particle at $x$):

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) x \Psi(x,t) \, dx = \int_{-\infty}^{+\infty} u^*(x) x u(x) \, dx \quad \text{Definition of BRA–KET notation}$$

we will use $\langle x \rangle$ to describe the dipole

$$\langle p \rangle = -e \langle x \rangle \quad \rightarrow \quad \langle \chi \rangle \quad \text{etc.}$$

- The stationary solutions $\Psi(x,t)$ are, in order to be stationary ($E=\text{const}$.), non-radiating, resp. free of a dipole moment.
Definition of bra-ket notation:

The expectation value $\langle f \rangle$ of an observable $f(x)$ of a QM-system is defined as:

$$\langle f \rangle = \int_{-\infty}^{+\infty} \Psi^*_a(x,t) f(x) \Psi_b(x,t) \, dx \equiv \langle \Psi_a | f | \Psi_b \rangle$$

Non-stationary states with a perturbing optical field: Time dependent Schrödinger-Equation

It is expected that the nonstationary state with an interacting optical field changes the occupation probabilities $|IC_j(t)|^2$ by exciting or de-exciting charge carriers by optically induced state transitions between energy states $E_i, E_j$.

- the coefficients $C_i(t)$ become time functions
- State transitions will be described by transition probabilities $r$ and transitions rates $R$ of charge carriers

Electron dynamics in an optical EM-field $(\vec{E}(\vec{r},t), \vec{H}(\vec{r},t))$:

The optical EM-field exerts forces $\vec{F}(\vec{r},t)$ on the moving electron

a) time-dependent electrostatic force $\vec{F}_{\text{elektrisch}} = -e\vec{E}(x,t)$

and

b) time-dependent magnetic force $\vec{F}_{\text{Lorentz}} = e\mu_0 \vec{v} \times \vec{H}$

- producing energy exchange and state transitions

In most cases we can neglect the H-field because $\vec{F}_{\text{elektrisch}} \gg \vec{F}_{\text{Lorentz}}$
Schematic representation of basic interactions of a 2-level system and an optical field:

Photon Absorption  Spontaneous Photon-Emission  Stimulated Photon-Emission

(Electron-Hole-Pair Generation)  Photon-Annihilation  (Electron-Hole-Pair Annihilation)  Photon-Generation

e-transition from:  $E_1 \rightarrow E_2$  $E_2 \rightarrow E_1$  $E_2 \rightarrow E_1$

EM-Radiation field changes occupation probabilities by level-transitions
What are the transition rates $R$ and how do they depend on the optical field?

In historical order:

1) **Einstein Theory**: (A. Einstein, 1905 without QM)

The 2-level system exchanges energy with the EM-field of frequency $\omega$ only if the photon energy $E=\hbar\omega=E_2-E_1$ (resonance)

1) electrons in the ground state $E_1$ absorb a photon and make an **upward transition** to the excited (upper) state $E_2$.

2) electrons in the excited state $E_2$ make a **downward transition** to the ground state $E_1$ emitting an **incoherent spontaneous photon** or emit a **coherent stimulated photon**, if a stimulating field is present.

3) Stimulated absorption and emission are **proportional to the energy density of the optical field**, the probabilities of the occupation of the initial state and the final state being empty.

**Definition: Transition-Pair** $(E_2, E_1) =$ initial and final state:

The initial and final state ($E_2$ and $E_1$) of an atom form a local transition pair. In isolated atoms the occupation of a level means that the other level is necessarily empty and available for a transition.

Details see p.5-16.

2) **Quantum Mechanics**: (after ~1930)

The motion of the bound electron in an optical field (where the energy $E$ of the 2-level system is not constant) is described by the matter wave $\Psi(x,t)$ of the electron in the **time dependent potential** $V(x,t) = V(x) + V_{opt}(t)$.

- The time-dependent EM-forces induce a microscopic dipole extracting (attenuation) or transferring (amplification) energy from or to the field depending on the relative phase.

- The energy-exchange excites electron transition from the ground to the excited state and vice versa if the optical frequency $\omega_{opt}$ is close to the transition frequency $\omega_{21}$.  

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Electronics Laboratory: Optoelectronics and Optical Communications 22.03.2010
Time-dependent Schrödinger equation with the time-dependent Hamilton-Operator $H_{ww}(x,t)$ of the optical field:

$$\left[ H(x) + H_{ww}(x,t) \right] \psi(x,t) = jh \frac{\partial}{\partial t} \psi(x,t) \quad \text{time-dependent Schrödinger equation}$$

$$H(x) = \left( \frac{p^2}{2m} + qV(x) \right) \quad \text{Static Energy-Operator } H(x) \text{ for the interaction with the positive charge of the nucleus } V(x)$$

$$H_{ww}(x,t) = ? \quad \text{time-dependent Energy-Operator for the interaction electron - optical field}$$

(how does the EM energy of the electron in the optical field formally enter $H_{ww}$)

**Task:** find the time-dependent solution $\psi(x,t)$ for $H_{ww}(t)$ of the harmonic optical field $E(t)$ of the form (weak perturbation assumption):

$$\psi(x,t) = C_1(t)\psi_1(x,t) + C_2(t)\psi_2(x,t) \quad C_1(t), \ C_2(t) = \text{time dependent}$$

$|C_1(t)|^2$ and $|C_1(t)|^2$ are the time-dependent probabilities of finding the system at $E_1$ or $E_2$ at a time $t$ ; $|C_1(t)|^2 + |C_1(t)|^2 = 1$

The solution-“Ansatz” for “weak” perturbation is a time-dependent superposition of the stationary solutions.

⇒ the occupation probabilities $|C(t)|^2$ of the levels become time dependent due to the energy exchange with the field.

⇒ Details in Chap.5.4.1.1 ,

first we consider the classical Einstein-Theory:
5.1.3 Einstein-Theory of the optical transition in 2-level systems

(see lit: Loudon)

**Concept:** Phenomenological theory of A. Einstein (1905).

Light fields and matter interact by EM-field induced stimulated and spontaneous level-transitions in 2-level atomic systems by photon emission and absorption at the transition frequency.

The transition modify the occupation probabilities $p_i$ of the energy levels $E_i$ in the atomic system (rate equations).

1) **Transition Postulate:**

- Matter is built from **quantized 2-level systems** (transition pairs) representing atoms undergoing interaction with a classical optical wave.

- Interaction with the EM-field induces “upward or downward” transition between the levels (absorption, emission).

The ⤷- or ⤸-transitions between levels $i$ and $j$ are described by changes in occupation probability $|IC_i(t)|^2$ and $|IC_j(t)|^2$:

(a) **Definition:** Transition Probability $r_{ij}$ ($i \rightarrow j$)

change of level occupation probability $p_j$ per unit time in a single 2-level system

$$ r_{ij} = \frac{\partial p_j}{\partial t} = \frac{\partial |C_j|^2}{\partial t} \quad i = \text{initial state} \quad ; \quad j = \text{final state} $$

(b) **Transition Rates** $R_{ij}$ ($i \rightarrow j$)

change of the particle density $N_j$ in state $E_j$ per unit time and volume of a collection of atomic density $N$

$$ R_{ij} = \frac{\partial^2 N_j}{\partial t \partial V} = r_{ij} N_i = r_{ij} N |C_i|^2 $$
Describing the **occupation probability** of state $i$ of the transition as

$$p_i(t) = |C_i(t)|^2$$

we get for the 2-level system $E_2$ and $E_1$ with

$$|C_2(t)|^2 \text{ and } |C_1(t)|^2 \text{ fulfilling } |C_2(t)|^2 + |C_1(t)|^2 = 1$$

$$r_{ij} = \frac{\partial |C_j(t)|^2}{\partial t} = -\frac{\partial |C_i(t)|^2}{\partial t} \quad \text{i= initial state, j= final state}$$

and obtain for the **transition rate of** $N_i$ identical pairs

$$R_{ij} = N_i \frac{\partial |C_j(t)|^2}{\partial t} = -N_i \frac{\partial |C_i(t)|^2}{\partial t} \quad \text{N}_i=\text{density of transition pairs } i \to j, \text{ resp. atoms}$$

### 2) **Spontaneous emission Postulate:**

For thermodynamic reasons or due to the additional quantization of the optical field (zero-point energy) **spontaneous emission transitions** (downward transitions) are possible **without** an exciting optical field.

Spontaneous emission is spatially isotropic.

### 3) **Stimulated emission Postulate:**

The **stimulated emitted photon** induced by an external field has the same **frequency** $\omega$, **phase** $\phi$ and **propagation direction** (wave number) $\vec{k}$ as the **stimulating** photon.

- The two photons are **indistinguishable**.
- Stimulated emission results in a **coherent amplification** of the EM-field.
5.1.3.1 Transition rates $R_{ij}$ between discrete energy levels in atoms

**Goal:**

We want to relate the “up” and “down” transition rate $R_{12}$, $R_{21}$ and $R_{21,\text{spont}}$ to the properties of the spectral energy density $W(\omega)$, resp. $W(E)$ or photon density $s_{\text{ph}}$ of the optical field and the densities of the available transition pairs $N_1$ (level $E_1$ for up-ward transitions) and $N_2$ (level $E_2$ for up-ward transitions).

$N_i$ is the occupation density of level $E_i$.

**Definition: spectral energy density $W(\omega)$ (SED)**

Optical broad-band fields $E(r,t)$, $H(r,t)$ are characterized in the frequency domain by their cycle averaged spectral energy density $W(\omega)$

$$W(\omega) = \frac{\partial^2 E}{\partial \omega \partial V}; \quad W(E = \hbar \omega) = \frac{\partial^2 E}{\partial E \partial V} \quad \text{with the relation: } W(\omega) = \hbar W(E) \quad \text{(SED)}$$

For a monochromatic, harmonic optical fields (as an ideal case):

$$E(t) = E_0 \cos(\omega t) = Re\{e^{\pm j\omega_{\text{opt}}t}\} = E_0 / 2 \left(e^{\pm j\omega_{\text{opt}}t} + e^{-j\omega_{\text{opt}}t}\right)$$

→ the SED $W(\omega)$ becomes a δ-function (1-sided spectrum):

$$W(\omega) = \frac{1}{2} \bar{E} \bar{D} = \frac{\varepsilon_0 E_0^2}{2} \delta(\omega - \omega_{\text{opt}}) = s_{\text{ph}} \hbar \omega \delta(\omega - \omega_{\text{opt}}) \quad \text{E}_0 \leftrightarrow s_{\text{ph}}$$

using the concept of the photon as a energy quantum $E=\hbar \omega_{\text{opt}}$ and the photon density $s_{\text{ph}}$

At Einstein’s time lasers producing quasi-ideal monochromatic fields (cos-field) did not exist. Only optical broadband (thermal) sources characterized by $W(\omega)$ were available.

So it was natural to formulate the dependence of the transition probability $r_{ij}$ related to $W(\omega)$. 

a) Graphical representation of the transition rates for a discrete 2-level system:

We consider \( N \) identical atomic 2-level systems with a atom density \( N \) and a occupation density \( n_2 \) for the \( N \) upper level 2 (\( \downarrow \)-pairs) and a occupational density \( n_1 \) (\( \uparrow \)-pairs) for the \( N \) lower level 1.

Therefore \( N = n_1 + n_2 \).

\( N \) states at \( E_2 \) occupied with a density \( n_2 \)

\( N \) states at \( E_1 \) occupied with a density \( n_1 \)

Rate of stimulated absorption

\[ R_{12} = R_{12,\text{abs}} = \frac{\partial}{\partial t} n_1 = r_{12} n_1 \]

Rate of stimulated emission

\[ R_{21} = R_{21,\text{stim}} = \frac{\partial}{\partial t} n_2 = r_{21} n_2 \]

Rate of spontaneous emission

\[ R_{21,\text{spont}} = \frac{\partial}{\partial t} n_2 = r_{21,\text{spont}} n_2 \]

Net-Rate of stimulated Emission

\( \text{net down-ward transition, defines gain if } >0 \)

\[ R_{21,\text{net}} = R_{21} - R_{12} = r_{21} n_2 - r_{12} n_1 \]

Resulting in a total particle rate in (+) and out(-) flow for \( N \) levels at \( E_2 \) occupied with \( n_2 \) electrons:

Rate-Equation

\[ \frac{\partial n_2}{\partial t} = -R_{21,\text{stim}} + R_{12,\text{abs}} - R_{21,\text{spont}} = -r_{21} n_2 + r_{12} n_1 - r_{21,\text{spont}} n_2 = -\frac{\partial n_1}{\partial t} \]

\[ \frac{\partial n_1}{\partial t} = +R_{21,\text{stim}} - R_{12,\text{abs}} + R_{21,\text{spont}} = +r_{21} n_2 - r_{12} n_1 + r_{21,\text{spont}} n_2 \]
Relations between transition rates $R$ and $W$, $n_1$ and $n_2$:

We are looking for a relation of the rates $R_{ij} = r_{ij}N_i$ between energy levels $E_i \rightarrow E_j$ and

1) the electron occupation density $n_i = Nf_i$ of the levels $E_i$ and the occupation probability function $f(E_i)$  

\[ f_i = f(E_i) = \text{occupation probability function of level } E_i, \text{ eg. Boltzmann- or Fermi-distribution} \]

2) the total transition pair (corresponding initial and final state) or atomic density $N$ and

3) the SED $W(\omega)$ or $W(E)$ of the exciting optical field

4) the values and microscopic dependence of transition probabilities $r_{ij}$

A. Einstein proposed in 1905 based on plausible arguments the following assumptions for the transition probabilities $r_{ij}$ and the transition rates $R_{ij}$ (which will be proven quantum mechanically later):

1) the transition probability $r$ for a 2-level transition pair (1,2) is postulated as:

\[
\begin{align*}
    r_{21} &= B_{21}W(\omega_{21}) & \text{stimulated Emission } 2 \rightarrow 1 \\
    r_{12} &= B_{12}W(\omega_{21}) & \text{“stimulated“ Absorption } 1 \rightarrow 2 \quad \text{A. Einstein postulates} \\
    r_{\text{spont}} &= A_{21} & \text{spontaneous Emission into all modes } 2 \rightarrow 1
\end{align*}
\]

\[ \omega_{21} = (E_2 - E_1) / \hbar \text{ transition frequency} \]

- the transition probabilities $r_{ij}$ of the stimulated processes are related by the Einstein-coefficient $B_{ij}$ to spectral energy density $W(E_{ji})$, resp. $W(\nu_{ji})$ assuming an optical field with a spectral density much broader than the sharp atomic transitions.
- The spontaneous transition probability $A_{ji}$ is independent of the photon field.
Remark:

\( W(E_{ji}) \) is the energy of the light field per unit volume and energy, \( W(\omega_{ji}) \) is the energy of the light field per unit volume and frequency

\[ \hbar W(E_{ji}) = W(\omega_{ji}) \quad \text{and} \quad B(E) = B(\omega) \hbar \]

2) the transition rate \( R_{ij} \) (\( i \rightarrow j \)) for atomic 2-level systems:

- \( R_{ij} \) is proportional to \( n_i \) the carrier density of the occupied "Start"-levels \( E_i \) (resp. transition pair density)
- \( R_{ij} \) is proportional to \( W(\omega_{21}) \) the spectral energy density
- for atoms all final states \( E_j \) of a transition pair with density \( n_j \) are per definition unoccupied, \( n_j = N - n_i \).

3) level occupation probability functions \( f_i(E_i) \) for a transition-pair:

\( f_i(E_i) \) is the occupation probability function that the level \( i \) is occupied by an electron.

Per definition: \( f_j = (1 - f_i) = \) probability that state \( j \) is empty

Transition Rates:

1) Stimulated Emission \( 2 \rightarrow 1 \):

\[ R_{21,\text{stim}} = W B_{21} n_2 = W B_{21} N f_2 \quad \text{for isolated atoms} \]

\( B_{21} \) is the Einstein-coefficient for stimulated Emission.

\( W(\omega) B_{21} \) is the transition probability per excited energy state at \( E_2 \)

2) stimulated Absorption \( 1 \rightarrow 2 \):

\[ R_{12,\text{abs}} = W B_{12} n_1 = W B_{12} N f_1 \quad \text{for isolated atoms} \]

\( B_{12} \) is the Einstein-coefficient for stimulated Absorption
3) spontaneous Emission $2 \rightarrow 1$ per mode:

$$R_{21,\text{spont}} = A_{21} n_2 = A_{21} N f_2$$

for isolated atoms

$A_{21}$ is the Einstein-coefficient for spontaneous Emission

4) net stimulated Rate $R_{21,\text{net}}$ $2 \rightarrow 1$:

$$R_{21,\text{net}} = R_{21,\text{stim}} - R_{12,\text{abs}} = R_{21,\text{net}} = W \left( B_{21} n_2 - B_{12} n_1 \right) = W B_{21} N f_2 - W B_{12} N f_1$$

for isolated atoms

$n_1$ = density of the transition pairs with the electron in the ground state $E_1$ (Valence band)

$n_2$ = density of the transition pairs with the electron in the excited state $E_2$ (Conduction band)

$N$ = density of all atomic transition pairs, resp. density of the atoms

$f_1$ = occupation probability for an electron in the ground state $E_1$ (eg. Boltzmann or Fermi-Function)

$f_2$ = occupation probability for an electron in the excited state $E_2$ (eg. Boltzmann or Fermi-Function)

**Condition for optical amplification and population inversion:**

- The net-rate of stimulated emission (difference between stimulated Emission und Absorption) must be $R_{21,\text{net}} > 0$, in order that the photon density in the optical field is increased ➔ optical gain $g$ is possible.

For $B_{12} = B_{21}$ the occupation probability of the upper energy level 2 must be larger than the lower level 1:

⇒ POPULATION INVERSION $n_2 = N f_2 > n_1 = N f_1$, ➔ $f_2(E_2) > f_1(E_1)$

Important Remark:

In thermal equilibrium with the thermal blackbody radiation at a finite temperature $T$ the electrons are distributed according to a Boltzmann-Distribution with $n_2 << n_1$.

This means that no gain is possible in thermally excited materials.

Electrons have to be “pumped” or transferred actively to the upper level to create population inversion by non-equilibrium.
5.1.3.2 Concept of thermodynamic equilibrium, optical pumping and population inversion

**Problem:**

Is it possible to establish a population inversion \( n_2 > n_1 \), resp. amplification \( R_{21,net} > 0 \) by optical absorption in a 2-level system to “pump” the upper level?

Introducing a 2-level system with an atom density \( N \) in an optical field of a resonant spectral energy density \( W(\omega_{21}) \) leads to a change in the level population densities \( n_1 \) and \( n_2 \) until a stationary state is reached when the down- and up-ward transition rates are equal and no change in \( n_1 \) and \( n_2 \) occurs any more.

→ **no optical population inversion is possible in a 2-level system.**

\[ \frac{\partial n_2}{\partial t} / \frac{\partial t}{\partial t} = 0 \rightarrow \text{equilibrium} \]

\[ R_{12} = R_{21} + R_{\text{spont}} \quad \text{equilibrium condition (rate equation)} \]

by insertion of the expressions for the rates \( R \) gives:

\[ W B_{12} n_1 = W B_{21} n_2 + A_{21} n_2 \rightarrow \]

with \( n_1 + n_2 = N \)

\[ W B_{12} (N - n_2) = W B_{21} n_2 + A_{21} n_2 \]

\[ W B_{12} N = (W (B_{21} + B_{12}) + A_{21}) n_2 \rightarrow \]

\[ n_2 = \frac{W B_{12} N}{(W (B_{21} + B_{12}) + A_{21})} ; \quad n_1 = N - n_2 \]

for \( W \rightarrow \infty \)

\[ n_2 = \frac{B_{12}}{B_{12} + B_{21}} N < N / 2 \quad \text{resp.} \quad R_{21} < R_{12} \]

Absorption \( N_2 < N/2 \) → Transparency \( N_2 \sim N/2 \)
The rate of absorption is always larger than the rate of stimulated emission, therefore

- **a simple 2-level system** “optically pumped” by a light field remains always absorbing or at most becomes transparent \( n_2 = n_1 \).

- **No population inversion** \( n_2 > n_1 \) or gain can be reached by optical pumping at the transition frequency!

The same formalism as above can be used for the

**Thermal Boltzmann equilibrium with the blackbody radiation:** \( W(\omega) = \rho_{bb}(\omega) \) (see chap.5.2.1)

In reality a 2-level system with no external light field \( W = 0 \) must be in equilibrium with the always present “black body radiation“ with the spectral energy density \( \rho_{bb}(\omega) \) and exhibit an electron distribution according to a Boltzmann-distribution, where \( n_1 >> n_2 \), resp.

\[
n_2 / n_1 = \exp \left( - \frac{E_2 - E_1}{kT} \right)
\]

The resulting relationship was used by A. Einstein to relate the constant A to B.
Optical population inversion in a 3-Niveau-System:

Reaching **optical amplification** $g>0$ in a 2-level system requires: $R_{21,\text{stim}} > R_{12,\text{abs}}$ resp. $R_{21,\text{not}} > 0$ resp. $n_2 > n_{2,\text{transp}} > N/2$

To enforce a **population inversion**, resp. inverting the population in a $2 \rightarrow 1$ transition ($\omega_{21}$) by an optical „pump“ field $W_{\text{pump}}(\omega_{\text{pump}})$ such that $n_2 > n_{2,\text{transp}} > n_i$ it is necessary to introduce a **3rd level** for artificially injecting carriers in level $E_2$ without removing them by stimulated emission of the pump light again.

