

English Summary :

4. Quantum Statistics

4.1 Density matrix - statistical operator $\hat{\rho}$: $\langle \hat{M} \rangle = \text{tr}(\hat{\rho} \hat{M})$
(mixed state)

Von Neumann eq. $\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}]$

distrib. fct. of electrons $f_e(\underline{k}) = \langle a_{\underline{k}}^\dagger a_{\underline{k}} \rangle$
of holes $f_h(\underline{k}) = \langle d_{\underline{k}}^\dagger d_{\underline{k}} \rangle$

makroskop. Polarisation $\underline{P}(\underline{r}, t) = \langle \hat{\underline{P}} \rangle = \langle e \hat{\psi}^\dagger(\underline{r}, t) \underline{r} \hat{\psi}(\underline{r}, t) \rangle$

• Blochdarstellung $\hat{\psi}(\underline{r}, t) = \sum_{\underline{n}, \underline{k}} a_{\underline{n}, \underline{k}} \psi_{\underline{n}, \underline{k}}(\underline{r})$
↳ Blochfkt. $e^{i \underline{k} \cdot \underline{r}}$ $u_{\underline{n}, \underline{k}}(\underline{r})$

$$\hat{\underline{P}}(\underline{r}, t) = \sum_{\substack{\underline{n}, \underline{k} \\ \underline{n}', \underline{k}'}} a_{\underline{n}, \underline{k}}^\dagger a_{\underline{n}', \underline{k}'} \psi_{\underline{n}, \underline{k}}^\dagger(\underline{r}) \underline{r} \psi_{\underline{n}', \underline{k}'}(\underline{r})$$

• Fouriertrafo $\hat{\underline{P}}(\underline{q}, t) = \int d^3r \hat{\underline{P}}(\underline{r}, t) e^{-i \underline{q} \cdot \underline{r}}$

- Def.: el. Dipolmatrixelement $\underline{\mu}_{\underline{n}, \underline{n}'}(\underline{k}) = \frac{1}{V} \int d^3r u_{\underline{n}, \underline{k}}(\underline{r}) \underline{r} u_{\underline{n}', \underline{k}'}(\underline{r})$
(oft auch mit $d_{\underline{n}, \underline{n}'}$ bezeichnet, $e < 0$) *ähnlich*
- Näherung: schwache \underline{k} -Abhängigkeit der Blochfkt. $u_{\underline{n}, \underline{k}}$

längere Rechnung $\Rightarrow \underline{P}(\underline{q}, t) = -\sum_{\underline{n}, \underline{n}'} \underline{\mu}_{\underline{n}, \underline{n}'}(\underline{k}) \langle a_{\underline{n}, \underline{k}}^\dagger a_{\underline{n}', \underline{k}+\underline{q}} \rangle$

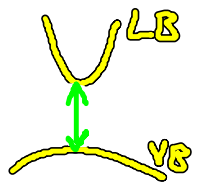
Näherung für opt. Grenzfall :

- (1) $q \approx 0$ (Impuls der Photonen klein gegen)
Quasiimpuls der Elektronen



(2) Bandkantenoptik $\hbar \omega \approx E_g$ (Bandlücke)

\Rightarrow nur Interbandübergänge (LB \leftrightarrow VB)



(3) 2-Band-Modell: $n = L, V$ und $\underline{\mu}_{LV}(\underline{k}) \approx \underline{\mu}_{LV}(0)$
konstantes Dipolmatrixel.

Elektron-Loch-Bild :

Interbandpolarisation (makr.)

$$\underline{P}^{\text{inter}}(\underline{q}, t) \approx \underline{P}(0, t) \equiv \underline{P}(t) = \sum_{\underline{k}} \underline{\mu} \left(\langle d_{\underline{k}} a_{\underline{k}} \rangle + \langle a_{\underline{k}}^{\dagger} d_{\underline{k}}^{\dagger} \rangle \right)$$

\downarrow
 $P(\underline{k}, t)$

em.

\downarrow
 $P^*(\underline{k}, t)$

ab.

mikroskop. Interbandpolarisation

eines Zustandes \underline{k} :

$$P(\underline{k}, t) = \langle d_{\underline{k}} a_{\underline{k}} \rangle$$

$$P^*(\underline{k}, t) = \langle a_{\underline{k}}^{\dagger} d_{\underline{k}}^{\dagger} \rangle$$

4.2.2 Elektron-Feld-WW-Op.

$$\hat{H}_{\text{opt}} = - \int d^3r \varphi^{\dagger}(\underline{r}, t) e_{\underline{r}} \underline{E}(\underline{r}, t) \varphi(\underline{r}, t)$$

Fouriertrafo $\underline{E}(\underline{r}, t) = \frac{1}{V} \sum_{\underline{q}} e^{i\underline{q} \cdot \underline{r}} \underline{E}(\underline{q}, t)$

$$\Rightarrow \hat{H}_{\text{opt}} = \frac{1}{V} \sum_{\substack{\underline{k}, \underline{q} \\ n, n'}} \underline{E}(\underline{q}, t) a_{n, \underline{k}}^{\dagger} a_{n', \underline{k}+\underline{q}} \mu_{nn'}(\underline{k})$$