Establishment of such a non-equilibrium (Inversion) $n_2 > n_{2,\text{transp}}$ is called **Pumping or Inversion of the medium**

Optical pumping of a 3-level system:
The simplest way to achieve population inversion between level $E_2$ and $E_1$ is the introduction of a third, lower level $E_0$

$$\omega_{\text{pump}} = \omega_{20} = (E_2 - E_0) / \hbar$$
$$\omega_{21} = (E_2 - E_1) / \hbar \quad \text{(active transition 1-2)}$$

and $\omega_{20} > \omega_{21}$

$n_1 + n_2 + n_0 = N$

Assumptions:
- active optical transitions (eg. gain) occur only between $1 \leftrightarrow 2$
- optical pumping take place between $0 \leftrightarrow 2$
- the transition probability $r_{10} \rightarrow \infty$ (*“empty”* 1-level)
- $A_{20}$ should be small
Calculation of the equilibrium rates between the 3 levels leads to:

Lasing transition: 2-1 (without lasing $W_{12} = 0$), pump transition: 0-2 ($\rho_{\text{pump}}$)

\[
\frac{\partial}{\partial t} = 0 \quad ; \quad n_0 + n_1 + n_2 = N = \text{density of atoms} \quad ; \quad W_{12} = 0
\]

level 2:  $W_{\text{pump}}B_2(n_0 - n_2) - n_2(A_{20} + A_{21}) = 0$

level 1:  $A_{21}n_2 - A_{10}n_1 = 0 \quad \rightarrow \quad \text{condition for inversion } n_2 > n_1 \rightarrow 0$

\[
\frac{n_2}{n_1} = \frac{A_{10}}{A_{21}} > 1 \quad \rightarrow \quad \tau_{10} < \tau_{21}
\]

replacing $n_0$ and $n_1$ \rightarrow

\[
0 < n_2 = \frac{W_{\text{pump}}B_2n}{W_{\text{pump}}B_2\left(\frac{A_{21}}{A_{10}} + 2\right) + (A_{20} + A_{21})} < \frac{N}{2} < \frac{N}{2}
\]


\[
\text{and } n_1 = n_2 A_{21} / A_{10} < n_2
\]

Depending on the optical and electrical properties of the gain-medium the inversion of transition $2 \rightarrow 1$ is realized by:

a) absorption of pump-light of a shorter wavelength than the active transition
   (many solid state lasers, Er-doped fiber amplifiers etc.)

b) Injection of carriers by an electrical current in forward biased pn-diodes (SC-Diode Lasers)

c) Ionization in gases (eg. HeNe-Gas Laser)
5.1.4 Stimulated Emission Rate $R_{21,\text{net}}$ and Optical Amplification $g$

**Goal:**
- **Relation between gain and optical transition rate** \( g \leftrightarrow R_{21,\text{net}} \)
- Stimulated emission generates temporal and spatial coherent photons (ω, k, φ) which amplify the stimulating light field.
- **Relation between the net stimulated emission rate** $R_{21}$ or the **carrier densities difference** $n_2-n_1$ and the **gain constant** $g(R_{21,\text{net}}) = g(n_2,n_1)=\text{d}I/\text{d}x/\text{l}$.
- **Relation between the susceptibility** $\chi(n_2-n_1)$ for the wave-picture.

**Wave representation as a photon stream:** (necessary for coupling to transition rates)
- The optical field is represented as coherent superposition of elementary wave packets with an energy quantum $\hbar \omega$
- In analogy to the electrical current a **photon flux density (intensity)** can be associated to a **current of photons** with the photon density $s_{ph}$ which propagate with the **group velocity** $v_{gr}$ (particle picture of light)

**Relation between photon density $s_{ph}$ and field amplitude** $E=E_0\cos(\omega t)$ for a harmonic TE plane wave $s_{ph} \leftrightarrow E_0$

\[
\text{energy density} : \ w = \frac{1}{2} \varepsilon E_0 E_0^* = \hbar \omega s_{ph} \quad \rightarrow \quad E_0 = \sqrt{2\hbar \omega s_{ph}} / \varepsilon = E(s_{ph})
\]

or from the intensity $I$ :

\[
I = S = \frac{1}{2} E \times H = \frac{1}{2} E_0 \varepsilon E_0^2 \frac{\varepsilon}{\mu_0} = \frac{\varepsilon E_0^2}{\sqrt{\varepsilon \mu_0}} = \omega s_{ph} v_{gr} \quad \rightarrow \quad v_{gr} = \frac{1}{\sqrt{\varepsilon \mu}} \quad \rightarrow \quad E_0 = \sqrt{2\hbar \omega s_{ph}} / \varepsilon \quad ; \quad \varepsilon = \varepsilon_0 \varepsilon_r
\]

with the spectral energy density : (1-sided)

\[
W(\omega) = w \delta(\omega - \omega_{opt}) = \frac{1}{2} \varepsilon E_0 E_0^* \delta(\omega - \omega_{opt}) = \hbar \omega_{opt} s_{ph} \delta(\omega - \omega_{opt})
\]
Relation between the energy density $w$ and the photon density $s_{ph}$ of an optical field:

**classical energy density of optical EM-fields**

a) electric energy density $\frac{1}{2} DE$

b) magnetic energy density $\frac{1}{2} BH$

c) cycle and spatially averaged energy density of an harmonic optical field $w = \frac{\partial W}{\partial V} = \frac{\varepsilon}{2} E_0^2$

d) intensity (Pointing-Vector) $I = |S| = \frac{1}{2} E \times H = w \nu_{gr} = \hbar \omega n_{ph} \nu_{gr}$

**Graphical representation of photon-flux through a volume element:**

**associated photon density:** $n_{ph} = s_{ph} = \frac{w}{\hbar \omega} = \frac{\varepsilon E_0^2}{2 \hbar \omega}$

$E = \text{electrical field strength}$
$H = \text{magnetic field strength}$
$S = \text{Pointing-vector}$
$w = \text{energy density}$
$n_{ph} = \text{Photon density} = s_{ph}$
Calculation of the relation \( g(R_{\text{stim}}(n_2,n_1)) \):

- The net-rate of stimulated emission \( R_{21,\text{net}} \) changes the photon density \( s_{\text{ph}} \) in transit. Depending \( R_{21,\text{net}}>0 \) or \( <0 \) optical amplification \( g \) or attenuation \( \alpha \) will result.

The optical field with photon density \( s_{\text{ph}}(x,t) \), resp. intensity \( I(x,t)=s_{\text{ph}}(x,t)\hbar \omega v_{\text{gr}} \) travels with \( v_{\text{gr}} \) in the x-direction through a thin layer \( \Delta x \) of amplifying medium in time \( \Delta t \).

- The medium increasing its intensity by \( \Delta I \), resp \( \Delta s_{\text{ph}} \).

From the definition of the attenuation \( \alpha \):

\[
\alpha = -\frac{\partial I}{\partial x} \left( \frac{I(x)}{I(x)} \right) \rightarrow I(x) = I(0)e^{-\alpha x}
\]

using this definition of \( \alpha \): \( \alpha>0 \) means absorption, \( \alpha<0 \) gain!

because the intensity \( I=s_{\text{ph}}v_{\text{gr}}\hbar \omega \) is proportional \( s_{\text{ph}} \), we write:

\[
I(x+\Delta x) = I(x) + \Delta I \approx I(x) - I(x)\alpha \Delta x \quad \rightarrow \quad I \sim s_{\text{ph}}
\]

\[
s_{\text{ph}}(x+\Delta x) = s_{\text{ph}}(x) + \Delta s_{\text{ph}} \
\]

\[
s_{\text{ph}}(x) - s_{\text{ph}}(x) \frac{\Delta s_{\text{ph}}}{\Delta s_{\text{ph}}}
\]
To travel through the layer $\Delta x$ and increase its intensity by $\Delta I$, resp. $\Delta s_{ph}$ the wave needs the time $\Delta t$:

$$\Delta t = \Delta x / v_{gr}$$

during the time $\Delta t$ the wave increases its photon density by $\Delta s_{ph} = R_{21,netto} \Delta t$ of stimulated photons:

$$\Delta s_{ph} = R_{21,netto} \Delta t = (R_{21} - R_{12}) \Delta t = -s_{ph}(x) \alpha \Delta x = -s_{ph}(x) \alpha v_{gr} \Delta t = s_{ph}(x) g v_{gr} \Delta t$$

$$\alpha = -R_{21,netto} / \left( s_{ph}(x) v_{gr} \right) = -g$$

Important relationship to connect fields and rates: $g \Leftrightarrow R_{21}$
5.2 Spontaneous emission in 2-Level Systems

(see lit. Coldren, Yariv)

Goal:

To determine 2 relations between the 3 Einstein-coefficients $A$, $B_{21}$, $B_{12}$ we can use the thermodynamic equilibrium situation between a 2-level system and the Blackbody-Radiation with a spectral power density $W(E)=\rho_{bb}(E)$ (obtained from thermodynamics) and a carrier distribution obeying the Boltzmann-distribution (see Physik II, 2.Sem.)

Finally there is still one unknown remaining, e.g. $B$ which can only be determined only from a quantum mechanical description of atomic polarization or experimentally from an absorption measurement.

5.2.1 Spontaneous Emissions-Processes

$R_{21,\text{spont}}$ Spontaneous-Emission-Postulate

- The spontaneous transition of an excited QM-system without external optical disturbance into the lower energy-level has no classical equivalent.
  This can only be understood by QM if also the optical field is quantized into a harmonic oscillator (2.quantization, zero-point fluctuations of an optical mode)

- Spontaneous emission is a necessary process to explain that an optical 2-level system perturbed by an external optical field (resulting in non-equilibrium carrier densities $n_2+\Delta n_2$ and $n_1+\Delta n_1$ with $\Delta n =$ carrier disturbance) can relax back to equilibrium (Boltzmann-distribution) after switching off the disturbance.

⇒ Spontaneous emission is a thermodynamic necessity to establish equilibrium
5.2.2 Thermodynamic equilibrium: quantized atomic system ↔ blackbody radiation

Following A. Einstein we consider the rate equations for the electrons of a 2level system in thermodynamic equilibrium (Boltzmann) with the known blackbody EM-radiation field with a spectral energy density $\rho_{BB}(\omega)$ inside a ,,2-level blackbody“ of temperature $T$. The carrier distribution obeys Boltzmann distribution.

Idea: In thermodynamic equilibrium the spectral energy density is $W = \rho_{BB}$ and the electron densities $n_2$ and $n_1$ obey Boltzmann-statistics. In equilibrium the transition rates between levels $2 \rightarrow 1$ and $1 \rightarrow 2$ must be equal:

$$R_{21}(\rho_{BB}) + R_{21,spont} = R_{12}(\rho_{BB}) \quad \rho_{bb} = ?$$

Spectral mode $\rho_{mode}$ and energy $\rho_{BB}$ density of blackbody-radiation: (without proof, see Physik II)

We obtain the spectral energy density $\rho_{BB}$ of blackbody radiation by counting the EM-modes inside a Volume $V$ and multiplying the spectral mode density $\rho_{mode}$ with the average number of thermal photons per mode $\langle n \rangle$ and the photon energy $E$. $n=$refractive index.

$$\rho_{BB}(E) = \rho_{mode}(E) \langle n(E) \rangle E$$

$$\rho_{BB}(E) = \frac{8\pi n^3 E^3}{h^3 c^3} \frac{1+\left(E/n\right) \frac{d n}{d E}}{\exp(E/kT) - 1}$$

$$\rho_{BB}(\nu) = \frac{8\pi n^3 E^3}{h^3 c^3} \frac{1+\left(E/n\right) \frac{d n}{d E}}{\exp(E/kT) - 1} = \frac{d s_{ph,BB} \nu}{d \nu}$$

E=hf= energy of blackbody radiation photons $n=$ refractive index of blackbody
T= temperature of the blackbody $h=$ Plank constant

volume V

inter-
action

EM-blackbody
field

blackbody
at temp.T

elementary
blackbody mode i
$E_\nu, \omega_i, k_i$
For the derivation of the $\rho_{BB}$ we made use of:

**Spectral blackbody mode density:**

$$\rho_{\text{mode}}(E) = \frac{8\pi n^3 E^2}{\hbar^3 c^3} \left[ 1 + \frac{E}{n} \frac{dn}{dE} \right] \approx \frac{8\pi n^3 E^2}{\hbar^3 c^3} = \frac{d^2 N_{\text{mode}}}{dE d\text{Vol}} \quad \text{blackbody-mode density}$$

$$\rho_{\text{mode}}(\nu) \approx \frac{8\pi n^3 \nu^2}{c^3} = \frac{d^2 N_{\text{mode}}}{d\nu d\text{Vol}}$$

**Photon-occupation $\langle n(E) \rangle$ per mode in thermal equilibrium:**

In thermal equilibrium each mode $i$ carries according to the **Bose-Einstein-Statistic** for photons $\langle n_i \rangle$ photons.

**Bose-Einstein-Statistic:**

$$\langle n_i(E_i) \rangle = \frac{1}{\exp(E_i/kT) - 1} \ll 1$$

occupation probability of mode $i$ with photons of energy $E_i = \hbar \omega_i$

Therefore we get $\rho_{BB}(E) = \rho_{\text{mode}}(E)\langle n_i \rangle E_i$
5.2.3 Relation between the Einstein-coefficients $A_{21}$, $B_{21}$ and $B_{12}$

Example: atomic 2-level transition pairs

In the thermodynamic equilibrium with the spectral energy density $\rho_{BB}$ of the thermal radiation:

1) total emission rate = total absorption rate

\[ A_{21} n_2 + B_{21} n_2 \rho_{BB} = B_{12} n_1 \rho_{BB} \]

$A_{21} n_2$ = spont. photon emission rate into all vacuum modes with density $\rho_{bb}$

2) Boltzmann-equilibrium of the level occupation for $n_2$, $n_1$

\[ \frac{n_2}{n_1} = \exp\left(-\frac{E_{21}}{kT}\right) ; \quad E_{21} = E_2 - E_1 \]

insertion of the ratio of $n_2/n_1$ leads to:

\[ \rho_{BB}(E_{21}) = \frac{A_{21} / B_{21}}{(B_{12} / B_{21}) \exp\left(\frac{E_{21}}{kT}\right) - 1} = \frac{8 \pi n^3 E_{21}^3}{\hbar^3 c^3} \frac{1}{\exp\left(\frac{E_{21}}{kT}\right) - 1} = \rho_{mod\cdot E_21}(E_{21}) \langle n_{21} \rangle E_{21} \]

Comparison of the coefficients on both sides of the equation results in:

\[ B_{21} = B_{12} = B \]

\[ A = B(E) \left(\frac{8 \pi n^3 E_{21}^3}{\hbar^3 c^3}\right) = B(\nu) \left(\frac{8 \pi n^3 h \nu^3}{c^3}\right) = B \rho_{mode}(E) E \]

Relation between Einstein-coefficients $B$ and $A$
**Important remark:**

The relations are valid at a particular energy difference $E_{21} = E_2 - E_1$ of a particular mode.

The coefficient $A$ which is the inverse of a spontaneous carrier lifetime $A = 1 / \tau_{\text{spont}}(E_1)$ is the Einstein coefficient for the spontaneous emission into all modes of free space. (also not only lasing modes or resonator modes, see spont. emission factor $\beta$ in chap.6)

Considering the ratio between the net stimulated rate and the spontaneous rate:

(measure for the ease to invert the material)

$$R_{21,\text{net}} = R_{21} - R_{12} = B(n_2 - n_1) \rho_{\text{opt}}$$

$$R_{21,\text{spont}} = An_2 = B \left( \frac{8\pi n^3 h \nu^3}{c^3} \right) n_2$$

In thermal equilibrium $\rho_{\text{opt}}(E_{21}) = \rho_{bb}(E_{21}) = \rho_{\text{mode}}(E_{21}) \langle n_{21} \rangle E_{21}$ we have the following magnitude-relation of the net stimulated and spontaneous rates:

$$\frac{R_{21,\text{net}}}{R_{21,\text{spont}}} = \frac{1}{\exp(E/kT) - 1} = \langle n \rangle << 1 \quad \text{if} \quad E = h\nu > kT \quad \text{and} \quad n_2 << n_1$$

$$R_{21,\text{spont}} >> R_{21,\text{stim}}, \ R_{12,\text{abs}} \quad \text{Thermal} \ \text{Radiation Source}$$

**Conclusion:**

Systems in thermodynamic equilibrium (eg. lamps) do virtually not emit coherent, resp. stimulated radiation ($R_{\text{stim}} << R_{\text{spont}}$).

Only for LASERs, excited by pumping into a strong non-equilibrium state (inverted) with $n_2 > n_1$, optical gain and coherent radiation becomes possible and dominant.

Optical gain is more difficult to achieve at short wavelengths (microwave Masers have been invented before optical Lasers).
Relation between the Einstein coefficient B and the attenuation $\alpha$:

A direct experimental measurement of $A$ or $B$ is difficult, however we will show that there is a simple relationship between the Einstein coefficients and the attenuation $\alpha$.

The attenuation $\alpha$, describing the decrease of the optical beam intensity $I(L)=I(0)e^{-\alpha L}$ with propagation distance $L$ in the medium of known absorption state, is relatively easy to measure.

Assuming a weak monochromatic optical field (close to thermal equilibrium) with the spectral energy density:

$$W(\omega) = s_{ph} \hbar \nu \delta(\omega - \omega_0) \rightarrow R_{21,net} = B(n_2 - n_1)s_{ph} \hbar \nu$$

We have already shown that $\alpha$ and $R_{21,net}$ are related by:

$$\alpha(E) = -R_{21,net}(E)/(s_{ph}\nu_{gr}) = -s_{ph}\hbar \nu B(n_2 - n_1)/(s_{ph}\nu_{gr}) = -\hbar \nu B(n_2 - n_1)/\nu_{gr}$$

Using a weak optical beam for attenuation measurements, which does not disturb the equilibrium Boltzmann population:

$$\frac{n_2}{n_1} = \exp\left(-\frac{E_{21}}{kT}\right) \rightarrow \frac{n_2 - n_1}{n_1} \approx \frac{n_2 - n_1}{N} \approx \exp\left(-\frac{E_{21}}{kT}\right) - 1 \quad \text{with known } N=\text{atoms / unite volume}$$

$$B(E) = -\alpha(E) \frac{\nu_{gr}}{h \nu} \frac{l}{(n_2 - n_1)} = -\alpha(E) \frac{\nu_{gr}}{h \nu} \frac{l}{N \exp\left(-\frac{E_{21}}{kT}\right) - 1} \quad ; \quad E_2 - E_1 = h \nu$$

From the measurement of $\alpha$ with known atom density $N$ and group velocity $\nu_{gr}$ we obtain $B$ and also $A$. 
Conclusions:

- The Einstein model postulates
  1) the energy quantization of the medium and
  2) transition rates between the states
- The Einstein coefficients $B_{12}$, $B_{21}$ and $A_{21}$ have been introduced formally as postulates and can not be related directly to the material properties (eg. electronic potentials, eff. mass) on a microscopic level
- The model allows the description of optical gain $g$ by population inversion
- The spontaneous emission is a quantum-mechanical phenomenon and has no classical equivalent.
  However it is a thermodynamic necessity for the classical system to relax to thermal equilibrium.
- The model is also capable of representing the black-body radiation, resp. the relation between A and B
5.3 Pumping and Population Inversion

Optical amplification $\alpha<0$ or $g>0$ requires a population inversion $\rightarrow R_{21,\text{net}}>0 \rightarrow n_2>n_1$.

- A population inversion can not be realized in thermodynamic equilibrium (eg. heating $T\rightarrow\infty$).
- Non-equilibrium is enforced by an influx of carriers into the higher energy level $E_2$ PUMPING (pumping transitions in 3- or multi-level systems).

5.3.1 Optical and electrical pumping

Inverted transition pairs are realized by Absorption of „pump-light“ (optical pumping) in the isolating crystal matrix containing the active atoms. The atoms must provide at least an additional 3rd energy level $E_3$ (3-level-system), at $\lambda_{\text{pump}}<\lambda_{21}$.

For so called solid-state lasers based on active metal atoms like Nd, Er, Cr, etc. embedded in an isolating crystal matrix of eg. Erbium in Glass, Cr in Ruby, Nd in Glass etc. there is no possibility for pumping by an electrical current or impact-ionization.

a) Optical Pumping-Scheme of a 4-level system:

- It is assumed that the active atoms (often metals in isolators) provide the atomic levels
- In addition we assume that there is a very fast transition with a short life time $r=1/\tau$ between levels $3 \rightarrow 2$ and $1 \rightarrow 0$.
  $\Rightarrow n_3\sim0$, $n_1\sim0$, $n_2>0$
  \[ n_0 + n_1 + n_2 + n_3 = N \]

See also Er-doped-Fiber-amplifier in chap.6.
b) **Electrical Pumping:** (mostly used with semiconductor based components, see chap.6)

- Inversion of the excited states in the conduction and valence band of SC can be realized by optical pumping, impact ionization, but in particular by **current injection in pn-junctions**.

- **Minority carrier-injection** (electron-injection into the conduction band of a p-SC, hole-Injection into the valence band of n-SC) is realized simply by **current injection through a depletion layer of a forward biased pn-diode**.

**Schematic Carrier (**electrons / holes**) injection in forward biased PiN-Diode:**

- **a) amplification in SC** \((n_1<<n_2)\):
  - **Elektrons** \((n_2)\) in Conduction band, \(E_2\)
  - **Löcher** \((n_1)\) in Valence band, \(E_1\)

- **b) attenuation in SC** \((n_1>>n_2)\):

  **Carrier non-equilibrium by carrier injection**
  the active i-layer:
  
  \[ n >> n_0, \ p >> p_0 \]
  
  \[ n_{p} >> n_{l}^2 \]
  
  of a forward biased diode.
Technical Realizations of optical and electrical Pumping:


Excitation of Neodymium atoms (Nd) in an YAG-crystal-matrix by Absorption of pump-light from a gas discharge lamp.

Nd:YAG-Laser

YAG: Nd₃Y₃₋ₓAlₓO₁₂
Yttrium-Aluminium-Granat

2) Gas-Discharge-Pumping (electrical pumping) of Gas-Lasers (He-Ne)

Excitation of gas atoms (Ne) by Impact ionization in gas-discharge.

3) Current-Injection-Pumping of pn-Diodes Lasers: Band diagram-Representation

Inversion by minority carrier injection (chap. 6)

\[ V_D = 0 \ , \ I_D = 0 \]

\[ V_D > E_g/e \ , \ I_D > 0 \]

\[ V_D > E_g/e \] (High current-Injection)

d: area if inversion

Electronics Laboratory: Optoelectronics and Optical Communications
5.3.2 Carrier Rate Equations and total Spontaneous Emission

**Total Spontaneous Emission Rate** \( R_{21,\text{spont}} \): (see lit. Coldren)

The Einstein coefficient \( A \) describes the spontaneous emission rate \( R_{21,\text{spont}} \) into all modes of a particular frequency \( \omega_{21} \), in a spectral width \( \Delta \omega_{\text{spont}} \) and all propagation directions in a "given volume" \( V \).

Therefore an excited 2-level system can emit spontaneously

1) **in all spatial directions** resp. into all available optical modes \( \rho_{\text{mode}} \) in the a given device volume \( V_{\text{spont}} \)

2) **at all frequencies** \( \Delta \omega_{\text{opt}} \) of the involved active transition pairs

The **total spontaneous emission rate** \( R_{21,\text{spont}} \) (appearing in the carrier rate equation) is obtained as the spontaneous emission rate per mode \( R_{21,\text{spont,mode}} \) (eg. the lasing mode) multiplied by the **spatial mode-density** \( \rho_{\text{mode}}(\omega) \approx \frac{8 \pi n^3 v^2}{c^3} \), the spectral band-width \( \Delta \omega_{\text{spont}} \) of the total spontaneous transition and the “available” volume for spontaneous emission \( V_{\text{spont}} \):

\[
R_{21,\text{spont}} = R_{21,\text{spont,mode}} \rho_{\text{mode}}(\omega) \Delta \omega_{\text{spont}} V_{\text{spont}} \quad (\overset{\Delta}{=} n_2 A)
\]

\[
R_{21,\text{spont,mode}} = \gamma R_{21,\text{spont}}
\]

with \( \gamma = \beta = \text{spontaneous emissions factor} = \frac{1}{V_{\text{spont}} \rho_{\text{mode}}(\omega) \Delta \omega_{\text{spont}}} \ll 1 \)

(one often assumes as a first order approximation \( V_{\text{spont}} = V_{\text{mode}} \))

\( R_{21,\text{spont,mode}} = \gamma A n_2 \) is the spontaneous emission into a **single** mode (eg. lasing or amplified mode)
Carrier-Rate Equations including Pumping

Concept of Rate Equations: (carrier continuity equation for particle currents per energy level)

Optical transitions produce particle currents (rates) \( R \) into and from a particular energy level \( E_i \). Particles can also be stored in the energy states of the energy level \( E_i \) in the volume \( V_{\text{active}} \) (particle reservoir).

Rate equations are just the continuity equation for particle in an energy level (reservoir):

\[
\frac{\partial n}{\partial t} = \sum \text{in-flowing particle currents} - \sum \text{out-flowing particle currents}
\]

The pump-mechanism (optical, electrical) can be accounted by the continuity equation for the carrier densities \( n_2, n_1 \) by the addition of an inflowing carrier generation rate \( R_{\text{pump}} \).

\[
\frac{\partial n_2}{\partial t} = -\frac{\partial n_1}{\partial t} = R_{\text{pump}} - R_{21,\text{net}} - R_{21,\text{spont}}
\]

Rate equation of the carriers in the excited state \( E_2 \) and \( E_1 \)

We express the optical field by the photon density \( s_{\text{ph}} \) and relate it by the gain \( g \) to the transition rates:

\[
R_{21,\text{net}} = g(n_2, n_1) s_{\text{ph}} v_{gr}
\]

\[
R_{\text{spont}} = n_2 / \tau_{\text{spont}}
\]

\[
\frac{\partial n}{\partial t} = R_{\text{pump}} - g(n_2, n_1) v_{gr} s_{\text{ph}} - n_2 / \tau_{\text{spont}}
\]

Remark: the active volume for carriers \( V_{\text{active}} \) and the mode volume for photons \( V_{\text{mode}} \) must not necessarily be equal!
Amplification and Inversion:

Static: \( \partial / \partial t = 0 \)

\[
g(E_{21}, n_{tr}) = -\frac{R_{21,\text{net}}(E_{21}, n_{tr})}{s_{\text{ph}}v_{gr}} = 0 \quad \text{Transparency condition } g \geq 0 \text{ defines}
\]

\( \rightarrow n_{tr} \quad \text{transparency density} \)

**Pump rate for Transparency** \( n = n_{tr} \) and \( R_{\text{pump,tr}}(n_{2,\text{tr}}) : \)

\[
0 = R_{\text{pump,tr}} - 0 - n_{tr} / \tau_{\text{spont}} \quad \rightarrow \quad \text{with } R_{21,\text{net}} = 0
\]

\[
R_{\text{pump,tr}} = n_{tr} / \tau_{\text{spont}}
\]

Conclusions:

Materials without pumping are absorbing for the wavelength of interest. Pumping reduces the attenuation until the material becomes transparent and finally amplifying.

For low pump rates for transparency \( R_{\text{pump,tr}} \)

- small spontaneous emission ("lost" photons) and small density of atoms (gives also only small gain)
- small Einstein coefficient \( A \), eg. long carrier lifetime of the excited state
### 5.3.3 Photon Rate Equation

Photons propagate as photon streams of density $s_{\text{ph}}$ or are contained as standing waves in resonators.

Continuity equations per unit volume can also be formulated for in- and out-flowing photons into the propagating field of a single optical mode $i$. (note that here the spontaneous emission rate per mode $R_{21,\text{spont, mode}} = \gamma R_{21,\text{spont}}$ has to be used)

The photon density $s_{\text{ph}}$ is changed by:

1) the stimulated emission (net) $R_{21,\text{net}}$ and

2) the spontaneous emission per mode $R_{21,\text{spont, mode}} = \gamma R_{21,\text{spont}}$  
   ( $\gamma = \beta$ = spontaneous emission factor)

3) Scattering losses from the waveguide, $R_{\text{loss}}$ (residual absorption, scattering)

Photon number $S_{\text{ph}} = s_{\text{ph}} V_{\text{mode}}$ of the mode volume $V_{\text{mode}}$:

$$\frac{\partial S_{\text{ph}}}{\partial t} = \left( R_{21,\text{net}} + \gamma R_{21,\text{spont}} \right) V_{\text{active}} - R_{\text{loss}} V_{\text{mode}} \rightarrow : V_{\text{mode}}$$

$$\frac{\partial s_{\text{ph}}}{\partial t} = \left( R_{21,\text{net}} + \gamma R_{21,\text{spont}} \right) \frac{V_{\text{active}}}{V_{\text{mode}}} - R_{\text{loss}}$$

**Rate equation for photon density per mode**

$R_{\text{loss}}$ = losses per unit length due to scattering, different absorption mechanisms, etc.

For a 2-level system we get:

$$\frac{\partial s_{\text{ph}}}{\partial t} = \Gamma g \left( n_2, n_1 \right) s_{\text{ph}} v_{\text{gr}} + \Gamma \gamma n_2 / \tau_{\text{spont}} - R_{\text{loss}}$$
Example:
Graphical representation of particle “reservoirs” and particle flow rates:

Particle transition rates between an active, pumped medium and an optical mode field
5.4 Quantum Mechanics of Optical Transitions

5.4.1 Quantum-Mechanical concepts of the dynamic of bound electrons in an optical E/M-field

What do we need beyond the Einstein-Theory? (see lit: Loudon, Yariv)

- **Perturbation Theory** for the motion of electrons in the potential \( V(x) \) of atomic or crystal lattice forces and a superposed dynamic optical field (optical potential \( V_{opt}(t) \))

- Correlation of the transition rates \( R \) or Einstein coefficients \( A, B \) to microscopic properties (eg. \( V(x) \)).

**Quantum Mechanics (QM)** allows the self-consistent calculation of \( B \), resp \( A \) from first principles

**Procedure of solution:**

1) the classical EM light field superposes a time dependent, high frequency \((f \sim 200\;\text{THz})\) electrical potential \( V_{opt}(x,t) \) on the static microscopic potential field \( V(x) \) of the atom or crystal lattice.
   Assumption: weak perturbation \( V_{opt}(x,t) \ll V(x) \).

2) Weak Perturbation Theory solves approximately the **time-dependent Schrödinger-equation (TSE)** for \( \psi(x,t) \)

The interaction of the E(M) forces of the optical field appears as time-dependent electrical (magnetic) „potential“ in the time-dependent Energy (Hamilton)-Operator \( H_{WW}(t) \): \( V_{opt}(x,t) \Rightarrow H_{WW}(x,t) = ? \).

a) the solution \( \psi(x,t) \) of the TSE, allows the calculation of statistical QM expectation values of:

   - position: \( \langle x(t) \rangle = \int \psi(x,t)x\psi^*(x,t)dx \rightarrow \) dipole: \( \langle p(t) \rangle = -e\langle x(t) \rangle \rightarrow \) susceptibility: \( \langle \chi(\omega) \rangle \)
   
   \(- C_1(t); C_2(t) \rightarrow r_{12}; r_{21} \)

b) the **transitions probabilities** \( r_{ij} = \frac{\partial}{\partial t}|C_i|^2 \) between discrete atomic states
5.4.1.1 Time dependent Schrödinger-Equation for a 2-level system in an optical field (perturbation theory):

**Questions:**

What is the electron motion \( <x> \) in a one-electron atom exposed to the EM-forces of a harmonic optical field with frequency \( \omega_{\text{opt}} \) and field strengths \( E \) and \( (H) \)?

**Assumptions:**

The forces acting on the moving electron result from:

1) time invariant potential field of nucleus or crystal field \( V(x) \)

2) time variant, oscillating (with \( e^{i\omega_{\text{opt}} t} \)) EM-potential of the light field \( V_{\text{opt}}(t) \)

simplified optical potential \((H)\) neglected

\[
E(t,x) = E_0 \, e^{i\omega_{\text{opt}} t}
\]

using the definition

\[
E = -\frac{\partial V_{\text{opt}}}{\partial x}, \quad V_{\text{opt}} = -E(t)x
\]

\[
H_{\text{wv}}(t,x) = -eV_{\text{opt}}(t) = +eE_0 x \, e^{i\omega_{\text{opt}} t}
\]

(Note: we assume the positive time dependence \( e^{i\omega_{\text{opt}} t} \) with \( \frac{\partial}{\partial t} \cdot -\infty + j\omega \) )

We neglect the magnetic forces for simplicity and consider only the electrical force.

The TSE describes the probabilistic electron motion by the wave function \( \psi(r,t) \), resp.by the spatial probability \( |\psi(r,t)|^2 \) of finding the electron at position \( x \).
Time dependent Schrödinger-equation:

\[ H(t,x)\Psi(x,t) = \left[ H_{\text{pot}}(x) + H_{\text{WW}}(t,x) \right] \Psi(x,t) = i\hbar \frac{\partial}{\partial t} \Psi(x,t) \]

H=Hamilton-Energy Operator, \( H_{\text{pot}} \gg H_{\text{WW}} \)

\( H_{\text{ww}}(t,x) \) is the Hamilton-Operator of the optical field. 2 is the upper excited level, 1 is the lower ground state with \( E_2 > E_1 \).

Stationary solutions \((H_{\text{ww}}=0)\): (\( \rightarrow \) discrete energy levels without the optical field)

without an optical field: \( H_{\text{ww}} = 0 \)

\[ H\Psi(x,t) = i\hbar \frac{\partial}{\partial t} \Psi(x,t) = E \Psi(x,t) \quad \text{time independent Schrödinger equation} \]

\[ \rightarrow H \mu(x) = E \mu(x) \]

with the two stationary solutions (eigenfunctions) and the energy-eigenvalues: \( E_1 , E_2 \)

Eigenfunctions for \( H_{\text{ww}} = 0 \)

\[ E_1 : \quad \Psi_1(x,t) = u_1(x)e^{-jE_1/h t} = u_1(x)e^{-j\omega_1 t} ; \quad \omega_1 = E_1 / \hbar \]

\[ E_2 : \quad \Psi_2(x,t) = u_2(x)e^{-jE_2/h t} = u_2(x)e^{-j\omega_2 t} ; \quad \omega_2 = E_2 / \hbar \]

The solutions \( u_i(x) \) fulfill the Orthonormalization Relations (orthogonal and normalized):

\[ \int u_k(x)u_l^*(x)dx = \Delta_{kl}, \quad \int u_k(x)u_l^*(x)dx = \Delta_{kk} = 1, \quad \int_{k \neq l} u_k(x)u_l^*(x)dx = \Delta_{kl} = 0 \quad \text{(without prove)} \]

The stationary total solution for the 2-level-system is a superposition:

\[ \Psi(x,t) = C_1 u_1(x)e^{-j\omega_1 t} + C_2 u_2(x)e^{-j\omega_2 t} \]

with \( |C_1|^2 + |C_2|^2 = 1 \), \( \omega_i = E_i / \hbar \)
Interpretation:

\[ |C_1|^2, (|C_2|^2) \text{ is the probability of finding the electron in the state } E_1 (E_2) \text{ resp. } \Psi_j(x,t), (\Psi_2(x,t)) \].

C_1 and C_2 are constants for the stationary state, H_{ww}=0.

System in Ground state: C_1=1, C_2=0 System in Excited state: C_2=1, C_1=0 System in Mixed state: C_2 \neq 0, C_1 \neq 0

5.4.1.2 Optical Perturbation calculation of the transition probability r_{ij} or transition rate R_{ij}

1) Non-stationary solution for a harmonic perturbation H_{ww} \neq 0:

\[ H \Psi(x,t) = \left[ H_{pot}(x) + H_{ww}(t) \right] \Psi(x,t) = i \hbar \frac{\partial}{\partial t} \Psi(x,t) \]

with the postulated solution as a superposition of the stationary ground and excited states described by C_1(t), C_2(t) as time functions

\[ \Psi(x,t) = C_1(t)u_1(x)e^{-j\omega_1 t} + C_2(t)u_2(x)e^{-j\omega_2 t} \]

with \[ |C_1(t)|^2 + |C_2(t)|^2 = 1 \]

- The perturbation of the 2-level-system by the optical field (switched on at t=0 with eg. the system initially in the ground state |C_1(0)|^2=1 and |C_2(t)|^2=0) causes an absorption Process E_1 \rightarrow E_2 changing the occupation probabilities |C_1(t)|^2 and |C_2(t)|^2.

- For simplicity the system is at t=0 in a „pure“ state, either at E_1 (leading to absorption) or at E_2 (leading stimulated emission).
Knowing $C_1(t)$, $C_2(t)$, we calculate the **transition probabilities** $r_{ij}(t)$ as change of the occupation probability per unit time:

$$r_{21} = \frac{\partial}{\partial t} |C_1(t)|^2 = -\frac{\partial}{\partial t} |C_2(t)|^2$$

**Transition probability** $r_{21}$

**Generic solution-procedure for $C_i(t)$:**

1) insertion of the assumed solution $\psi(x,t)$ into the TSE, then
2) we first **right** multiply both sides of the TSE with $u^*_k(x)$ and then
3) we **left** multiply the TSE by $u_l(x)$ and finally
4) we integrate both sides by $\int_{-\infty}^{+\infty} dx$ using the **orthonormality** of the static solutions $u_i(x)$ and $u_k(x)$ and the abbreviation:

$$\langle u_i | H | u_k \rangle = \int_{\text{volume}} u^*_i H u_k dx$$  **Matrix element between the states $i$ and $k$ of Energy Operator $H$**

Considering only the **time-dependent** part of the TSE, we get (after a simple but lengthy calculation, see appendix !) the fundamental nonlinear and coupled 1.order differential equations of for $C_1(t)$ und $C_2(t)$:

$$\frac{\partial}{\partial t} C_1 = -j \frac{\hbar}{\omega_1} [C_1 \langle u_1 | H_{WW} | u_1 \rangle + C_2 \langle u_1 | H_{WW} | u_2 \rangle \exp(-j(\omega_2 - \omega_1)t)]$$

$$\frac{\partial}{\partial t} C_2 = -j \frac{\hbar}{\omega_2} [C_1 \langle u_2 | H_{WW} | u_1 \rangle \exp(-j(\omega_1 - \omega_2)t) + C_2 \langle u_2 | H_{WW} | u_2 \rangle]$$

**Coupled Differential-Equation for $C_1(t)$ and $C_2(t)$**

with the definition

$$H_{kl} = \langle u_k | H_{WW} | u_l \rangle = \int u^*_k H_{WW} u_l dx$$  **Perturbation - Matrix Element**

With the definition $\omega_2 - \omega_1 = (E_2 - E_1)/\hbar = \omega = \omega_{21} > 0$  **Transition frequency**
Observe that Matrix element $\langle u_k | H_{ww} | u_l \rangle$ is the key parameter containing the materials parameter and the optical perturbation with the frequency $\omega_{\text{opt}}$ because $H_{ww} = H_{ww}(E_0, \omega_{\text{opt}})$.

$\langle u_k | H_{ww} | u_l \rangle$ contains only the spatial parts $u_i(x)$ of the solutions $\Psi(x)$.

2) Calculation of the Interaction Hamilton Operator $H_{WW}(x,t)$ for monochromatic harmonic optical fields:

We calculate the interaction hamiltonian $H_{ww}(t,x)$ as the time dependent potential energy $-eV_{opt}(x,t)$ of a bound electron in the time dependent potential of the electrical field strength $E(t)$ of the harmonic optical field (magnetic energy is neglected).

The matrix element $H_{kl}$ describes the atomic forces acting on the electron inducing the transition $k \leftrightarrow i$ resp. $2 \leftrightarrow 1$.

**Potential energy of electrons in the optical E-field** (atomic nucleus at $x=0$):

On atomic dimension (few Å) the optical field is considered spatially constant $E(x,t) \sim E(0,t)$.

\[
V_{\text{opt}}(x,t) \approx -x E(0,t) \quad \rightarrow \quad H_{WW}(t,x) = -eV_{\text{opt}}(t,x) = e x E(0,t)
\]

because $F_{\text{electrical, opt}}(x) = -eE(x)$ and $V_{\text{opt}}(x) = -\int_0^x E(x)dx = -E(0,t)x$

Considering only harmonic optical fields with frequency $\omega_{\text{opt}}$:

\[
E(t) = E_0 \cos(\omega_{\text{opt}} t) = \frac{1}{2} E_0 \left[ \exp(i\omega_{\text{opt}} t) + \exp(-i\omega_{\text{opt}} t) \right] = \frac{1}{2} E_0 \left[ e^{i\omega_{\text{opt}} t} + cc \right]
\]

Remark: we just use the positive frequency $e^{+i\omega_{\text{opt}} t}$ term

\[\Rightarrow H_{ww}(t) = ex E_0 \cos \omega_{\text{opt}} t \quad \text{Interaction-Hamiltonian}\]

The atomic resonance occurs at the transition frequency:

\[
\omega = \omega_{12} = \frac{E_2 - E_1}{\hbar} = \omega_2 - \omega_1 \approx \omega_{\text{opt}}
\]

Inserting $H_{ww}(t)$ into the differential equation for the coefficients $C_1(t)$ und $C_2(t)$ we obtain:
using \( H_{kl} = \langle u_k | H_{WW} | u_l \rangle = \int_{vol} u_k^* H_{WW} u_l \, dx = eE_0 \cos \omega_{opt} t \langle u_k | x | u_k \rangle \) Interaction Hamiltonian

and the definition: \( \langle u_k | x | u_l \rangle = \int u_k^* x u_l \, dx \) dipole matrixelement of the transition \( k \leftrightarrow l \)

leading to: \( H_{11} = H_{22} = 0 \) (because \( x \) is an odd function)

Inserting \( H_{WW} \) and \( \omega_{21} = \omega \) in the diff. equation for \( C_i \) \( \Rightarrow \)

\[
\frac{\partial}{\partial t} C_1 = j \frac{1}{2\hbar} \left[ \exp \left( j \left( \omega_{opt} - \omega \right) t \right) + \exp \left( - j \left( \omega_{opt} + \omega \right) t \right) \right] C_2 \langle u_1 | eE_0 x | u_2 \rangle ;
\]

\[
\frac{\partial}{\partial t} C_2 = j \frac{1}{2\hbar} \left[ \exp \left( j \left( \omega_{opt} + \omega \right) t \right) + \exp \left( - j \left( -\omega_{opt} + \omega \right) t \right) \right] C_1 \langle u_2 | eE_0 x | u_1 \rangle
\]

Coupled differential equation for \( C_1(t) \) and \( C_2(t) \) for harmonic optical excitation

Remark: \( C_i(t) \) is determined by \( \omega_{21}, \omega_{opt} \) and \( \langle u_2 | eE_0 x | u_1 \rangle \)

For the calculation of the transition \( (\uparrow, \downarrow) \) rates we will solve this diff. eq. for 2 different situations (initial conditions):

1) Switching on the field at \( t=0 \) if the system is initially either
   - in the ground state \( 1 (C_1(0)=1) \) \( \rightarrow \) absorption, upward transition or \( \rightarrow r_{12} \)
   - in the excited state \( 2 (C_2(0)=1) \) \( \rightarrow \) stimulated emission, downward transition \( \rightarrow r_{21} \)

3) Calculation of the photon absorption (ground state transition 1 \( \rightarrow \) 2):
   we simplify the solution for \( C_1(t), C_2(t) \) for a weak perturbation (only small changes from the initial condition at \( t=0 \) !) of the system, which is assumed to be initially in the ground state.