Bandkantenoptik wie in 4.2.1 :

$$\hat{H}_{\text{opt}} = \sum_{\underline{k}} \underline{\mu} \cdot \underline{E}(t) (a_{\underline{k}}^{\dagger} d_{\underline{k}}^{\dagger} + d_{\underline{k}} a_{\underline{k}})$$

4.3 Halbleiter - Blochgleichungen

- Zeitentwicklung folgender Größen :

Verteilungsfkt. $f_e(\underline{k}, t) = \langle a_{\underline{k}}^{\dagger} a_{\underline{k}} \rangle$

$f_h(\underline{k}, t) = \langle d_{\underline{k}}^{\dagger} d_{\underline{k}} \rangle$

mikr. Polarisation $P(\underline{k}, t) = \langle d_{\underline{k}} a_{\underline{k}} \rangle$

$P^*(\underline{k}, t) = \langle a_{\underline{k}}^{\dagger} d_{\underline{k}}^{\dagger} \rangle$

- Ansatz : Bewegungsgl. für Erwartungswerte (Fundamentalrelation der Quantentheorie)

$$\frac{d}{dt} \langle \hat{F} \rangle = \left\langle \frac{i}{\hbar} [\hat{H}, \hat{F}] + \frac{\partial \hat{F}}{\partial t} \right\rangle \quad (\text{Bildmethode.})$$

Berechne Kommutatoren ① $[\hat{H}, a_k^\dagger a_k]$

② $[\hat{H}, a_k^\dagger a_k^\dagger]$

Ham.op. $\hat{H} = \hat{H}_0 + \hat{H}_{e-e} + \hat{H}_{ii} + \hat{H}_{e-ph} + \hat{H}_{opt}$

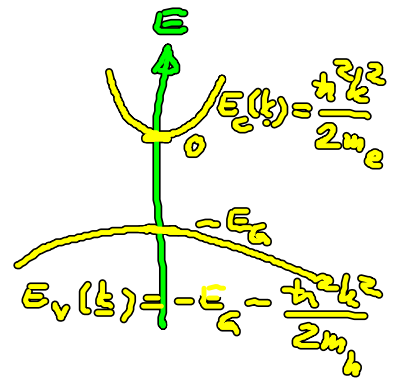
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 $\S 3.6.1 \quad \S 3.6.2 \quad \S 3.7.2 \quad \S 4.2.2$

1. Fall: Vernachlässigung der WW $\hat{H}_{e-e}, \hat{H}_{ii}, \hat{H}_{e-ph}$

$$\hat{H} = \hat{H}_0 + \hat{H}_{opt}$$

Elektron-Loch-Bild:

$$\hat{H}_0 = \sum_{\mathbf{k}} E_c(\mathbf{k}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} - \sum_{\mathbf{k}} E_v(\mathbf{k}) d_{\mathbf{k}}^\dagger d_{\mathbf{k}}$$



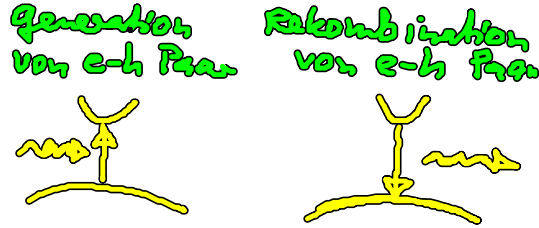
Bezüge zum Kommutator ①:

$$\begin{aligned}
 [\hat{H}_0, a_1^\dagger a_2] &= \sum_{\mathbf{k}} \left[E_c(\mathbf{k}) (a_{\mathbf{k}}^\dagger a_{\mathbf{k}} a_1^\dagger a_2 - a_1^\dagger a_2 a_{\mathbf{k}}^\dagger a_{\mathbf{k}}) \right] - \sum_{\mathbf{k}} E_v(\mathbf{k}) (\dots) \\
 &= \sum_{\mathbf{k}} \left[E_c(\mathbf{k}) (-\cancel{a_{\mathbf{k}}^\dagger a_{\mathbf{k}} a_1^\dagger a_2} + \cancel{a_1^\dagger a_2 a_{\mathbf{k}}^\dagger a_{\mathbf{k}}}) \right. \\
 &\quad \left. + \delta_{\mathbf{k}1} a_1^\dagger a_2 - \delta_{\mathbf{k}2} a_1^\dagger a_2 \right] - \sum_{\mathbf{k}} E_v(\mathbf{k}) (\dots) \\
 &= 0
 \end{aligned}$$

d.h. \hat{H}_0 liefert keine Zetahl. von f_e und f_h

$$\begin{aligned}
 [\hat{H}_{opt}, a_1^\dagger a_2] &= \sum_{\mathbf{k}} \left\{ \mu E \left[\cancel{a_{\mathbf{k}}^\dagger d_{\mathbf{k}} a_1^\dagger a_2} - \cancel{a_1^\dagger a_2 a_{\mathbf{k}}^\dagger d_{\mathbf{k}}} \right] + \cancel{(d_{\mathbf{k}} a_1^\dagger a_2 - a_1^\dagger a_2 d_{\mathbf{k}})} \right\} \\
 &= \sum_{\mathbf{k}} \left\{ \mu E \left[(-\delta_{\mathbf{k}1} a_1^\dagger d_{\mathbf{k}}) + \delta_{\mathbf{k}2} d_{\mathbf{k}} a_2 \right] \right\} \\
 &= -\mu E \left(\underbrace{a_1^\dagger d_1^\dagger} - \underbrace{d_2 a_2} \right)
 \end{aligned}$$