1) Initial condition for Absorption: \( C_1(0) = 1 , C_2(0) = 0 \) ground state \( E_2 > E_1 \)

2) the changes of \( C_1(t) \) and \( C_2(t) \) are still small with respect to the initial state, \( C_1(t) \approx 1 - \varepsilon , C_2(t) \approx \varepsilon << 1 \)
With these simplification a simple integration \( \int_0^t dt' \) of the differential eq. for \( C_2(t) \) leads to simple solution (appendix):

\[
C_2(t) = \frac{j}{2\hbar} \langle u_2|eE_0 x|u_1 \rangle \exp \left( j \left( \omega - \omega_{\text{opt}} \right) t / 2 \right) \frac{\sin \left[ \left( \omega - \omega_{\text{opt}} \right) t / 2 \right]}{\left( \omega - \omega_{\text{opt}} \right) / 2}
\]

and

\[
|C_2(t)|^2 = \frac{1}{4\hbar^2} \left| \langle u_2|eE_0 x|u_1 \rangle \right|^2 \frac{\sin^2 \left[ \left( \omega - \omega_{\text{opt}} \right) t / 2 \right]}{\left( \omega - \omega_{\text{opt}} \right)^2 / 2} \approx E_0^2 \approx \text{Intensity } I ; \quad |C_2(t)|^2 < < 1
\]

Approximation for a weak perturbation
Approximation of the evolution of the occupation probability $|C_2(t)|^2$ of the excited state at $E_2$:

(excitation with both exactly defined optical frequency $\omega_{\text{opt}}$ and transition frequency $\omega$ of the 2-level system, unphysical)

The occupation probability $|C_2(t)|^2$ of the excited state 2 increases resulting in absorption. The evolution of $|C_2(t)|^2$ depends on time $t$ and frequency detuning $\omega - \omega_{\text{opt}}$ between transition and monochromatic E-field.

- only close or at resonance $\omega \approx \omega_{\text{opt}}$ there is a substantial absorption
- at resonance $\omega = \omega_{\text{opt}}$ the occupation probability of the excited state increases with $t^2$ (experimental $~t^2$!)
  → unphysical, in most experimental situations, because state energies $E$ and photon energies $h\omega_{\text{opt}}$ need to be exactly defined over long times without any perturbation.

- at resonance $\omega = \omega_{\text{opt}}$ \[ |C_2(t)|^2 = \frac{e^2 E_0^2}{4\hbar^2} |\langle u_2 | x | u_1 \rangle|^2 t^2 \] increases $~t^2$, the „width“ of the resonance decreases as $\Delta\omega \sim \frac{2\pi}{t}$,
  ➞ the area under the curve $|C_2(t)|^2$ increases $~2\pi t$ (→ constant rate at constant field).
4) Fermi’s Golden Rule

To get out of the dilemma we use a procedure known as “Fermi’s Golden Rule”:

- The calculation contains the unphysical assumptions
  1) the light field is ideal **monochromatic**, characterized by a $\delta$-function for the SDF $W(\omega)$ (infinite duration of the light wave !)
  2) the energy levels $E_i$ are defined **exactly** and characterized by a $\delta$-function for the density of state function
     (assuming infinite duration of atomic states $\rightarrow$ no collisions, dephasing processes, etc.).

In reality the density of state function of the electrons is broadened and $\Psi_i$ shows an energy $\Delta E_i$ uncertainty due to the short (~0.1ps) lifetime of the state.

**Solution: Averaging the transition probabilities over the optical power density $\rho_{opt}(\omega)$**

We average the transition functions over the energy width of the optical field or the electronic states by an integration over the frequency domain of $C_2(t, \omega)$.

For averaging over the optical spectral width of the transition we replace the field amplitude term $E_0^2$ by the spectral energy density $\rho_{opt}$, defined with the relation $\varepsilon E_0^2 / 2 = \int \rho_{opt}(\omega_{opt}) \cdots d\omega_{opt}$, and integrate the time-dependent probability $|C(t, \omega_{opt})|^2$ weighted by $\rho_{opt}(\omega_{opt})$ over the **finite spectral width of $W(\omega)=\rho_{opt}(\omega)$ of the field**:

$$\frac{e^2}{4\hbar^2} \int \frac{2W(\omega_{opt})}{\varepsilon} \left|\langle u_2 | x | u_1 \rangle \right|^2 \frac{\sin^2\left[\frac{(\omega - \omega_{opt})t}{2}\right]}{\left[\frac{(\omega - \omega_{opt})}{2}\right]^2} d\omega_{opt} = e^2 \frac{W(\omega_{opt})}{\varepsilon} \frac{\pi}{2\hbar^2} \left|\langle u_2 | x | u_1 \rangle \right|^2 t$$

$$\lim_{\omega_{opt} \rightarrow \omega} 2\pi t \delta(\omega - \omega_{opt})$$

**⇒ the averaged occupation probability** increases **linear with** $t$ **leading to a constant transition probability** $r_{12}$ **which is proportional to the spectral energy density** $W(\omega)=\rho_{opt}(\omega)$. 

a) the term dipole matrix element $\langle u_2 | x | u_1 \rangle$ contains the dynamic microscopic properties of the 2-level system

b) a transition with a matrix element $\langle u_2 | x | u_1 \rangle = 0$ is not possible and is called forbidden transition.

c) detuned transitions $\omega_{opt} \neq \omega$ only show weak oscillations of $|IC(t)|^2$ → polarization mode

- Interpretation of the dipole matrix elements: $\langle u_k | x | u_l \rangle = \int u_k^* x u_l \, dx$

The dipole moment $<p>=-e<x>$ is proportional to $\langle u_k | x | u_l \rangle$. For strong polarization and absorption $\langle u_k | x | u_l \rangle$ has to be large, meaning that the wave functions $u_k$ and $u_l$ should reach large values at large values of $x$ → only weakly bound electrons.

Stimulated emission proceeds in the same way but with changed initial conditions giving the same results:

$C_1(0) = 0, C_2(0) = 1 \quad \text{excited state as "start" state}$

**Einstein's Coefficient with an optical field of finite spectral energy density $W(\omega)$:**

From $|C_2(t)|^2 = \frac{e^2}{4\hbar^2} \frac{1}{\epsilon} |\langle u_2 | x | u_1 \rangle|^2 \rho_{opt}(\omega) 2\pi t$ → averaged occupation probability (linear in time $t$)

Per definition the transition rate $r_{12}$ per transition pair $1 \rightarrow 2$:

$r_{12} = \frac{\partial |C_2|^2}{\partial t} = \frac{e^2}{2\hbar^2} \frac{\pi}{\epsilon} |\langle u_2 | x | u_1 \rangle|^2 W(\omega) = BW(\omega)$

$B(\omega) = \frac{e^2}{2\hbar^2} \frac{\pi}{\epsilon} |\langle u_2 | x | u_1 \rangle|^2$

Einstein-coefficient $B$ for stimulated transitions (Absorption)

From $A = \left( \frac{n^2 \hbar \omega}{\pi^2 c_0^3} \right) B(\omega)$ →

$A = \frac{e^2 \omega^3}{2\pi \hbar c_0^3 \epsilon} |\langle u_2 | x | u_1 \rangle|^2 = 1/\tau_{spont}$

Einstein-coefficient $A$ for spontaneous emission
Calculation of transition rates with a spectral energy density: (self-study)

In order to avoid the averaging by the Fermi-Golden Rule we consider that the optical field is not monochromatic but described by a spectral power density $\rho_{\text{opt}}(\omega)$. For being able to work with Fourier-transforms we consider all signal to be time-limited (compare chap.7).

The optical field amplitude is described by a time-limited envelop-function $A(t)$ and we consider the situation of absorption:

\[
E_T(t) = \frac{A_T(t)}{2} \left( e^{j \omega_{\text{opt}} t} + e^{-j \omega_{\text{opt}} t} \right) \quad \text{for} \quad 0 < t < T \quad ; \quad E_T(t) = 0 \quad \text{for} \quad T < t \quad \text{and} \quad t < 0
\]

Differential equation for occupation probability for absorption with $C_j(t) \approx 1$: (p.49)

\[
\frac{\partial}{\partial t} C_2(t) = \frac{jeE(t)}{\hbar} \langle 1|x|2 \rangle e^{j \omega_2 t} = \frac{jeA(t)}{2\hbar} \langle 1|x|2 \rangle \left( e^{+j(\omega_{21}+\omega_{\text{opt}})t} + e^{+j(\omega_{21}-\omega_{\text{opt}})t} \right)
\]

Initial condition: $C_1(0) = 1$ ; $C_2(0) = 0$ ; $\omega_{21} = (E_2 - E_1)/\hbar$

Integrating both sides over $t$: $\int_0^T dt$ and considering time-limited functions:

\[
C_2(T) - C_2(0) = C_2(T) = \frac{je}{2\hbar} \langle 1|x|2 \rangle \int_0^T A(t) e^{+j(\omega_{21}+\omega_{\text{opt}})t} dt + \int_0^T A(t) e^{+j(\omega_{21}-\omega_{\text{opt}})t} dt = \frac{je}{2\hbar} \langle 1|x|2 \rangle \left( A_T(\omega_{21}+\omega_{\text{opt}}) + A_T(\omega_{21}-\omega_{\text{opt}}) \right)
\]

\[
|C_2(T)|^2 = \frac{e^2}{4\hbar^2} \langle 1|x|2 \rangle^2 \left( A_T(\omega_{21}+\omega_{\text{opt}}) A_T^*(\omega_{21}+\omega_{\text{opt}}) + A_T(\omega_{21}-\omega_{\text{opt}}) A_T^*(\omega_{21}-\omega_{\text{opt}}) \right)
\]

Using the relation between sectral power density and spectral amplitude density (chap.7):

\[
\frac{E_T^2}{E} = \frac{2}{\pi} \int_0^{\infty} S_T(\omega) d\omega = \frac{\lim_{T \to \infty}}{T \to \infty} \frac{1}{T 2\pi} \int_0^{2\pi} E_T(\omega) E_T^*(\omega) d\omega \quad \text{if} \quad T \to \infty \quad S_T(\omega) T 2\pi = E_T(\omega) E_T^*(\omega) \quad \text{(one - sided spectrum)}
\]

\[
|C_2(T)|^2 = \frac{e^2 \pi}{2\hbar^2} \langle 1|x|2 \rangle^2 S(\omega) T = \frac{e^2 \pi}{2\hbar^2} \langle 1|x|2 \rangle^2 \rho_{\text{opt}}(\omega) T \quad \text{(same result as Fermi – Golden – Rule)}
\]
5.4.1.3 Expectation value $\langle x(t) \rangle$ and $\langle p(t) \rangle$ of the dipole oscillator (field viewpoint)

**Goals:**

Transition rates $R$ and their dependency on carrier density $n$ do not describe the frequency dependent properties of the QM dipole, in particular the expectation value of the **expectation value of the susceptibility** $\langle \chi(\omega) \rangle$.

$$\langle \chi(\omega, N_1, N_2) \rangle$$?

we need to determine $\langle x(\omega) \rangle$ first!

Knowing $C_1(t)$ and $C_2(t)$ gives the **transient mixed state** $\Psi(x,t) = C_1(t)u_1(x)e^{-j\omega_1 t} + C_2(t)u_2(x)e^{-j\omega_2 t}$ and the time dependent expectation value $\langle x(t) \rangle$ and $\langle p(t) \rangle = -e\langle x(t) \rangle$ by the basic definition

$$\langle x(t) \rangle = \langle \Psi | x | \Psi \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)x \Psi(x,t) \, dx .$$

$C_1(t)$ and $C_2(t)$ can be related to $\langle x(t) \rangle$ (Appendix 5A):

$$\langle x(t) \rangle = \frac{C_1(t)C_2^*(t)}{\omega_{21}} \langle u_2 | x | u_1 \rangle + cc$$

depending on occupation, resp. carrier densities $n_1, n_2$ and $\omega_{opt}, E_{opt}$

**Expectation value of position** $\langle x(C) \rangle$ of the electron of the atomic DP (only in mixed state $\neq 0$ during 1-2, 2-1 transition)

**Graphical interpretation of the Dipole-Formation during the level transition:** (see also chap. 5.4.1.5)

- $\langle x(t) \rangle$ oscillates with **transition frequency** $\omega = \omega_2 - \omega_1 = \left( E_2 - E_1 \right) / h$.
- the functions $C_1(t)C_2^*(t)$ of $\langle x(t) \rangle$ depend on the optical field by $E_0^2$ and $\omega_{opt}$ and are calculated from the coupled Dgl. for $C_i(t)$
- stationary pure states have no dipoles because $C_1=0$, $C_2=1$ (excited state) or $C_1=1$, $C_2=0$ (ground state) $\rightarrow$ $\langle x(t) \rangle = 0$.
- $\langle x(t) \rangle$ has a well defined phase relation ship to the exciting field $E_o(t)$
Dipole oscillation for the transition between a **symmetric** ground state \( u_{100} \)- and a **nonsymmetric** excited state \( u_{210} \) of the H-Atom:

Consider the total mixed wave function \( \Psi(z,t) \) and \( |\Psi(z,t)|^2 \), where we moved the phase factor out of the bracket expression:

\[
\Psi(x,t) = C_a(t)u_{100}(x)e^{-j\omega_a t} + C_b(t)u_{210}(x)e^{-j\omega_b t}
\]

\[
= e^{-j\omega_b t}\left( C_a(t)u_{100}(x)e^{-j(\omega_a-\omega_b)t} + C_b(t)u_{210}(x) \right) = e^{-j\omega_b t}\Psi'(x,t)
\]

where \( |\Psi(x,t)|^2 = |\Psi'(x,t)|^2 \)

\[
t_n = 2\pi n / (\omega_b - \omega_a) = nT_{ba}, \quad n = 0,1,2,3 \ldots \rightarrow \text{phase term } e^{-j2\pi n} = 1
\]

\[
t_{n'} = \pi(2n+1) / (\omega_b - \omega_a) = (n+1)T_{ba}, \quad n = 0,1,2,3\ldots
\]

\[
\rightarrow \text{phase term } e^{-j\pi(2n+1)} = -1
\]

Dipole-oscillation occur only during the transition between \( 100 \leftrightarrow 210. \)

**The transient mixed state** \( \psi(z,t) \) **is asymmetric and forms a oscillating charge dipole** \( <p> \) **with the transition frequency** \( \omega_{ba}=\omega_b-\omega_a \)
Remark:

the electron charge distribution $\sim u_i u_i^*$ is symmetric to the nucleus for a pure state, therefore stationary pure states have no dipole moment (für $\rho_{\text{opt}}=0$).

The phase of the dipole relative to the exciting field depends on the relative phase of $C_i$ resp. carrier occupation $n_2$, $n_1$ and the opt. Frequency $\omega_{\text{opt}}$

Depending on the phase the dipole absorbs or emits radiation.

**5.4.1.4 Dipole-Matrix-Elements for allowed and forbidden transitions**

**Possible Dipole-Matrix-Elements of a 2-level system:**

The time invariant potential $V(x)$ has been assumed as symmetric around $x=0$ for our 1-dimensional case. Therefore the solutions $u(x)$ are either symmetric or anti-symmetric. However the probability density $uu^*(x)$ must be symmetric.

**The dipole operator $x$ in $\langle u_2 | x | u_1 \rangle$ is a asymmetric function,** therefore we have 4 possibilities:

<table>
<thead>
<tr>
<th>Initial state:</th>
<th>final state:</th>
<th>transition:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_1$ symmetric</td>
<td>$u_2$ symmetric</td>
<td>forbidden, because $\langle u_2</td>
</tr>
<tr>
<td>$u_1$ asymmetric</td>
<td>$u_2$ asymmetric</td>
<td>forbidden, because $\langle u_2</td>
</tr>
<tr>
<td>$u_1$ symmetric</td>
<td>$u_2$ asymmetric</td>
<td>allowed, because $\langle u_2</td>
</tr>
<tr>
<td>$u_1$ asymmetric</td>
<td>$u_2$ symmetric</td>
<td>allowed, because $\langle u_2</td>
</tr>
</tbody>
</table>
5.4.1.5 QM-calculation of the Susceptibility $\langle \chi(\omega) \rangle$

Procedure: we show that the quantum-mechanical expectation value of $\langle x(t) \rangle$ leads to the same differential equation of motion as for the classical oscillator for $x(t)$.

The important difference is that $\langle x(t) \rangle$ depends on the populations $n_1$ and $n_2$, and the initial occupation state leading to negative absorption, resp. gain.

- For the analysis we consider the stationary harmonic solutions of the differential equation for $C_1(t)$ and $C_2(t)$ with weak harmonic optical excitation.

- Calculation of the expectation value of the “dipole distance“ $\langle x(t) \rangle$, resp $\langle X(\omega) \rangle$ determines the quantum mechanical Susceptibility $\langle \chi(\omega) \rangle$.

Classical mechanics: $D = \varepsilon_0 E + P = \varepsilon_0 E + \varepsilon_0 \chi E = \varepsilon_0 \left(1 + \chi\right) E = \varepsilon_0 E$ (electrons on springs)

Quantum mechanics: $\langle D(\omega) \rangle = \varepsilon_0 E + \langle P(\omega) \rangle = \varepsilon_0 E + eN \langle X(\omega) \rangle = \varepsilon_0 E + \varepsilon_0 \langle \chi(\omega) \rangle E \rightarrow \langle \chi(\omega) \rangle = eN / \varepsilon_0 \langle X(\omega) \rangle$

expectation values of physical observables

Solution-Procedure:

To calculate the quantum mechanical susceptibility $\langle \chi(\omega) \rangle$, we determine from the diff.eq. for $C_1$ and $C_2$ first an oscillator equation of motion for $\langle x(t) \rangle$, resp. $\langle X(\omega) \rangle$ having the same form as the classical diff.eq. for $x(t)$:

$$\ddot{x} + \omega_0^2 x + \gamma_D \dot{x} = -e / m_e E_x \cos(\omega t)$$

classical driven oscillator with damping $\gamma_D$ and resonance frequency $\omega_0$.

1) from the oscillator differential equation of $\langle x(t) \rangle$ we calculate $\langle \chi(\omega) \rangle$, resp. $\langle n(\omega) \rangle$, $\langle k(\omega) \rangle$ as for $x(t)$.

Definitions and assumptions:
Definition of position expectation value: \[ \langle x \rangle = \int \Psi^*(x,t)x \Psi(x,t) \, dx \]

\[
E(t) = \frac{E_0}{2} \left( e^{j\omega_{opt}t} + e^{-j\omega_{opt}t} \right) \quad \text{assuming: harmonic optical field with positive frequency } e^{j\omega_{opt}t}
\]

\[
P(t) = \frac{E_0 E_0}{2} \left( \chi(\omega_{opt}) e^{j\omega_{opt}t} + \chi(-\omega_{opt}) e^{-j\omega_{opt}t} \right) \quad \text{harmonic polarization (assumption)}
\]

\[
H_{\psi\psi}(t) = \text{ex} E(t) = \text{ex} \frac{E_0}{2} \left( e^{j\omega_{opt}t} + e^{-j\omega_{opt}t} \right)
\]

\[
\Psi(x,t) = C_1(t) u_1 e^{-j\omega_1 t} + C_2(t) u_2 e^{-j\omega_2 t} \quad \text{assumed solution for harmonically perturbed wavefunction}
\]

Therefore the differential equations for \( C_1, C_2 \) (p.5-42) transform to:

\[
\dot{J} C_1 \approx \frac{E_0 e}{2\hbar} \langle u_2 | x | u_1 \rangle \left[ \exp \left( j(\omega_{opt} - \omega)t \right) + \exp \left( -j(\omega_{opt} + \omega)t \right) \right] C_2
\]

\[
\dot{J} C_2 \approx \frac{E_0 e}{2\hbar} \langle u_2 | x | u_1 \rangle \left[ \exp \left( -j(\omega_{opt} - \omega)t \right) + \exp \left( j(\omega_{opt} + \omega)t \right) \right] C_1
\]

with \( \dot{C} = \frac{\partial}{\partial t} C \)

By insertion of the of assumed solution for \( \psi(x,t) \) into \( \langle x \rangle \) we obtain:

\[
\langle x \rangle = C_1(t) C_2^*(t) \langle u_1 | x | u_2 \rangle e^{j\omega t} + C_1^*(t) C_2(t) \langle u_1 | x | u_2 \rangle^* e^{j\omega t}
\]

with transition frequency: \( \omega = \omega_2 - \omega_1 \)

(used p.5-49)

For the derivation of the QM-equation of motion of \( \langle x(t) \rangle \) we evaluate the first and second derivatives \( \langle \dot{x} \rangle = \frac{\partial}{\partial t} \langle x \rangle \)

and \( \langle \ddot{x} \rangle = \frac{\partial^2}{\partial t^2} \langle x \rangle \) (see appendix Chap.5). Making use of the above differential equation for \( C_1(t) \) and \( C_2(t) \) gives finally an:
QM Oscillator-Equation of the expectation value $\langle x(t) \rangle$:

$$\langle \ddot{x} \rangle + \omega^2 \langle x \rangle = \frac{E_0 e}{\hbar} \left| \langle u_2 | x | u_1 \rangle \right|^2 \omega \cos(\omega_{opt} t) \times \left\{ \left| C_2(t) \right|^2 - \left| C_1(t) \right|^2 \right\}$$

(without damping force!)

determines the phase of the oscillator relative to the driving optical field

fundamental driven oscillator equation for $\langle x(t) \rangle$ with the self-resonance $\omega = \omega_21$

$$-1 \leq \left\{ \left| C_2(t) \right|^2 - \left| C_1(t) \right|^2 \right\} \leq 1$$

depends on the occupation $n_1, n_2$ of $E_1, E_2$ determines the phase of the DP to the driving E-field

F-transforming gives: $x(t) \rightarrow X(\omega) = F(x(t))$

$$\rightarrow \langle X(\omega) \rangle = \frac{\omega}{\omega^2 - \omega_{opt}^2} \left( \frac{2E_0 e}{\hbar} \right) \left| \langle u_2 | x | u_1 \rangle \right|^2 \left\{ \left| C_2(t) \right|^2 - \left| C_1(t) \right|^2 \right\}$$

(frequency domain with undamped resonance at $\omega$)

Remark: Incomplete solution, because we do not know the time-dependence of $C(t)$!

The equation simplifies ($C \sim$ constant and known) under the assumption of
1) a weak field, that does not change the initial condition for $C_1$ and $C_2$ substantially during time $t$ and
2) that the system was initially eg. in the ground state $E_1$ (absorption process):

$$C_1(t) \sim 1 \quad \text{and} \quad C_1(t) \gg C_2(t) \rightarrow \text{medium is absorbing} \quad \left\{ \left| C_2(t) \right|^2 - \left| C_1(t) \right|^2 \right\} \sim -1$$

Quantum mechanic equation of oscillation for the charge position $\langle x \rangle$ for ABSORPTION ($C_2(t) \sim 0, C_1(t) \sim 1$)

$$\langle \ddot{x} \rangle + \omega^2 \langle x \rangle = \left( - \frac{E_0 e}{\hbar} \right) \left| \langle u_2 | x | u_1 \rangle \right|^2 \omega \cos(\omega_{opt} t)$$

undamped driven oscillator for absorption

Inphase or antiphase oscillating DP (classical situation)
\[
\left\langle X(\omega_{\text{opt}}) \right\rangle = -\frac{\omega}{\omega^2 - \omega_{\text{opt}}^2} \left( \frac{2E_0e}{\hbar} \right) \left| \langle u_2 | x | u_1 \rangle \right|^2
\]
(frequency domain solution for absorption)

The QM-equation for the harmonic oscillator \( \langle x(t) \rangle \) for absorption is formally equivalent to the classical undamped dipole, therefore all relations for the frequency dependence of the real part \( (\chi') \) and imaginary part \( (\chi'') \) of the QM-susceptibility \( <\chi> \) will be equal (no damping \( \gamma_D=0 \)).

**Substitution / equivalence classical ↔ QM: (absorption)**

<table>
<thead>
<tr>
<th>classical:</th>
<th>Quantum mechanical dipole:</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \omega_0 )</td>
<td>( \omega = \left( E_2 - E_1 \right) / \hbar )</td>
</tr>
<tr>
<td>( -\frac{e}{m_e} E_x )</td>
<td>( -2 \frac{E_0e}{\hbar} \left</td>
</tr>
<tr>
<td>( \gamma_D )</td>
<td>( \gamma_D = 0 ) (undamped -&gt; no loss, gain)</td>
</tr>
</tbody>
</table>

Depending if the system is initially in the a) **ground state** (absorption) or b) **excited state** (emission), there is a change in the sign of the driving field in the oscillator equation (dipole phase relative to the optical field \( E \)):

**a) ground state:** \( C_1(0)=1, C_2(0)=0 \) \( \rightarrow \left( \left| C_2(0) \right|^2 - \left| C_1(0) \right|^2 \right) \approx -1 \) Absorption [ ] \( (n_1\sim N, n_2\sim 0) \)

**b) excited state:** \( C_1(0)=0, C_2(0)=1 \) \( \rightarrow \left( \left| C_2(0) \right|^2 - \left| C_1(0) \right|^2 \right) \approx +1 \) Emission \( (n_2\sim N, n_1\sim 0) \)

- **the susceptibility for absorption and stimulated emission have opposite signs.**
  - similar to the classical case \( \chi''=0 \) results in no optical gain at this level of QM-oscillator model. Only by introducing damping \( \gamma \) we will be able to realize \( \chi''\neq0 \).
  - The necessary damping mechanism (deexcitation of excited state) by the spontaneous emission can not be introduced in the semi-classical QM-model self-consistently (Quantization of the optical field is required).
Relation of polarization density and transition pair densities $n_1$, $n_2$:

We have a transition pair density $N (=\text{atomic density})$ with an excited (E2) transition pair density $n_2$ and a ground-level (E1) density $n_1$, so that $N=n_1 + n_2$.

From $\langle x \rangle$ we get the polarization density $\langle P \rangle = -n_i \epsilon \langle x_i \rangle$ per type of transition pair density $n_i$:

$$\langle \chi_i(\omega_{\text{opt}}) \rangle = -\langle x_i \rangle / \epsilon_0 , \quad + \text{gain}, \quad - \text{absorption}$$

For a medium containing a mixture of transition pair in the ground state ($n_1$) for absorption and the excited state ($n_2$) for gain with the densities $n_1$ and $n_2$, we get for the total polarization density the superposition (using phase change for emission $2 \rightarrow 1$ transitions):

$$\langle \chi(\omega_{\text{opt}}) \rangle = \langle \chi_1(\omega_{\text{opt}}) \rangle + \langle \chi_2(\omega_{\text{opt}}) \rangle = \left( -n_1 e \langle X_1(\omega_{\text{opt}}) \rangle + n_2 e \langle X_2(\omega_{\text{opt}}) \rangle \right) / \epsilon_0 = e \langle X_1(\omega_{\text{opt}}) \rangle \left( n_2 - n_1 \right) / \epsilon_0$$

The susceptibility depends on the OCCUPATION DENSITY DIFFERENCE ($n_2-n_1$)!

From the QM-oscillator equation for $\langle x \rangle$ we obtain for an assumed solution $\langle x(t) \rangle = \langle X(\omega) \rangle e^{j\omega t}$

$$
\langle P \rangle = n_1 \langle p_1 \rangle + n_2 \langle p_2 \rangle = -n_1 e \langle X_1(\omega_{\text{opt}}, E_o) \rangle + n_2 e \langle X_2(\omega_{\text{opt}}, E_o) \rangle = -\left( n_2 - n_1 \right) e^2 \left| \langle u_1 | x | u_2 \rangle \right|^2 \frac{2\omega}{\omega^2 - \omega_{\text{opt}}^2}, E_0 = \epsilon_0 \langle \chi(\omega_{\text{opt}}) \rangle E_0
$$

$$
\langle \chi(\omega_{\text{opt}}) \rangle = \frac{\left( n_2 - n_1 \right) e^2 \left| \langle u_1 | x | u_2 \rangle \right|^2}{\epsilon_0 \hbar}, \quad \frac{2\omega}{\omega^2 - \omega_{\text{opt}}^2}
$$

Absorption: $n_2=0$, $n_1=N$

Stimulated emission: $n_1=N$, $n_1=0$
**QM: absorption, n₁=N  (stimulated emission, n₂=N)**

\[
\chi'(\omega_{\text{opt}}) = (-) \frac{N e^2 |\langle u_1 | x | u_2 \rangle|^2}{\varepsilon_0 h} \frac{2\omega}{\omega^2 - \omega_{\text{opt}}^2},
\]

Susceptibility of the undamped, lossless QM-Dipole with density N in absorption

\[
\chi''(\omega_{\text{opt}}) = 0
\]

with \( N = \text{dipole density} = n_1 ; n_2 = 0 \)  absorption

**Klassisch:**

\[
P = -N \chi(\vec{E}_0) = \frac{N e^2}{m} \frac{2}{\omega^2 - \omega_{\text{opt}}^2} E_0 = \varepsilon_0 \chi' \vec{E}_0
\]

\[
\chi'(\omega_{\text{opt}}) = + \frac{N e^2}{m \varepsilon_0} \frac{2}{\omega^2 - \omega_{\text{opt}}^2}, \quad \chi'' = 0
\]

---

**Formal introduction of QM damping by spontaneous emission:** (Appendix 5A)

**Goal:**

The QM-model assumed unrealistically „sharp“ energy levels and exact optical frequency meaning infinite carrier lifetimes.

As can be seen from the differential equations for \( C_1 \) and \( C_2 \):

An excited system can not return to equilibrium after switching-off of the optical field \( (E_0=0) \) because the is no damping term in the diff.eq. for \( C_1, C_2 \) (same argument as in Einstein-model) \( \rightarrow \frac{\partial}{\partial t} C_i = 0 \).
To formally introduce damping and optical gain ($\chi'' \neq 0$) into the diff.eq. for $C_1$, $C_2$ we modify them by additional a damping term $\gamma$ (representing finite carrier lifetime $\tau \sim 1/\gamma$):

**Only the introduction of damping als the QM representation of loss and gain!** (from first principles required the quantization of the optical field)

$$\frac{\partial}{\partial t} C_2 = -\frac{jE_0e}{2\hbar} \langle u_2 | x | u_1 \rangle \left[ \exp\left(j(\omega_{opt} + \omega)t\right) + \exp\left(j(\omega - \omega_{opt})t\right) \right] C_1 - \gamma C_2$$

carrier lifetime damping of excited level E2

$$\gamma = A / 2 = 1 / \left(2\tau_{spont}\right)$$ damping constant

The damping $\gamma$ relaxes $C_2$ after a disturbance ($E_0 \rightarrow 0$) with the time constant $\tau_{spont}$ back to equilibrium $\rightarrow \frac{\partial}{\partial t} C_i = -\gamma C_i$.

We repeat the previous calculation as for the undamped case to get the frequency dependence of the susceptibility $\langle \chi(\omega) \rangle$ of the damped QM-oscillator:

$$\chi = \chi_{ground\ state}(n_1) + \chi_{excited\ state}(n_2) \quad n_1 = \text{transition pairs in ground state} \quad n_2 = \text{transition pairs in excited state} \quad n_1 + n_2 = N = \text{atom density}$$

$$\chi(\omega_{opt}) = \text{Re} \chi + j \text{Im} \chi = \chi' + j \chi'' = \frac{e^2}{\epsilon_0 2\hbar} |\langle u_2 | x | u_1 \rangle|^2 \frac{2\omega\left[\omega^2 + \gamma^2 - \omega_{opt}^2\right] - j2\gamma\omega_{opt}}{\left[\omega^2 + \gamma^2 - \omega_{opt}^2\right]^2 + (2\gamma\omega_{opt})^2} (n_1 - n_2)$$

$$\chi'(\omega_{opt}) = \frac{e^2}{\epsilon_0 2\hbar} |\langle u_2 | x | u_1 \rangle|^2 \frac{2\omega\left[\omega^2 + \gamma^2 - \omega_{opt}^2\right]}{\left[\omega^2 + \gamma^2 - \omega_{opt}^2\right]^2 + (2\gamma\omega_{opt})^2} (n_1 - n_2)$$

$$\chi''(\omega_{opt}) = -\frac{e^2}{\epsilon_0 2\hbar} |\langle u_2 | x | u_1 \rangle|^2 \frac{2\omega\gamma_{P\omega_{opt}}}{\left[\omega^2 + \gamma^2 - \omega_{opt}^2\right]^2 + (2\gamma\omega_{opt})^2} (n_1 - n_2) \neq 0$$

Positive frequencies have been assumed $e^{j\omega_{opt}t}$

Absorption $\chi'' < 0$

Gain $\chi'' > 0$

using the attenuation relation from chap. $\alpha = 2\beta_{\gamma,K} \approx -\chi'' / 2 / \sqrt{1 + \chi'}$ from chap.2.
Quantum mechanically susceptibility with damping

QM allows describing optical gain as a function of population inversion \((n_2 > n_1)\):

- \(n_2 > n_1 \rightarrow\text{Gain (for population inversion), } \chi'' > 0\)
- \(n_2 < n_1 \rightarrow\text{Attenuation, } \chi'' < 0\)

Real- and imaginary part of the QM-susceptibility with damping

- The frequency dependence of \(\chi'(\omega), \chi''(\omega)\) is similar to the classical damped dipole.
  
  However for population inversion \(n_2 > n_1\) we get \(\chi''(\omega) \leq 0\) and optical gain \(g(\omega) = -\sim \chi''(\omega)\)

- The detuned QM-resonance frequency is:

  \[
  \omega_{\text{res}} \approx \sqrt{\omega_0^2 - \gamma^2} \quad \frac{\gamma/\omega \ll 1}{\rightarrow} \quad \omega = (E_2 - E_1)/\hbar
  \]
Conclusions:

- QM showed us, that the emission of a stimulated, coherent photon becomes possible for $n_2>n_1$, because the 2-level oscillator can be synchronized in such a way, that there is a dipole component orthogonal to the exciting field, resp. that $\chi''>0$. In a classic description this was not possible ($\chi''<0$).
- In case of the population inversion $n_2>n_1$, then $\chi''>0$ and the medium produces optical gain $g>0$. Thus we succeeded to relate population $(n_2-n_1)$ to gain and absorption.
- The stimulated global optical field $E_0$ enforces a macroscopic synchronization of all atomic dipoles in a medium with a phase difference according to the frequency response of $\chi(\omega_{opt})$.
- The synchronized dipoles reemit (scatter) a macroscopic dipole field, that is synchronized with the exciting field and superimposes to a 1) amplified or attenuated ($\chi''$, $\alpha$) and 2) phase modified ($\chi'$, $n$) total field.
Linewidth functions and reduction of maximal gain: (self-study)

For weak damping \((\gamma >> \omega)\) \(g(\omega)\) simplifies to a Lorenzian-shaped frequency dependence \(L(\omega_{\text{opt}})\):

\[
g(\omega_{\text{opt}}) \approx -\alpha(\omega_{\text{opt}}) = \chi''(\omega_{\text{opt}}) = \frac{e^2}{\varepsilon_0 2\hbar} \left| \langle u_2 | x | u_1 \rangle \right|^2 \frac{2\omega_D \omega_{\text{opt}}}{\left( \omega^2 + \gamma^2 - \omega_{\text{opt}}^2 \right)^2 + \left( 2\gamma \omega_{\text{opt}} \right)^2} (n_1 - n_2) = \frac{e^2}{\varepsilon_0 2\hbar} \left| \langle u_2 | x | u_1 \rangle \right|^2 L(\omega_{\text{opt}})(n_1 - n_2)
\]

The width \(\Delta \omega\) of the linewidth function \(L(\omega_{\text{opt}})\) is:

\[
L(\omega_{\text{opt}}) = \frac{1}{2\gamma} \frac{1}{1 + \left( \omega_{21} - \omega_{\text{opt}} \right)^2 / \gamma^2} = \frac{\Delta \omega / 4}{\left( \Delta \omega / 2 \right)^2 + \left( \omega_{21} - \omega_{\text{opt}} \right)^2} ; \quad \Delta \omega = 2\gamma
\]

The width of linewidth function is proportional to the inverse of the spontaneous carrier lifetime \(\tau_{\text{spont}}\) (typ. \(\sim 1\)ns for SC). Additional lifetime effects such as carrier collisions leading to a dephasing of the dipole (typ. \(\sim 100\)fs in SC) cause much stronger broadening and reduction of the gain by the linewidth functions.

In the following we will neglect the effect of the linewidth functions for mathematical simplicity.

Remarks:

The damping \(\gamma\) of the level populations \(n_1\) and \(n_2\) is the origin for the appearance of the imaginary part \(\chi''\) of the susceptibility \(\chi\).

In the excited state the polarization is opposite to the “classical” polarization (180° out of phase).

In the excited state the dipole acts as a source of radiation or as an active source of the field.

The role of the external stimulating field is to synchronize the phases of \(C_1(t)\) und \(C_2(t)\) in such a way, that there results an active dipole, emitting radiation coherent to the simulating field.
5.5 Optical band-to-band transitions in Semiconductors

In Optoelectronics active (amplifying) III-V semiconductors, such as GaAs, AlGaAs, InP, InGaAsP, GaN etc. play a key role for optical component, therefore we will concentrate on optical processes in semiconductors (SC).

In the courses Physik II (3.Sem) and Bauelemente (4.Sem) it was demonstrated that the coupling of the atoms in the solid and the condensation into a periodic lattice leads to:

- energetic splitting of discrete energy levels of the electrons into energy-bands (Conduction-, Valence band)
- a band structure with a band gap $E_g$ and quantized, quasi-free electron states (no localized states as in atoms)
- distributed, non-localized matter waves $\psi(x,t)$ and quasi-free motion of the electrons in the bands

To analyze the optical gain in SC we extend the notion of discrete transition pairs from atoms to a quasi-continuum of state-pairs distributed over energy-bands (Conduction and Valence band) of the SC.

Similar to the averaging process for the transition rate over energy spectrum of the optical field $W(\omega)$, we assume here a mono-chromatic light field $E_0 \cos(\omega_0 t)$ (typical for modern optoelectronic devices) and average the transition over the energy state density distributions of the transition pairs $\rho_{\text{continuum}}(E)$ or $\rho_{\text{continuum}}(\omega)$ ($\neq \rho_C$ or $\rho_V$).

### Conduction band:
- density of energy states $\rho_C(E_2)$

### Valence band:
- density of energy states $\rho_V(E_1)$

Transition pair density $\rho_r(E_{21}) = \rho_r(\rho_C(E_2), \rho_V(E_1)) = ?$
Band-to-Band-Transition Rates between energy bands of semiconductors:

For SC the optical transitions occur between the densely distributed energy states $E_{c,i}$, $\psi_{c,j}(x)$ in the C-band and the $E_{v,i}$, $\psi_{v,j}(x)$ in the V-band forming transition pairs (defined by selection rules).

- For the total energy interval $\Delta E = \Delta E_2 + \Delta E_1$ we will prove later that a reduced transition-pair density (RTPD) $\rho_r(E_2-E_1)$ can be defined as the number of transition pairs pro unit volume and unit energy $\Delta E$.

- In SC the electrons are quasi-free to move and the final state is not necessary empty as in atoms. The final state can be occupied by an electron according to the Quasi-Fermi-occupation probability function $f_Q,c(E_2)$, resp $f_Q,v(E_1)$.

We consider incremental sub-populations $\Delta n_2$, $\Delta n_1$ around the energy levels at $E_2$ and $E_1$ and distributed in energy intervals $\Delta E_2$ and $\Delta E_1$ with the individual density of state functions $\rho_c(E_2)$ and $\rho_v(E_1)$.

Generalization of Einstein-Formalism:

![Diagram of band-to-band transitions showing conduction and valence bands, transition probability, and transition rate equations.]

- **Transition probability of a single transition pair**
  - **Stimulated Emission:**
    \[ r_{21} = W B_{21} f_c(E_2) \left( 1 - f_v(E_1) \right) \]
  - **Stimulated Absorption:**
    \[ r_{12} = W B_{12} f_v(E_1) \left( 1 - f_c(E_2) \right) \]
  - **Spontaneous Emission:**
    \[ r_{21,\text{spont}} = A_{21} f_c(E_2) \left( 1 - f_v(E_1) \right) \]

- **Transition rate in the energy interval $\Delta E$ with the postulated pair density $\rho_r(E_{12})$**
  - **Stimulated Emission:**
    \[ \Delta R_{21} = W B_{21} \rho_r(E_{21}) f_c(E_2) \left( 1 - f_v(E_1) \right) \Delta E \]
  - **Stimulated Absorption:**
    \[ \Delta R_{12} = W B_{12} \rho_r(E_{12}) f_v(E_1) \left( 1 - f_c(E_2) \right) \Delta E \]
  - **Spontaneous Emission:**
    \[ \Delta R_{21,\text{spont}} = A_{21} \rho_r(E_{21}) f_c(E_2) \left( 1 - f_v(E_1) \right) \Delta E \]
Transition rates $r_{ij} \sim$ to the density of transition pairs $\rho_r \times$ occupation probability $f_i$ of initial state $\times$ probability of final to be empty $1-f_j$

Generalization of transition rates for non-monochromatic light fields and distributed levels:

In the general case when optical field and transition pairs are described by spectral density functions, $W(E)$ and $\rho_r(E)$ we generalize the transition rates as for the example for the stimulated transition rate:

$$dR_{21}(E_{21}) = B_{21} W(E_{21}) \rho_r(E_{21}) f_c(E_{21})(1-f_v(E_i))dE \rightarrow \int \ldots dE$$

$$R_{21}(E_{21}) = \int_{-\infty}^{+\infty} B_{21} W(E_{21}) \rho_r(E_{21}) f_c(E_{21})(1-f_v(E_i))dE \quad \text{total transition rate} \quad C \rightarrow V$$

Considered the two extreme cases:

a) optical field described by a broadband spectral density function $W(E)$ and a “sharp” discrete transition-pair density $N_\delta(E-E_{21})$ (eg. atomic states with no collision processes)

$$W(E); \quad \rho_r(E) = N \delta(E-E_{21}); \quad N = \text{atom density}$$

$$R_{21}(E_{21}) = B_{21} \int W(E) N \delta(E-E_{21}) f_c(E)(1-f_v(E))dE = B_{21} W(E_{21}) N f_c(E_{21})(1-f_v(E_i))$$ Einstein-Ansatz (broad band sources)

b) monochromatic optical field $E(t)=E_0\cos(\omega_{\text{opt}}t)$ described by a spectral density function $W(E)=N_{ph}\hbar\omega_{\text{opt}} \delta(E-\hbar\omega_{\text{opt}})$ and a distributed transition-pair density $\rho_r(E)$ (eg. bands-to-band transition in semiconductors)

$$W(E) = N_{ph} \hbar \omega_{\text{opt}} \delta(E-\hbar\omega_{\text{opt}}) = \frac{E_0^2 \hbar^2}{2} \delta(E-\hbar\omega_{\text{opt}}); \quad \rho_r(E); \quad N_{ph} = \text{photon density}$$

$$R_{21}(E_{21}) = B_{21} \int N_{ph} \hbar \omega_{\text{opt}} \delta(E-\hbar\omega_{\text{opt}}) \rho_r(E) f_c(E)(1-f_v(E))dE = N_{ph} \hbar \omega_{\text{opt}} B_{21} \rho_r(E_{21} = \hbar \omega_{\text{opt}}) f_c(E_{21})(1-f_v(E_i))$$
c) monochromatic optical field \( E(t) = E_0 \cos(\omega_{opt} t) \) with \( W(E) = N_{ph} \hbar \omega_{opt} \delta(E - \hbar \omega_{opt}) \) and a “sharp” discrete transition-pair density \( N \delta(E - E_{21}) \).