4x Vertauschen



$$\Rightarrow \langle [\hat{H}_{opt}, a_e^+ a_e] \rangle = -\mu E (f_e^h(t) - f_e(t)) = \frac{\hbar}{i} \dot{f}_e$$

WV mit \hat{H}_{opt} führt zur Ankopplung an die Polarisation

② Dynamik der Polarisation

$$\frac{\partial}{\partial t} p_k(t) = \frac{i}{\hbar} \langle [H, d_k^+ a_k] \rangle$$

Beiträge zum Kommutator:

$$\begin{aligned}
 [\hat{H}_{opt}, d_e^+ a_e] &= \sum_k \mu E [(a_k^+ d_k^+ d_e a_e - d_e a_e^+ d_k^+) + (d_k d_k a_e - d_e a_e^+ d_k^+)] \\
 &= \sum_k \mu E [(a_k^+ a_e d_k^+ d_e - a_e^+ a_e d_k^+ d_e^+) + 0] \\
 &= \sum_k \mu E (a_k^+ a_e d_k^+ d_e + a_e^+ a_e d_k^+ d_e^+ - \cancel{\delta_{ek} d_k^+ d_e^+}) \\
 &= \sum_k \mu E (\cancel{a_k^+ a_e d_k^+ d_e} - \cancel{a_e^+ a_e d_k^+ d_e^+} + \delta_{ek} a_k^+ a_e - \delta_{ek} d_k^+ d_e^+) \\
 &= \sum_k \mu E (+\delta_{ek} a_k^+ a_e + \delta_{ek} d_k^+ d_e^+ - \delta_{ek} \delta_{ek}) \\
 &= \mu E (a_e^+ a_e + d_e^+ d_e - 1)
 \end{aligned}$$

$$\begin{aligned}
 \frac{\hbar}{i} \dot{p}(t) &= \langle [\hat{H}_{opt}, d_k^+ a_k] \rangle = \mu E (f_e(t) + f_h(t) - 1) \\
 &= -(1-f_e)(1-f_h) + f_e f_h \\
 &\quad \uparrow \text{Absorption} \quad \downarrow \text{Emission} \\
 &= \text{Inversion } f_e - (1-f_h)
 \end{aligned}$$

Polarisation getrieben durch klass. Lichtquelle

$$[\hat{H}_0, d_e^+ a_e] = \sum_k \{ E_c(t) (a_k^+ a_k d_e^+ a_e - d_e a_e^+ a_k^+ a_k) - E_v(t) (\dots) \}$$

$$= \sum_{\underline{k}} (-E_c(\underline{k}) \delta_{\underline{k}l} d_{\underline{k}} a_{\underline{k}} - (-1) E_v(\underline{k}) \delta_{\underline{k}l} d_{\underline{k}} a_{\underline{k}})$$

$$= - \underbrace{(E_c(\underline{k}) - E_v(\underline{k}))}_{\hbar \omega_p(\underline{k})} d_{\underline{k}} a_{\underline{k}}$$

$\hbar \omega_p(\underline{k})$ freie Osz. der komplexen Polarisation,
opt. Übergangsfrequenz $\omega_p(\underline{k}) = \frac{1}{\hbar} (E_c(\underline{k}) - E_v(\underline{k}))$

(i) Halbleiter- Bloch- gln. :

$$(1) \frac{\partial}{\partial t} f_c(\underline{k}, t) = \frac{1}{i} \Omega_p (p^*(\underline{k}, t) - p(\underline{k}, t))$$

$$(2) \frac{\partial}{\partial t} p(\underline{k}, t) = \frac{1}{i} \omega_p(\underline{k}) p(\underline{k}, t) + \frac{1}{i} \Omega_p \underbrace{(1 - f_c - f_v)}_{\text{- Inversion}}$$

$$(3) \frac{\partial}{\partial t} f_v(\underline{k}, t) = \frac{\partial}{\partial t} f_c(\underline{k}, t)$$

$$\text{Rabi-Frequenz } \Omega_p = \frac{\mu \cdot E}{\hbar}$$

Bem. : Kohärente Dynamik eines Ensembles unabh.
durch klass. Lichtquelle getriebene 2-Niveau-Systeme
(Opt. Bloch gln.)

Also : Ladungsträgergeneration als kohärenter 2-Stufen-Prozess
(e-h Paar)