Here the transition rate diverges because the situation is unphysical.
5.5.1 Dipole-Matrix-Element of the transitions between energy bands

For the calculation of the transition rates between valence-continuum and conduction-continuum we have to determine the dipole-matrix element \( \langle u_c | x' | u_v \rangle \) between a delocalized discrete valence and a delocalized discrete conduction-band state \( \psi_{c,j}(x,t) \) and \( \psi_{v,j}(x,t) \) of the continuum:

\[
\text{continuum-to-continuum transition} \quad \sum_j \psi_{v,j}(x,t) \frac{E_0 \cos(\omega_{opt})}{E_0 \cos(\omega_{opt})} \sum_i \psi_{c,i}(x,t)
\]

In a SC the wave functions \( \psi_{c,j}(x,t) \) and \( \psi_{v,j}(x,t) \) are extended and periodic with the lattice (lattice-modulated plane waves). The calculation of total transition rates in SC is further complicated because the transition pairs are distributed over two continuums in the conduction and valence bands.

\[ \rightarrow \text{Summation, resp. integration over allowed band-to-band (interband) transitions} \sum_{ij-pairs} r_{ij} \]

Assumptions:

1) The light field is monochromatic with an amplitude \( E_0 \) and a frequency \( \omega_{opt} \) resulting in a \( \delta \) spectral energy density:

\[
\rho_{opt}(\omega) = \frac{1}{2}E_0^2\delta(\omega - \omega_{opt}) \quad (1\text{-sided})
\]

2) Wave functions in SC are non-localized Bloch-functions \( u_j(x) \), having the periodicity \( a \) of the lattice.

\[
\Psi_j(x,t) = F_j(x)u_j(x)e^{-jE_j t / h} \quad \text{resp.} = \psi_0 e^{j(k_j x)}u_j(x)e^{j(k_j x)}e^{-jE_j t / h}
\]

\( F_j(x) \) slow spatial envelope function, determined by the macroscopic crystal-potential (macroscopic crystal dimension \( L \))

\( u_j(x) \) fast varying, lattice-periodic Bloch-function, determined by the microscopic lattice potential (a lattice period \( a \sim 5\text{A} \))

\( k_j(\omega) \) crystal wave vector

\( \psi_0 \) normalization constant
Schematic representation of the wave function and e-h-dipoles in SC:

3) For transitions in SC the final states are not necessarily empty, but are occupied by electrons according to the Fermi-statistics $F(E, E_{F0})$ (in atoms the final state of an atomic transition-pair was per definition empty).

- Dipole-transitions are represented as a superposition of wavefunctions $\psi_C$, $\psi_V$ of the conduction- and valence-band.
5.6 Basic Properties of Electrons in Semiconductors

(Recapitulation, 4.Sem. Habibleiterbauelemente)

For the calculation of the rates of stimulated $R_{21,\text{netto}}$ and spontaneous $R_{21,\text{spont}}$ emission, as well as optical amplification $g$ in SC and their relation to the electron- and hole-densities $n$ and $p$ we review the following basic relations on wavefunctions in conduction (valence) band $\psi_{c(v)}(\vec{r}, \vec{k}_{c(v)}, t)$

- **Dispersion relation**, $E_{c(v)}(\vec{k}_{c(v)})$
- **Effective mass** $m_{\text{eff}}$
- **Density of states** $\rho_{c(v)}(E)$ and **carrier densities** in SC: $n$, $p$

**Density of states** $\rho_c(E_{ci})$, $\rho_v(E_{vi})$ and **carrier densities** $n$, $p$ in conduction- and valence-band at energy $E_{ci}$ and $E_{vi}$

**Reduced density of state-pairs** $\rho(r(E_{ij}))$, describing the density of electrons and holes of transition pairs having the same crystal momentum $p$, resp. the same propagation vector $k$ (conservation of $k$ of the transition) for an energy difference $E_{ij}$, resp. $E_{V1C2}$: $k_v(E_{vi})=k_c(E_{ci})$

**The dispersion relation** $E(k_i)$ for electron and holes, expressing the dependence of the quantized particle energy $E_i$ on its crystal momentum $p_i=\hbar k_i$, resp. wave vector $k_i$.

**The carrier occupation probability** in valence- and conduction-band described by assumed Quasi-Fermi-distribution functions $f_{c(v)}(E, E_{FQ})$ of the individual bands C, V. $E_{FQ}$ is the Quasi-Fermi-level of the particular band.
5.6.1 Density of states and dispersion-relation of electrons in an ideal SC

Electrons of a precise total energy \( E = E_{\text{kinetic}} + E_{\text{potential}} \) moving in the periodic potential \( V_{\text{lattice}}(r) \) of a crystal can be represented quantum mechanically by a planar Bloch-wave \( \Psi(\vec{r},t) \) as solution of the stationary Schrödinger equation.

Planar matter wave for a particle of energy \( E = h\nu \), of mass \( m \) and a crystal momentum \( p = \hbar k \):

\[
\Psi(\vec{r},t) = u(\vec{r}) \exp \left( j \frac{E}{\hbar} t - j \frac{p}{\hbar} \cdot \vec{r} \right) = u(\vec{r}) \exp \left( j \omega t - j \frac{k}{\hbar} \cdot \vec{r} \right)
\]

\( u(\vec{r}) \) has the periodicity of the crystal lattice (a)

To first order the motion of the electron in an energy band can be described as a quasi-free “classical” particle with

1) an effective mass \( m_{\text{eff}} \),
2) a kinetic energy \( E_{\text{kin}} = E - E_{c} \) (for the electrons in the conduction band and \( E_{\text{kin}} = E_{v} - E \) for holes in the valence band) and
3) a crystal momentum \( p = \hbar k \)

**Dispersion-Relation \( E(k) \) and density of states \( \rho \):**

The kinetic energy \( E_{\text{kin}} \) of the electron as a quasi-free particle in the SC-crystal is related to its momentum \( p \) in the same way as for a free particle:

\[
E_{\text{kin}} = \frac{p^{2}}{2m_{\text{eff}}} = \frac{\hbar^{2}k^{2}}{2m_{\text{eff}}}
\]

In analogy to classical particles there is a square law relation between the quantized crystal momentum \( p \), resp. \( k \) and the quantized \( E_{\text{kin}} \):

\[
p = \hbar k \quad k = \text{wave vector of matter wave}
\]
\[
\omega = E / \hbar \quad \omega = \text{frequency of the matter wave}
\]
the kinetic energy $E_{\text{kin}} = E - E_c$ of the electron is positive from the conduction band edge $E_c$ into the band (similar for holes in the valence band)

**Dispersion-Relation $E_{\text{kin}}(k)$ for quantized matter waves in (1D) semiconductors:**

$$E_{\text{kin}}(p) = \frac{1}{2m_{n,p}} p^2$$

$$E_{\text{kin}}(k) = \frac{\hbar^2}{2m_{n,p}} k^2$$

$$E_{\text{kin},n} = E - E_c \quad \text{(electrons)}$$

$$E_{\text{kin},p} = -E + E_v \quad \text{(holes)}$$

$m_{n(v)}$ = effective electron (hole) mass

Unlike a classical particle the **crystal momentum** $p$ and **wave vector** $k$ are quantized (by the boundaries of the macroscopic crystal volume $L_x$):

$$k_x = \frac{2\pi}{L_x} n = n\Delta k \quad ; \quad n = 0, 1, 2, 3, \ldots$$

$$\Delta k = k_n - k_{n-1} = \frac{2\pi}{L_x}$$

Therefore also the energy levels $E$ are quantized:

$$E_{\text{kin}}(k_n) = \frac{\hbar^2}{2m_{n,p}} k_n^2 = \frac{2\pi^2 \hbar^2}{L_x m_{n,p}} n^2$$

$n = 0, 1, 2, 3, 4 \ldots \text{the energy level quantization is not equidistant!}$

The **allowed** energy-levels and momentums on the dispersions-relation $E(k)$ are quasi-continuous, because $\Delta k$ and $\Delta E$ very small.
Occupation of states in the $k$-diagram:

(undoped SC $\rightarrow$ in thermal equilibrium Fermi-Energy $E_F$ lies in the band gap)

For each wave vector $k_n$ there are two associated energy-levels $E_C(k_n)$ and $E_V(k_n)$ in the conduction and valence band forming a discrete transition pair ($E_C(k_n) \leftrightarrow E_V(k_n)$) at $k_n$. 
Repetition: carrier densities in C- and V-bands:

In the course „Halbleiterbauelemente“ (4.Sem) the number $N$ of solution of the Schrödinger equation in k-space has been calculated per unit volume and unit energy interval – this density is called 1. Density of states $\rho(E)$ (DOS), resp. $\rho(k)$ for electrons and holes as a function of Energy $\rho_c(E), \rho_v(E)$ using a constant effective masse for parabolic bands

$$\rho_c(E) = 4\pi \left( \frac{2m_e}{h^2} \right)^{3/2} \sqrt{E - E_c}, \quad \rho_v(E) = 4\pi \left( \frac{2m_h}{h^2} \right)^{3/2} \sqrt{E_v - E}$$

$\rho$ describes the state density in a band at a particular energy, it does not describe the transition pair density $\rho_r$ directly.

2. Fermi-Occupation Probability of the energy level $E$ by an electron

$$f(E, E_{QF}) = \frac{1}{1 + e^{(E-E_{QF})/kT}}, \quad E_{QF} = E_F \text{ (Quasi-)} \text{Fermi-Energy of the corresponding band for equilibrium}$$

resp. Quasi-Fermi-Distribution for electrons and holes in non-equilibrium $E_{QF,n} \neq E_{QF,p}$

$$f_{Q,n}(E) = \frac{1}{1 + e^{(E-E_{QF,n})/kT}}; \quad f_{Q,p}(E) = \frac{1}{1 + e^{(E-E_{QF,p})/kT}}$$

3. Electrons- and Hole-Density $n, p$ for parabolic Bands as a function of Fermi-energies

From the DOS $\rho(E)$ and from $f(E, E_{QF})$ the carrier densities $n, p$ are determined by integration over the corresponding band

$$n = \int_{E_C}^{E_{C,\text{Top}}} \rho_c(E) f_c(E) \, dE = \frac{4 \sqrt{\pi} \left( \frac{2m_{e,\text{eff}}}{h^2} \right)^{3/2}}{F_{1/2} \left( \frac{E_F - E_C}{kT} \right)} \left( \frac{2m_{e,\text{eff}}}{h^2} \right)^{3/2} F_{1/2} \left( \frac{E_F - E_C}{kT} \right)$$

$$p = \int_{E_v}^{E_{V,\text{Bottom}}} \rho_v(E) f_v(E) \, dE = \frac{4 \sqrt{\pi} \left( \frac{2m_{h,\text{eff}}}{h^2} \right)^{3/2}}{F_{1/2} \left( \frac{E_F - E_v}{kT} \right)} \left( \frac{2m_{h,\text{eff}}}{h^2} \right)^{3/2} F_{1/2} \left( \frac{E_F - E_v}{kT} \right)$$

$$N_{\text{eff}} = \text{effective density of states}$$

with the Fermi-Integral

$$F_{1/2}(x, x_F) = \int_0^\infty \frac{x^{1/2}}{1 + e^{x-x_F}} \, dx$$
4. Carrier Transport by Drift and Diffusion

\[ j_n = en\mu_n E + eD_n \frac{\partial n}{\partial x}, \quad j_p = ep\mu_p E - eD_n \frac{\partial p}{\partial x} \]

Drift current Diffusion current

\(\mu = \) mobility, \(D = \) diffusion constant

Important for carrier transport in photodiodes and current-injection in Laser diodes and LEDs
Graphical representation of the density of states $\rho_C$, $\rho_V$ and electron and hole occupation $n$, $p$ in the density of states diagram:

(at different temperatures $T$ and for different positions of the Quasi-Fermi-levels $E_{QF,C}$, $E_{QF,V}$)

For equilibrium:

$n_p = n_i^2$, $E_{QF,n} = E_{QF,p} = E_F$

Quasi-Neutrality for undoped SC:

$n = p$, $np \neq n_i^2$, $E_{QF,n} \neq E_{QF,p}$ (nonequilibrium)
5.7 Optical Transition Rates and Amplification in SC

Band-to-band Transitions in SC are continuum-to-continuum transitions and the total transition rates are obtained by an integration over all involved allowed state-pairs (state-pair = initial + final state):

- allowed pair transition are (in most cases) energy (E) and momentum (k)-conserving
- the matrix element is determined by the Bloch-wave function for the C- and V-band
- the transition-pair density function $\rho(T_2,T_1)$ is given by the bandstructure (dispersion relation $k(\omega)$) and the density of state functions of the C- and V-band, $\rho_n(E_2)$ and $\rho_p(E_1)$.

**Goal:**
- Extension of the transition rate $R(\omega,n)$ for Band-to-Band-transitions
  - Calculation of the reduced transition pair density $\rho_r(\omega)$ for parabolic conduction- and valence-bands
  - Determination of the spectral dependence of the transitions $R(\omega)$
  - Relation between transition rate $R(n)$ and the carrier densities $n$ and $p$, resp. the quasi-Fermi-levels and pump current $I_{pump}$

5.7.1 Optical Interaction between C- and V-band electrons in direct SC

**Schematic Band-to-Band-Transitions with momentum (k)-conservation**

We will show that the matrix element $H_{ik}$ between 2 discrete states out of the continuum is only non-zero (allowed) if the transition is between 2 states with the same momentum $p$, resp. $k$

**Vertical or direct transitions** (in the dispersion diagram)

The common k-vectors $k=k_{ci}=k_{vj}$ defines with the dispersion relations of the bands $k_c(\omega_{ci})$ and $k_v(\omega_{vj})$ the corresponding transition energy $E_{cv,i,j}(k)=E_{ci}(k) - E_{vj}(k)$
The k-conserving optical Band-to-Band-Transitions $E_2(k) \Leftrightarrow E_1(k)$ in the dispersion diagram $E(k)$:

Individual dipole-transitions can only take place between wave functions of the same $k$-vector.

Postulated momentum conservation: $\Rightarrow$ $k$ of start- and final state are equal (vertical transitions)

\[
\begin{align*}
\text{no momentum } k_v & \neq k_c \\
\text{momentum (k) } k_v & = k_c \quad (k_{\text{initial}} = k_{\text{final}}) \\
\text{conservation} & \quad \text{allowed}
\end{align*}
\]

Dispersions-Diagram represents energy- and momentum-conservation:

From a $k$ the corresponding energy difference of the pair are:

\[
E(k) = \hbar \omega = E_g + E_C(k) + E_V(k) = E_g + \frac{\hbar^2}{2m_{\text{eff},c}} k^2 + \frac{\hbar^2}{2m_{\text{eff},v}} k^2 \quad \rightarrow \quad k(\omega) \text{ or } \omega(k)
\]

The reduced pair state density $\rho_r$ has to be determined separately from the densities of states $\rho_c$, $\rho_v$. 

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5.7.2 Direct Semiconductors

The transition rates between C- and V-band levels $j$ and $k$ depend essentially of the matrix-elements $\langle u_j | x | u_k \rangle$.

If $\langle u_j | x | u_k \rangle = 0$ then this optical transition is forbidden.

Transition energy $\Psi_j(E_j) \rightarrow \Psi_k(E_k) ; E_{jk} = E_j - E_k = \hbar \omega$ conserved by converting potential/kinetic energy into a radiation quantum:

$\hbar \omega = E_j - E_k$  \hspace{1cm} Energy-conservation

During band-to-band transitions in SC the momentum of the electron-hole pair must be identical ("vertical" transitions, other transitions are forbidden):

$k_j = k_k$  \hspace{1cm} momentum conservation

5.7.2.1 Momentum conservation in optical transitions in undoped SC

Simple calculations will show that in ideal SC:

1) the transition matrix element is large for k-conservation and small (forbidden) for non-k-conserving transitions.

2) indirect transitions need a 3\textsuperscript{rd} particle (eg. phonon) for k-conservation \rightarrow low interaction probability for 3 particle interaction.

- a transition is \textbf{direct} if the \textbf{energy-minimum of the C-band} and the \textbf{energy –maximum of the V-band} have the same k-vector

- a SC with a direct optical transition (usually at k~0) is called a \textbf{direct Semiconductor} (eg. AlGaAs, InGaAsP, GaN, etc. but not Si, Ge)

\textbf{electrons} occupy the \textbf{energy minimum} of the conduction band and \textbf{holes} occupy the \textbf{maximum} of the valence band with high probability.
Allowed and forbidden transitions in SCs:
Direct, momentum conserving transitions

To proof the \textit{k-conservation} we calculate the dipole matrix-element for the electron and hole wave function in the C-, resp. V-band:

\begin{align*}
\Psi_{c,k}(x) &= u_{c,k}(x)e^{-jk_c x} \quad \text{matter wave of } e \text{ in conduction-band} ; \quad E_C = \hbar \omega_c \\
\Psi_{v,k}(x) &= u_{v,k}(x)e^{-jk_v x} \quad \text{matter wave of } h \text{ in valence-band} ; \quad E_V = \hbar \omega_v \\
E(x) &= e^{-j\beta x} \quad \text{optical wave with propagation vector } \beta = 2\pi / \lambda ; \quad \omega = (\omega_c - \omega_v)
\end{align*}

Not all transitions between \( \Psi_{c,k,j}(x,k_{c,j},t) \rightarrow \Psi_{v,k,j}(x,k_{v,j},t) \) are allowed. Allowed transitions (\( \langle u_{c,j} | x | u_{v,j} \rangle \neq 0 \)) conserve:

1. Energy conservation: \( \hbar \omega_{opt} = E_{c,j} - E_{v,i} \)
2. Momentum conservation: \( k_{c,j} = k_{v,j} \)

The dipole-matrix-element of the valence-conduction band transition \( \Psi_v \rightarrow \Psi_c \) becomes for an extended polarized (\( \vec{e}, \vec{\beta} \)) optical plane EM-wave:

\[ \vec{e} E_0 \cos(\omega t - \vec{\beta} \vec{r}) = \vec{e} E_0 \text{Re} \left\{ e^{-j(i\omega t - \vec{\beta} \vec{r})} \right\} = \frac{\vec{e} E_0}{2} e^{j\vec{\beta} \vec{r}} e^{-j\omega t} + cc \]

\[ E(\vec{r}) = E_0 \vec{e} e^{-j\vec{\beta} \vec{r}} \quad \text{and} \quad E(\vec{r},t) = \vec{E}(\vec{r}) e^{+j\omega t} ; \quad \vec{r} = \text{spatial coordinate} \]
Electrical potential:

\[ V(\vec{r},\vec{r}') = -E_0 e^{-j\vec{p} \cdot \vec{r}'} \]  \( \vec{r}' = \text{dipole displacement coordinate at position } \vec{r} \)

Including the distributed wave and EM-wave functions in the dipole matrix elements gives integrated over the total crystal volume:

\[
H_{21} = \left\langle \psi^*_c(\vec{r}) \right| H_{ww}(\vec{r},\vec{r}',t) \left| \psi_v(\vec{r}) \right\rangle = \left\langle \psi^*_c(\vec{r}) \right| eE_0 e^{-j\vec{p} \cdot \vec{r}'} \left| \psi_v(\vec{r},t) \right\rangle = eE_0 \left\langle u^*_c \right| x' \left| u_v \right\rangle
\]

\[
\equiv \iiint_{\text{crystal volume}} u^*_c(\vec{r}) e^{+jk_c \cdot \vec{r}} \left( eE_0 e^{-j\vec{p} \cdot \vec{r}'} \right) u_v(\vec{r}) e^{-jk_v \cdot \vec{r}'} \, d\vec{r} = eE_0 \iiint_{\text{crystal volume}} u^*_c(\vec{r}) u_v(\vec{r}) (\vec{e} \cdot \vec{r}') e^{-j(k_v-k_c+\vec{p}) \cdot \vec{r}'} \, d\vec{r} = eE_0 \left\langle u^*_c \right| \left( \vec{e} \cdot \vec{r}' \right) \left| u_v \right\rangle
\]

The function \( u(\chi) \) is periodic with the lattice-constant \( a \) and the exp-term containing \( [k_C-k_V-k_{opt}]x \) oscillates with unity absolute value in the integral and thus the volume integral over \( L^3 \) averages to \( <uCIxIuV>=0 \) if \( [k_C-k_V-k_{opt}] \neq 0 \).

\[ \vec{k}_v - \vec{k}_c + \vec{\beta}_{opt} = 0 \]  momentum conservation in optical transitions

momentum of a photon:

\[ \beta_{opt} = \frac{2\pi}{\lambda} \quad \rightarrow \beta_{opt} \approx 10^4 \text{ cm}^{-1} \]

momentum of a electron with the thermal energy \( E_k=kT \):

\[ p_c = \hbar k_c \quad k_c \approx \frac{\sqrt{2m_e kT}}{\hbar} \approx 10^9 \text{ cm}^{-1} \]

Because the photon wave vector \( k_{opt} \) is much smaller than the electron-momentum \( k_c \), \( k_v >> \beta_{opt} \) we get:

\[ \vec{k}_c \approx \vec{k}_v \]  Direct Optical Transition requirement
Remarks:

- The matrix element in a crystal is often a function of the optical propagation direction $\vec{\beta}$, resp. of the polarization $\vec{e}$ of the optical field, therefore in SC the optical properties are often non-isotropic.

- The lattice constant ($a\sim 5\text{Å}$) is much smaller than the wavelength $\lambda$ ($\sim 1\mu\text{m}$) of the light, $a<<\lambda$. The optical field is homogenous for atomic dimensions, resp. over the lattice cell.

### 5.7.3 Stimulated and spontaneous transition rates in direct SC

We extended from Chap.5.5 Einstein’s-transition rates to the transition probabilities and differential transition rates in $\Delta E$ as:

- **Conduction band**

  - Transition probability of a transition pair

  - **Stimulated Emission:**
    
    \[
    r_{21} = W B_{21} f_c(E_2) (1 - f_v(E_1))
    \]

  - **Stimulated Absorption:**
    
    \[
    r_{12} = W B_{12} f_v(E_1) (1 - f_c(E_2))
    \]

  - **Spontaneous Emission:**
    
    \[
    r_{21,\text{spont}} = A_{21} f_c(E_2) (1 - f_v(E_1))
    \]

- **Valence band**

  - **Transition rate in the energy interval $\Delta E$ with the pair density $\rho_r(E_{12})$**

    - **Stimulated Emission:**
      
      \[
      \Delta R_{21} = W B_{21} \rho_r(E_{21}) f_c(E_2) (1 - f_v(E_1)) \Delta E
      \]

    - **Stimulated Absorption:**
      
      \[
      \Delta R_{12} = W B_{12} \rho_r(E_{12}) f_v(E_1) (1 - f_c(E_2)) \Delta E
      \]

    - **Spontaneous Emission:**
      
      \[
      \Delta R_{21,\text{spont}} = A_{21} \rho_r(E_{21}) f_c(E_2) (1 - f_v(E_1)) \Delta E
      \]

  

\[
B = \frac{\pi e^2}{2\hbar^2} \langle u_c \mid x \mid u_v \rangle
\]
Wave functions of electrons in bands of SC are **not localized** and the final state may already be occupied by a particle according to the Fermi-statistic thus blocking the transition (because of Pauli exclusion principle):

- the transition rate $r_{12}$ (eg. absorption $1 \rightarrow 2$) is $\sim$ to the probability $f(E_1)$, that the start-level $E_1$ is occupied
- the transition rate $r_{12}$ (eg. absorption $1 \rightarrow 2$) is $\sim$ to the probability $[1-f(E_2)]$, that the final-level $E_2$ is empty
- $r_{ij} \sim f(E_i)(1-f(E_j))$

occupied state: [ ] empty state: [ ]

$f_x = $ Fermi-Function of band $x$

**Concept of the reduced density $\rho_r(E)$ for k-conserving pairs and the reduced mass $m_r$:**

**Concept:**

For optical transitions rates with k-conservation we are interested in the **number of energy-pairs** (in the 2 bands) with the same k-vector in the interval $\Delta k$, resp. per energy interval $\Delta E$ at $E_2(k)$ and $E_1(k)$ in C- and V-band.

(the density of states $\rho_n$ and $\rho_p$ describe only the number of energy-levels (not pairs !) per energy interval $\Delta E$ in one band)

**Definition of the Reduced Density $\rho_r$ for transition-pairs in conduction and valence bands:**

the **reduced density** $\rho_r(E)$ is defined as **number of energy level-pairs** with the energy-difference $E$ per energy interval $\Delta E$ where the initial and final states in the conduction and valence band have the **same k-vector**

---

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The continuum-continuum transition rates $R$ are proportional to the so defined reduced pair density $\rho_r$ weighted by the occupation probabilities of the initial and final state-pair.

**Graphical representation of continuum $\rightarrow$ continuum transitions 2 (C) $\rightarrow$ 1 (V)**

All $\Delta N$ transition pairs of the momentum interval $\Delta k$ are distributed in the total energy interval $\Delta E_{21}$:

$$
\Delta E_{21} = \Delta E_2 + \Delta E_1
$$

Remark:

$k$ determines (by the dispersion relation $E(k)$) the energy levels $E_2(k)$ and $E_1(k)$, $E(k) = E_2(k) - E_1(k)$ of an individual pair.
Procedure for the calculation of the reduced density $\rho_r$:

- calculate the reduced density $\rho_r$ for direct transition ($k_2=k_1$) between $E_2$ and $E_1$ as a function of the known densities of states of conduction and valence band $\rho_c(E_2)$, $\rho_v(E_1)$ and as a function of $k$, resp $E_{21}$:

$$\rho_r(E_{21}) = \rho_r(\rho_c(E_2),\rho_v(E_1)) = ?$$

- The calculation of the number of transition pairs $\Delta N(\Delta k)$ in the momentum interval $\Delta k$ is simple, because all states are separated by the equal momentum quantization $\delta k$. We then transform the interval $\Delta k$ into the associated energy interval $\Delta E_{21}(\Delta k)$ with the help of the dispersion relation of the C- and V-bands.

In addition we also use the fact that $\Delta N$ can also be expressed by both energy state densities

$$\Delta N = \rho_v(E) \Delta E_1 = \rho_c(E) \Delta E_2$$

with $\Delta E_1(\Delta k) \neq \Delta E_1(\Delta k)$.

a) Calculation of the number of transition pairs $\Delta N$ in the interval $\Delta k$ and $\Delta E$:

Due to the quantization $\delta k$ of $k_n$ there are $\Delta N$ pairs in the momentum interval $\Delta k$:

$$k_n = n \delta k \quad \text{with} \quad \delta k = \frac{h}{L} \quad (1-D \text{ case}) \quad \text{resp.} \quad \delta^3 k = \frac{h}{L^3} \quad (3-D \text{-case})$$

$$\Delta N = \frac{\Delta k}{\delta k} \quad \text{transition pairs} \quad \text{distributed over the total energy interval} \quad \Delta E_{21} = \Delta E_2 + \Delta E_1$$

$\Rightarrow \Delta N$ transition pairs are distributed in each energy interval $\Delta E_2$ and $\Delta E_1$ at $E_2$ and $E_1$.

b) Calculation of the relation between $\Delta E_2$, $\Delta E_1$, $(E_2-E_c)$ and $(E_v-E_1)$ with $k$ and $\Delta k$:

$\Delta k$, $\Delta E_{21}$, $\Delta E_2$, $\Delta E_1$ are related by the dispersion relation $E(k)$

$$\left( E_2(k) - E_c \right) = \frac{\hbar^2}{2m_n} k^2 \quad \text{and} \quad \left( -E_i(k) + E_v \right) = \frac{\hbar^2}{2m_p} k^2 \quad ; \quad \rightarrow \quad \text{differentiation by} \quad k:$$

$$\Delta E_2 = \frac{\hbar^2}{m_n} k \Delta k \quad \text{and} \quad \Delta E_i = \frac{\hbar^2}{m_p} k \Delta k$$
\[
\Delta E_{21}(k) = \Delta E_2 + \Delta E_1 = \left(\frac{\hbar^2 k}{m_n} + \frac{\hbar^2 k}{m_p}\right)\Delta k = \frac{\hbar^2 k}{m_n} \left(\frac{m_n + m_p}{m_p}\right)\Delta k
\]

\[
E_{21}(k) = E_2(k) - E_1(k) = E_g + \frac{\hbar^2}{2m_n}k^2 + \frac{\hbar^2}{2m_p}k^2 = E_g + \left(\frac{\hbar^2}{2m_n} + \frac{\hbar^2}{2m_p}\right)k^2 \Rightarrow
\]

\[
E_{21}(k) = E_g + \frac{\hbar^2}{2m_r}k^2
\]

Dispersion relation for the transition pairs

with \( m_r = \frac{m_n m_p}{m_n + m_p} \) Reduced mass (definition)

c) calculation of the relation between \( \Delta N \) and the density of state functions \( \rho_n, \rho_p \):

Because the number \( \Delta N \) of electron and hole states are equal in \( \Delta k, \Delta E_{21}, \Delta E_2, \Delta E_1 \) it follows:

\[
\Delta N = \rho_c(E_2)\Delta E_2 = \rho_v(E_1)\Delta E_1 \quad \Rightarrow \quad \rho_r(E_{21})\Delta E_{21} = \rho_r(E_{21})(\Delta E_2 + \Delta E_1) \quad \rightarrow \quad \rho_r(E_{21}) = \frac{\Delta N}{\Delta E_{21}} = \frac{\Delta N}{\hbar \Delta \omega_{21}}
\]

\[
\Delta E_2 = \frac{\rho_r}{\rho_c(E_2)}\Delta E_{21} \quad \text{und} \quad \Delta E_1 = \frac{\rho_r}{\rho_v(E_1)}\Delta E_{21} \quad \rightarrow
\]

\[
\Delta E_{21} = (\Delta E_2 + \Delta E_1) = \rho_r\left(\frac{1}{\rho_c(E_2)} + \frac{1}{\rho_v(E_1)}\right)\Delta E_{21}
\]

from the equality \( \rightarrow \)

\[
\rho_r(E_{21}) = \frac{\rho_c(E_2)\rho_v(E_1)}{\rho_c(E_2) + \rho_v(E_1)} = \rho_r(E_2, E_1) \quad \text{Reduced Density (Definition)}
\]

if \( \rho_v >> \rho_c \) then \( \rightarrow \rho_r(E_{21}) = \rho_c(E_2) \quad (\text{is the case for many III} - V - \text{SC})\)
we get with \( \rho_r(E) = \frac{\partial^3 N}{\partial \text{Vol} \partial E} \) for the Transition Rates \( R(E) = \frac{\partial^3 N}{\partial \text{Vol} \partial E \partial t} \) by generalizing to continuum (C:2) – continuum (V:1) transition with a monochromatic field \( W(E_{21}) = \frac{\partial^3 E}{\partial \text{Vol} \partial E} = \frac{eE_0^2}{2} \delta(E - (E_2 - E_1)) \):

\[
R_{21,abs}(E_{21}) = \frac{\pi e^2 E_0^2}{2\hbar^2} \left( u_{c,j} \left| X \left| u_{v,0} \right> \right. \right)^2 \rho_r(E_{21}) (1 - f_c(E_2)) f_v(E_1) = eE_0^2 B \rho_r(E_{21}) (1 - f_c(E_2)) f_v(E_1)
\]

\[
B = \pi e^2 \left/ \left( 2\hbar^2 \varepsilon \right) \right. \left( u_{c,j} \left| X \left| u_{v,0} \right> \right. \right)^2
\]

\[
R_{21,stim}(E_{21}) = eE_0^2 B \rho_r(E_{21}) (1 - f_v(E_1)) f_c(E_2)
\]

\[
R_{21,net}(E_{21}) = eE_0^2 B \rho_r(E_{21}) (f_c(E_2) - f_v(E_1))
\]

\[
\Delta R_{21,spont}(E_{21}) = A \rho_r(E_{21}) (1 - f_v(E_1)) f_c(E_2) \Delta E \quad \rightarrow \quad R_{spont} = \int dR_{21,spont} = \int A \rho_r(E_{21}) (1 - f_v(E_1)) f_c(E_2) dE
\]

with \( \omega = \frac{E_2 - E_1}{\hbar} \)

\( f_v, f_c \) are the Quasi- Fermi-functions at \( E_1 \) and \( E_2 \)

Remark:

if \( (E_2 - E_1) = E_{21} = \hbar \omega \) in a practical situation is specified, we get the corresponding k by solving a quadratic equation for \( E_{21}(k) \).

From k we obtain \( E_2, E_1 \) and \( \rho_r(E_2, E_1) \) by using the corresponding dispersion relations of the C- and V-band.
Transform $E_0$ to photon density $s_{ph}$ of the monochromatic field:

Modern optoelectronic devices often operate with almost monochromatic fields compared to the energy width of the band-to-band transitions in SC. Therefore we use **discrete field-amplitudes** $E_0$ or photon densities.

Using $$ w = \varepsilon |E_0|^2 / 2 = s_{ph} \hbar \omega_{opt} $$

$$ R_{21,netto}(\omega_{opt}) = \frac{1}{2} \varepsilon |E_o|^2 B \rho_r (f_2 - f_1) = s_{ph} \hbar \omega_{opt} B \rho_r (f_2 - f_1) $$

$$ R_{21} = w B \rho_r f_2 (1 - f_1) = \frac{1}{2} \varepsilon |E_o|^2 B \rho_r f_2 (1 - f_1) = s_{ph} \hbar \omega B \rho_r f_2 (1 - f_1) $$

$$ R_{12} = w B \rho_r f_1 (1 - f_2) = \frac{1}{2} \varepsilon |E_o|^2 B \rho_r f_1 (1 - f_2) = s_{ph} \hbar \omega B \rho_r f_1 (1 - f_2) $$

5.7.4 Optical Amplification and Attenuation in ideal SCs

Goals:
Combining the transition pair density $\rho_r$ and the Fermi-functions $f$ for the occupation probability of the energy-levels we can in principle calculate all transition rates $R$ (at least numerically) and their frequency dependence, determined mainly by $\rho_r(\omega)$ and $f(E_F,\omega)$:

- Emissions-/Absorption rates $R_{21,\text{net}}(\omega)$, $R_{21}(\omega)$, $R_{12}(\omega)$ and $R_{21,\text{spont}}(\omega)$ versus $\omega$ resp. $\lambda$, $E_{21}$ (rates per unit volume at the optical energy $\hbar \omega_{21}$ or wavelength $\lambda_{21}$) as a function of
  1) the Quasi-Fermi-Levels $E_{FQc}$ and $E_{FQv}$ or
  2) the carrier densities $n$ and $p$ (to combine with the carrier rate equation !) because $n=n(E_{FQc})$ and $p=p(E_{FQv})$

- Amplification $g(\omega)$ versus carrier density $n$ or finally as a function of pump current: $g(\omega,n)$, resp. $g(\omega,I)$

- Wavelength $\lambda_{\text{max}}(n)$ and value of the maximal optical gain $g_{\text{max}}(n, \lambda_{\text{max}})$

These rates will be fundamental for the design of the characteristics of diode lasers and optical amplifiers in chap.6.

5.7.4.1 Gain spectrum $g(\omega,E_{QF,n}, E_{QF,p}) ; g(\omega,n=p)$

Procedure:
For the computation of the frequency dependence of $g(\omega,n=p)$, $g(\omega,E_{QF,n}, E_{QF,p})$ the transition rates $R_{21,\text{net}}(E=\hbar \omega)$, $R_{12}(E)$, $R_{21}(E)$, $R_{\text{spont}}(E)$, $R_{21,\text{spont}}$ are evaluated at
a) given optical energy $E=\hbar \omega$, resp. a wavelength $\lambda$ and

b) given quasi-Fermi-level $E_{FQ,n}$, $E_{FQ,p}$, resp. carrier density $n(E_{FQ,n})=p(E_{FQ,p})$ assuming carrier neutrality $E_{FQ,n}$, $E_{FQ,p}$ are not independent because of the charge neutrality $n=p$ condition (pumped undoped SC)!
Relation between optical amplification $g(\omega, n)$ and netto-rate of stimulated emission $R_{21, \text{netto}}(\omega, n)$:

From $R_{21, \text{netto}}(\omega, n)$ we obtain immediately the important spectral gain function $g(\omega, n)$ often used in device design.

Assuming given quasi-Fermi-energies $E_{FQc}$, $E_{FQv}$ (with the restriction $n=p$) and using the fundamental relation between the gain $g(\omega, E_{FQc}, E_{FQv})$ and $R_{21, \text{netto}}$

$$g(\omega) = \frac{1}{s_{ph}} \frac{\partial s_{ph}}{\partial x} = \frac{1}{v_{gr}s_{ph}} \frac{\partial s_{ph}}{\partial t} = \frac{1}{v_{gr}s_{ph}} R_{21, \text{netto}} = \frac{1}{v_{gr}s_{ph}} (R_{21} - R_{12}) = g(\omega) \quad \to$$

$$g(\omega, E_{FQc}, E_{FQv}) = \frac{s_{ph}h\nu}{v_{gr}s_{ph}} \left( B \rho_r(E_{21}) \left[ f_c(E_{2}, E_{FQ,c}) \left( 1 - f_v(E_1, E_{FQ,v}) \right) \right] - B \rho_r(E_{21}) \left[ f_v(E_1, E_{FQ,v}) \left( 1 - f_c(E_{2}, E_{FQ,c}) \right) \right] \right)$$

$$= \frac{h\nu}{v_{gr}} \left( B \rho_r(E_{21}) \left[ f_c(E_{2}) - f_v(E_{1}) \right] \right)$$

with $B(E_{21}) = \frac{\pi e^2}{2\hbar^2 \epsilon_0} \left| u_c \right| \left| u_v \right|^2$, $\rho_r(E_{21})$, $\hbar \omega = E_{21} = (E_2 - E_1)$ and the relation between $E$ and $E_2, E_1$ we express $g(\omega)$ as $\to$

$$g(\omega) = g_{\text{max}}(E_{21}) \underbrace{\left[ f_c(E_{2}) - f_v(E_{1}) \right]}_{>0} \quad ; \quad g_{\text{max}}(E_{21}) = \frac{\hbar \omega}{v_{gr}} B \rho_r(E_{21})$$

$\left[ f_c(E_{2}) - f_v(E_{1}) \right]$ defines pumping condition and “parabolic or bell-shaped” frequency dependence of $g(\omega)$

For the numerical evaluation of $g(\omega)$ the energies $E_1(\omega)$, resp. $E_2(\omega)$, assuming k-conservation, are determined first followed by the computation of $f(E_2)$ and $f(E_1)$ using the charge neutrality $n=p$. 
From the functional dependence of $g(\omega, n)$ some basic conclusions about the gain-spectrum can be drawn:

**Condition for amplification in SC (Bernard-Duraffourgh condition)**

**a) SC in thermal equilibrium (no population inversion)**

In thermal equilibrium in undoped SC the Fermi level is approx. in the middle of the bandgap: $E_{FQ,c} = E_{FQ,v} = E_F \approx (E_c + E_v)/2$ therefore $f_c(E_2) < f_v(E_1)$ (few electrons in the C-band)

As a result $g$ is negative and the SC is for all frequencies absorbing (attenuating), so stimulated absorption is the dominating rate.

$$g(\omega) = g_{max}(\omega) \left[ f_c(E_2) - f_v(E_1) \right] \sim -g_{max}(\omega) f_v(E_1)$$

with $$g_{max}(\omega) \approx \frac{\pi e^2}{2 \hbar} \frac{2\omega}{E} \left\langle u_c^* \right| x \left| u_v \right\rangle^2 \rho_r(E_{21})$$

Remark: here $\rho_r$ is the density per energy interval!

for $\omega \approx E_g/\hbar$ (Absorption at the Bandedge)

In general we can estimate $g(\omega)$ by considering:

- for the term $[f_c(E_{c,2}) - f_v(E_{v,1})]$ we have the following inequality: $-1 < [f_c(E_{c,2}) - f_v(E_{v,1})] < 1$

- the dependence of $g_{max}(\omega)$ is dominated by $\rho_r(E) \approx \rho_c(E) = 4\pi \left( 2m_{eff,c} / \hbar^2 \right)^{3/2} \sqrt{E - E_g}$, if $\rho_c << \rho_v$ as is the case for many III-V-SC

then $$g_{max}(\hbar \omega) \approx \sqrt{(E_{21} - E_g)/\hbar}$$

max. absorption for parabolic bands (assuming that the matrix element is only weakly dependent on the transition energy $E_{21}$)

- Optical amplification is only possible if $f_c(E_2) > f_v(E_1)$, that means $[f_c(E_2) - f_v(E_1)] > 1$

**⇒ POPULATION-INVERSION**
b) Properties of the spectral dependence of optical gain $g(\omega)$ and absorption $\alpha(\omega)$:

For simplicity we assume $T=0$.

1) Intrinsic SC at $T=0$ and in thermal equilibrium: $n=n_i$, $p=n_i$  (no gain-situation)

\[ E_{FQ,c} = E_{FQ,v} = E_F \simeq E_i \]

\[ g(\omega) = g_{\text{max}}(\omega) \left[ f_c(E_2) - f_v(E_1) \right] = g_{\text{max}}(\omega) \left[ 0 - 1 \right] = -g_{\text{max}}(\omega) < 0 \quad (\sim \sqrt{E - E_g}) \]

\[ \Rightarrow \text{the semiconductor absorbs at all frequencies } \hbar \omega > E_g \]

\[ \Rightarrow \text{Absorption becomes stronger for shorter wavelengths.} \]

\[ \Rightarrow \text{Above the bandgap wavelength the material becomes transparent.} \]
2) Intrinsic SC at $T=0$ and in thermal non-equilibrium (Inversion) $n>n_i$, $p>p_i$ but $n=p$ (quasi-neutrality)

Assumption: $E_{FQ,c} > E_c$, $E_{FQ,v} < E_V$ \ $\rightarrow$ $E_{FQ,c} - E_{FQ,v} > E_g$ (degenerated SC)

\[ g(\omega) = g_{\text{max}}(\omega) [f_c(E_2) - f_v(E_1)] \]

\[ g(\omega) = g_{\text{max}}(\omega) \quad [+1] = g_{\text{max}}(\omega) \quad \text{for} \quad E_g < E_{21} < E_{FQ,c} - E_{FQ,v} \quad \text{range of amplification} \]

\[ g(\omega) = g_{\text{max}}(\omega) \quad [-1] = -g_{\text{max}}(\omega) \quad \text{for} \quad E_{21} > E_{FQ,c} - E_{FQ,v} \quad \text{range of absorption} \]

Quasi-Neutrality: $n=p$

⇒ the SC amplifies in the frequency range $E_g < h\omega < E_{FQ,c} - E_{FQ,v}$

In the frequency range $h\omega > E_{FQ,c} - E_{FQ,v}$, the SC is absorbing.

⇒ Condition for amplification in SC by Bernard-Duraffourgh

the condition $E_g < h\omega < E_{FQ,c} - E_{FQ,v}$ is called the amplification-condition of Bernard-Duraffourgh.
3) Intrinsic SC at $T > 0$ and thermal non-equilibrium (population inversion):

For $T \neq 0$ the expression for $g(\omega, n)$ is “smeared out” due to the continuous distribution of the Fermi-function at $E_{\text{QF}}$.

The following figure gives a qualitative picture of the role of the factor $[f_c(E_2) - f_v(E_1)]$ in the expression for $g(\omega) = g_{\text{max}}(\omega)[f_c(E_2) - f_v(E_1)]$.

**Thermal broadening of $g(\omega)$: graphical construction of the spectral dependence of the gain $g(\omega)$**

Band-filling and thermal broadening:

The spectral width $\Delta \omega$ of $g(\omega, n)$ is determined by:

- **Filling of the bands** by the carrier density $n$
- **Temperature dependence** of the Fermi-function

The higher the carrier density $n$ or the higher the temperature $T$

- the broader the positive gain-spectrum
- the smaller the peak gain

transparent \ I \ gain \ I \ losses/absorption
If the quasi-Fermi-levels are assumed to be known under the constraint of charge neutrality n=p, then the electron density n in the conduction band can be determined and we will calculate the gain g(\(\omega, n\)) vers. carrier density n.

This dependence is essential for device design and combining g with the rate-equations.

**Numerical example of gain spectra** \(g(\lambda, n)\) for GaAs and InGaAs at different carrier densities n=p:

Parameter: carrier density (electron density /10^{18} \text{cm}^3)

\(\Delta \lambda \sim 0.1 \lambda\)

**Remark on densities of states and quasi-Fermi-levels:**
For the self-consistent calculation of \(g(\omega,n)\) we have to eliminate the quasi-Fermi-levels \(E_{\text{FQC}}(n), E_{\text{FQV}}(p)\).

As \(E_{\text{FQC}}, E_{\text{FQV}}\) determine n and p and together with the boundary condition of quasi-neutrality in the SC n=p, the elimination can be carried out numerically as no analytical inverse Fermi-function \(F_{1/2}^{-1}\) exists.

\[
n = \int_{E_{\text{C,top}}}^{E_{\text{C,bottom}}} \rho_n(E) f_n(E) dE = N_{C,\text{eff}} F_{1/2} \left( \left( E_{\text{FQn}} - E_C \right) / kT \right)
\]

\[
p = \int_{E_{\text{V,bottom}}}^{E_{\text{V,top}}} \rho_p(E) f_p(E) dE = N_{V,\text{eff}} F_{1/2} \left( \left( E_V - E_{\text{FQV}} \right) / kT \right)
\]

\[
n(E_{\text{Q,F,C}}) = N_{C,\text{eff}} F_{1/2} \left( \left[ E_{\text{Q,F,C}} - E_C \right] / kT \right)
\]

and with the inverse function \(E_{\text{Q,F,C}} - E_C = F_{1/2}^{-1}(n/N_{C,\text{eff}})\)

\[
p(E_{\text{Q,F,V}}) = N_{V,\text{eff}} F_{1/2} \left( \left[ E_V - E_{\text{Q,F,V}} \right] / kT \right)
\]

and with the inverse function \(E_{\text{Q,F,V}} + E_V = F_{1/2}^{-1}(p/N_{V,\text{eff}})\)

To achieve substantial gain in SC the “transparency” carrier density \(n_{tr}\) must be in the range of \(3-4 \times 10^{18} \text{ cm}^{-3}\)
5.7.4.2 Spontaneous Emission versus carrier density \( n \) and wavelength \( \lambda \)

**a) incremental spontaneous emissions rate** \( R_{21,\text{spont}} \) into all modes

In the analysis of the thermal equilibrium with the blackbody radiation, we considered the radiation equilibrium with all modes of the blackbody-radiation.

⇒ so the Einstein-coefficient \( A \) for discrete energy states describes the spontaneous emission rate into all modes.

The incremental spontaneous emission rate \( \Delta R_{21,\text{spont}}(\omega) \) for a frequency \( \omega \), resp. energy \( E = \hbar \omega \) can be calculated from

\[
A(\omega) = B \left( \frac{\hbar \omega^3}{\pi^2 c^2} \right)
\]

Einstein-Relation.

• the spontaneous emission rate results from downward-transitions and has to be weighted by the level-occupancy (Fermi-functions \( f_c \) and \( f_v \):

\[
\Delta R_{21,\text{spont}}(\hbar \omega) = A \rho_r(\hbar \omega) \left[ f_c(E_{c,2})(1 - f_v(E_{v,1})) \right] \Delta E = B \left( \frac{\hbar \omega^3}{\pi^2 c^2} \right) \rho_r(\hbar \omega) \left[ f_c(E_{c,2})(1 - f_v(E_{v,1})) \right] \Delta E
\]

**Spontaneous Emission in \( \Delta E \)**

**b) Total spontaneous emission rate** \( R_{\text{spont}} \) into all possible spatial and frequency modes:

- The total spontaneous emission is generated isotropic in all directions by all transition pairs distributed over the whole energy range \( \Delta E = \hbar \Delta \omega_{\text{spont}} \). For the total spontaneous emission rate \( R_{\text{spont}} \) we have to integrate over all filled states in the bands resp. to the carrier density \( n \) under assumption f charge neutrality \( n = p \).

The total spontaneous emission rate \( R_{\text{spont}} \) enters the carrier rate-equation for \( n \) and \( p \).

- \( R_{\text{spont}} \) is emitted into all modes keeping in mind that \( R_{\text{spont}} >> R_{21,\text{spont} \text{,mode}} \).

\[
R_{\text{spont}} = \int_0^\infty A(\omega) \rho_r(\omega) \left[ f_c(E_{c,2})(1 - f_v(E_{v,1})) \right] d\omega = \frac{1}{\gamma} R_{21,\text{spont,mode}}
\]

**DEFINITION of \( \gamma \)**
For lasers also need the fraction $\gamma, \beta$ of spontaneous emission into a single mode $R_{21,\text{spont}, \text{mode}}$:

**Definition of the spontaneous emissions factor $\gamma = \beta$:**

$$
\gamma = 1/ \int_{\Delta \omega_{\text{spont}}} \rho_{\text{mode}}(\omega)V_{\text{spont}} \, d\omega \approx 1/(V_{\text{spont}}\rho_{\text{mode}}(\omega)\Delta \omega_{\text{spont}})
$$

$\rho_{\text{mode}} = \text{mode density of free space}$

If $A$ and $B$ are approximately frequency independent, we can use for simplicity the following

**life-time approximation** for $R_{\text{spont}}$:

$$
R_{\text{spont}} = A \int_0^\infty \rho_r(\hbar \omega) \left[ f_c(E_{c,2})(1-f_v(E_{v,1})) \right] d\omega \approx \frac{n}{\tau_{\text{spont}}} \quad \rightarrow \quad \tau_{\text{spont}} = n / \int_0^\infty A \rho_r(\hbar \omega) \left[ f_c(E_{c,2})(1-f_v(E_{v,1})) \right] \approx 1/n \quad \text{(not constant!)}
$$

$$
R_{\text{spont}} = n / \tau_{\text{spont}} \approx B_{\text{BM}} n^2 \quad \text{(Bimolecular Recombination)}
$$

**Numerical calculation** of $R_{\text{spont}}(n)$ confirms a square-law dependence $\sim n^2$ ($\sim n^3$) of the carrier density $n$ (Bimolecular Recombination).

- the spectral width $\Delta \omega_{\text{spont}}$ of the spontaneous emission $R_{21,\text{spont}}(\omega)$ is in general larger than the width $\Delta \omega_{\text{stim}}$ of stimulated emission $R_{\text{stim}}(\omega)$

- for mathematical simplicity spontaneous emission rates are often approximated by a constant carrier lifetime $\tau_{\text{spont, tot}}$. 

---

**Numerical Simulation of Gain- and spontaneous emission-spectra for GaAs:**

![Graph showing gain and spontaneous emission spectra for GaAs with photon energy plotted against intensity in arbitrary units.](image)
5.7.4.3 Numerical simulations of optical gain-spectra $g(\omega,n)$:

The numerical simulation of $g(\omega,n)$ using the appropriate material parameters gives for the practically important SC like InP ($\lambda=1.3\,\mu m$ und $1.5\,\mu m$) und GaAs ($\lambda=0.85\,\mu m$) demonstrated the following generic properties:

Amplification and absorption spectrum $g(\omega,n)$ for GaAs: (Simulation)

With increasing carrier density $n$ the bands are filled with carriers to higher energy levels resulting in

1) Increase of maximum gain
2) decrease of the wavelength of the maximum gain
3) increase of the width of the gain-spectrum

Parabolic spectral approximation of $g(\omega,n)$:

$$g(\omega,n) \approx g_{\text{max}}(n) \frac{I}{1 + \left(\frac{\omega - \omega_{\text{max}}(n)}{\Delta \omega(n)}\right)^2},$$

$\omega_{\text{max}}(n)$ is the peak gain and $\Delta \omega(n)$ is the linewidth.

Gain-Spectrum vers. carrier density $n$

Maximum Gain $g_{\text{max}}(n)$ vers. carrier density $n$:
Linear Gain dependence for bulk semiconductors:

Simulation shows that the maximum gain $g_{\text{max}}$ is approximately linear dependent on the carrier density $n > n_{tr}$.

\[ g_{\text{max}}(\omega_{\text{max}}, n) \approx a(n - n_{tr}) \]

**Linear approximation of max. gain in function of n**

**Definition:** $n_{tr}$ = Transparency-carrier density ($g_{\text{max}}(\omega_{\text{max}}, n_{tr}) = 0$) and $a$ = differential gain $a(n) = \partial g_{\text{max}} / \partial n$

- at $n=0$ the material is absorbing with $f_1 \approx 1$ and $f_2 \approx 0$, $g(0) \approx -g_{\text{max}}(\omega)$
- at $n=n_{tr}$ (transparency density) the material is transparent, $g(n_{tr})=0$
- at $n>n_{tr}$ the material is amplifying with $f_1 \approx 0$ and $f_2 \approx 1$, $g(n) \approx +g_{\text{max}}(\omega)$

Nonlinear gain-carrier density relation for Quantum Wells (QW) in SCs:

$g_{\text{max}}(n)$ relations show in general the nonlinear behavior (logarithmic for QWs) of the figure below and a parabolic frequency dependence:

\[ g_{\text{max}}(\omega_{\text{max}}, n) \approx g_0 \ln(n/n_{tr}) \]

**Parabolic approximation of the spectral dependence of $g(\omega,n)$:**

\[ g(\omega,n) = g_{\text{max}}(\omega_{\text{max}}, n) \left/ \left( 1 + \left( \frac{\omega - \omega_{\text{max}}}{\Delta \omega} \right)^2 \right) \right. = a(n - n_{tr}) \left/ \left( 1 + \left( \frac{\omega - \omega_{\text{max}}}{\Delta \omega} \right)^2 \right) \right. \]

Valid approximation because often only the gain close to the maximum is relevant!
Temperature dependence of the optical gain $g(\omega, n, T)$ in SC:

Thermal gain broadening and gain reduction

Because of the temperature $T$ dependence of the Fermi-functions and subsequent broadening of the carrier distribution:

- the spectral width $\Delta \omega$ of $g(\omega, n)$ increases with increasing temperature
- the maximum gain $g_{\text{max}}(\omega_{\text{max}}, n)$ decreases with increasing temperature

(RT-operation of diode lasers was a challenge)

The broadening and reduction of the optical gain with temperature has a very detrimental effect on devices such as diode lasers and amplifiers. It is also responsible for the high temperature sensitivity of these devices.
5.7.4.4 Rate equation for electrons and photons, electrical pumping

**Concept of carrier rate equations in SCs:**

Rate equations are *continuity equations for particle* (electrons, n, holes, p, and photons s\(_{ph}\)) *currents* flowing in and out of a particle reservoir (energy bands: energy states / volume, optical resonator for photons) per unit volume.

- Because each optical transition results in the generation or annihilation of a *electron-hole pair* in the conduction- and valence band, we formulate the continuity or rate equation for the carrier densities n and p.

We postulate that there is an external *pump mechanism* (eg. carrier injection in pn-junctions) available, which pumps electrons from the valence band up to the conduction band with a rate \( R_{pump} \):

\[
R_{pump} = \frac{\partial n_{pump}}{\partial t}.
\]

The continuity equation for n and p becomes for charge neutrality n=p:

\[
\frac{\partial}{\partial t} n = \frac{\partial}{\partial t} p = + R_{pump} - g(\omega, n) v_{gr} s_{ph} - R_{spont}(n) = - \frac{\partial}{\partial t} p
\]

_**Carrier (electron)-Rate equation** (assuming \( V_{active} = V_{mode} \))

\( R_{spont} = \) Rate of the total spont. emission in all modes in Vol\(_{spont} \) ; \( R_{21,spont,mode} = \) Rate of spont. emission in a single lasing mode

The stimulated emission \( R_{21,net} \) can be related to the gain \( g(w,n) \):

\[
R_{21,net}(\omega,n,s_{ph}) = g(\omega,n) v_{gr} s_{ph}
\]

**Photon-Rate-Equation:**

Because each optical transition *creates* (stimulated or spontaneous emission) or *destroys* (absorption) one photon in the optical field (mode) we formulate the continuity equation for the photon density s\(_{ph}\):

\[
\frac{\partial}{\partial t} s_{ph} = + R_{21,net} + R_{21,spont,mode} = + \Gamma g(\omega,n) v_{gr} s_{ph} + \beta \Gamma R_{spont}
\]

_**Photon-Rate Equation for 1 optical mode**

\( \beta = \gamma \) is the spontaneous emission factor (\( \beta \ll 1 \))
Conclusions SC:

- At low electron densities \( n < n_{tr} \) the SC is absorbing for all frequencies \( \omega \) with \( \hbar \omega > E_g \). This means that the simulated absorption is dominating for \( g(\omega, n) < 0 \)
- At the carrier density \( n_{tr} \) (transparency density) \( g(\omega, n_{tr}) = 0 \) for a particular frequency \( \omega \). Stimulated emission almost equals absorption – therefore the SC is transparent at \( \omega \).
- At carrier densities \( n > n_{tr} \) there is optical gain \( g(\omega, n) > 0 \) over a limited optical frequency range \( \sim (E_{QF,n} - E_{QF,n}) > \hbar \omega > E_g \).
  The optical bandwidth increases with increasing \( n \). The stimulated emission dominates.
- The frequency \( \omega_{max} \), where \( g(\omega) \) reaches a maximum \( g_{max}(\omega_{max}, n) \), increases with increasing \( n \) (filling the conduction- and valence band from the bottom)
- For bulk-SC \( g_{max}(\omega_{max}, n) \) increases approximately linear with \( (n - n_{tr}) \), for Quantum-Wells \( ~\ln(n - n_{tr}) \)
Conclusions:

- For the description of the interaction of the optical field with the quantized medium near resonance (amplification) needs an quantum-mechanical treatment

- The influence of the material properties on the dynamic of the dipole is described quantum-mechanically by the dipole-matrix-element

- Population inversion creates a non-classical net dipole with an out-of-phase component in anti-phase to the exciting field and which delivers energy to the field

- Populations-Inversion in quantized media allow a) optical amplification and b) generation of coherent optical wave

- The energy conservation in the interaction of optical field – carrier population can be described by rate equations for charge carriers and photons.

- The polarization and the e-h-pair generation can be described by the susceptibility and the transition probability, resp. by the quantum-mechanical transition rate of the carriers

- QM shows that the “electron-on-springs”-model is an adequate description for loss-less media

- Without the quantization of the optical field (photons) the spontaneous emission can not be calculated from first principles – it remains just a thermodynamic necessity for equilibrium
5.8 Population inversion by electrical pumping of pn-diodes
(optional, see Coldren)

To satisfy the condition of Bernard-Duraffourgh in SC a carrier pump mechanism is required for achieving population inversion between electrons and holes \( n > n_i \).

A simple, fast and efficient realization of electrical pumping is carrier injection through the depletion layer of a forward biased pn-diode or into the I-layer of a PIN-diode.

A key benefit electrical current pumping of a pn-diode is current modulation of the light generation up to high frequencies and with high efficiency.

5.8.1 Carrier injection and population inversion in homojunction pn-diodes

Considering a strongly forward biased GaAs-pn-diode with \( V_D \approx E_g/e \):

- electrons from the n-area (majority carriers in \( n^+ \)) are injected as minority carriers through the depletion layer into the p-area
- in the p-area the injected electrons diffuse for a distance of a diffusion length \( L_{D,n} \) (~2-3 \( \mu \)m) before they have mostly recombined by spontaneous emission and reach the electron equilibrium value \( n_{o,p} \) of the p-area.

- Within a diffusion length \( L_D \) in the p-area adjacent to the depletion layer we have \( n_p(x) >> n_{o,p} \). There is a local carrier non-equilibrium (\( np >> n_i^2 \)).

- Because the electrons in the conduction band and the holes in the valence band are not in equilibrium, the distribution of electrons and holes is described by 2 separate Quasi-Fermi-distributions characterized by 2 different Quasi-Fermi-levels \( E_{FQ,n} \) and \( E_{FQ,p} \).

\[
E_{FQ,n} - E_{FQ,p} \approx eV_D
\]

Same arguments hold for hole-injection from the p-area into the n-region.
The external diode voltage $V_D$ separates the quasi-Fermi-levels in the depletion-layer

**Carrier injection in forward biased pn-diodes:**

- **Equilibrium** $V_D=0$ \[ E_F = E_{FQn} = E_{FQv} \]
- **Region of gain**
  - **High injection** $V_D \sim E_g/e$ (forward polarized) \[ E_{FQn} = E_{FQv} \sim eV_D \]
  - Area of non-equilibrium carrier injection

Considering the inversion condition by Bernard-Duraffourg, $V_D$ must fulfill:

\[ eV_D \approx E_{QF,n} - E_{QF,p} > E_2 - E_1 = \hbar \omega > E_g \]

- Under this condition the material on both sides of the depletion layer is **inverted** within about one **diffusion length** $L$ and can be **optically amplifying** $g>0$ resp. ($n>n_{tr}$).
As long as there is no strong light field, which is amplified by stimulated emission, the injected minority carriers recombine only by spontaneous emission with a carrier-lifetime $\tau_{\text{spont}}$ (approximation):

$$\frac{\partial n}{\partial t} \approx \frac{n}{\tau_{\text{spont}}} = R_{\text{spont}}$$

It is obvious that for a given diode current $I$ the diffusion length $L$ must be a minimum in order to achieve a minority carrier density $n$ (or $p$) or an optical gain $g(n,p)$ as high as possible.

For simple homojunction-pn-diodes the diffusion length $L_D$ is as a material parameter in the order of a few $\mu$m leading to very high current densities for population inversion ($\sim$ several $10\text{kA/cm}^2$), resp. for achieving a certain optical gain $g(n)$.

**Quasi-Neutrality Condition in SCs:**

We will saw that in the electrical pumping of SCs by carrier injection in pn-diodes:

- The application of a forward diode voltage determines the separation of the quasi-Fermi-levels $E_{QF,n}$ and $E_{QF,p}$
  
  $$eV_D = (E_{QF,c} - E_{QF,v})$$

- $V_D$ also causes a very strong carrier-injection and current flow through the diode

It is assumed that at the high carrier injection levels, the minority carrier density is comparable to the majority carrier density. The carrier density is so high, so that there can be 1) no internal E-field or as an equivalent statement 2) the active area must be electrically neutral requiring:

**Quasi-Neutrality Condition for undoped SC:**

$$n = p$$

With the help of this equation it is possible to determine the positions of the quasi-Fermi-levels for a given $V_D$. 
5.8.2 Materials properties of direct Semiconductors (optional)

The crystal structure and composition of compound SC determines the bandstructure and thus the optical and electronic properties. Thus the composition of binary, ternary, quaternary crystals is used to control:

1) Bandgap $E_g \rightarrow$ Emission-wavelength $\lambda_g$ (direct $\leftrightarrow$ indirect SC)
2) Bandgap $E_g$, Electron Affinity $\chi \rightarrow$ Heterostructure-barriers, $\Delta E_C$, $\Delta E_V$
3) Refractive index $n \rightarrow$ Waveguides

Al$_x$Ga$_{1-x}$As-compound crystal:
(group III-element: Ga, Al group V-element: As)

Refractive index $n$ of Al$_x$Ga$_{1-x}$As vers. Al-concentration:
The Al-concentration $x$ is used to control the refractive index of Al$_x$Ga$_{1-x}$As.
Because the lattice constant of Al$_x$Ga$_{1-x}$As does not change with composition $x$ the layers are automatically
$\rightarrow$ crystallographically lattice matched

InGaAs and InGaAsP are only for a precise composition lattice-matched to InP-substrates (difficult growth)!