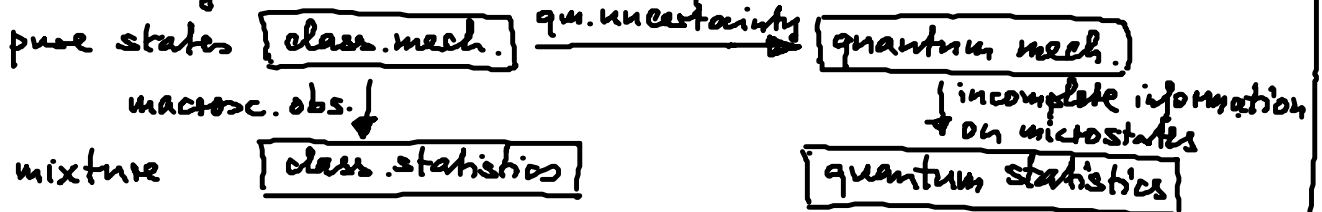


English Summary:

4. Quantum Statistics in Nonequilibrium

4.1 Density matrix - statistical operator



$$\text{statistical op. } \hat{\rho} = \sum_i p_i |\psi_i\rangle \langle \psi_i| = \sum_i p_i \hat{\rho}_{\psi_i} \approx \text{projector on pure states}$$

$$\langle \hat{M} \rangle = \text{tr}(\hat{\rho} \hat{M})$$

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

distribution fun. of electrons $f_e(k) = \langle a_k^\dagger a_k \rangle = \text{tr}(\hat{\rho} a_k^\dagger a_k)$

" " " holes $f_h(k) = \langle d_k^\dagger d_k \rangle$

4.2.1 Polarisation des Halbleiters

qm. Dipoldichte (vgl. klass. el. Dipolmomentdichte)

$$\underline{\hat{P}}(\underline{r}, t) = e \hat{\psi}^\dagger(\underline{r}, t) \underline{r} \hat{\psi}(\underline{r}, t) \quad \hat{\psi}^\dagger, \hat{\psi} \text{ sind Feldoperatoren}$$

$$\text{Erzeugungsup. } \hat{\psi}^\dagger(\underline{r}) := \sum_{\lambda} \psi_{\lambda}^*(\underline{r}) a_{\lambda}^{\dagger}$$

$$\text{Vernichtungsup. } \hat{\psi}(\underline{r}) := \sum_{\lambda} \psi_{\lambda}(\underline{r}) a_{\lambda}$$

$$\{\hat{\psi}(\underline{r}), \hat{\psi}^\dagger(\underline{r}')\} = \delta(\underline{r} - \underline{r}')$$

$$\text{Teilchendichtep. } \hat{n}(\underline{r}) = \hat{\psi}^\dagger(\underline{r}) \hat{\psi}(\underline{r})$$

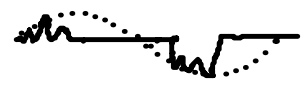
Def. makroskop. Polarisation \underline{P} als Erwartungswert des Dipoldichtep. $\underline{\hat{P}}$

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

nelle Größe

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

$$\hat{P}(\underline{r}, t) = \sum_{\substack{\underline{n}, \underline{k} \\ \underline{n}', \underline{k}'}} a_{\underline{n}, \underline{k}}^+ a_{\underline{n}', \underline{k}'} \psi_{\underline{n}, \underline{k}}^*(\underline{r}) e^{-i \underline{k} \cdot \underline{r}} \psi_{\underline{n}', \underline{k}'}(\underline{r})$$



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

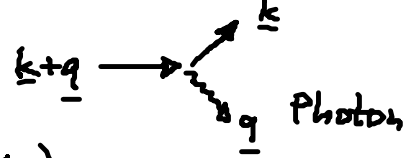
• Def.: el. Dipolmatrixelement $\mu_{\underline{n}, \underline{n}'}(\underline{k}) = \frac{1}{V_{\text{EZ}}} \int d^3r u_{\underline{n}, \underline{k}}(\underline{r}) e^{-i \underline{k} \cdot \underline{r}} u_{\underline{n}', \underline{k}}(\underline{r})$
(oft auch mit $d_{\underline{n}, \underline{n}'}$ bezeichnet, $e < 0$)

• Näherung: schwache \underline{k} -Abhängigkeit der Blochfkt. mod. $u_{\underline{n}, \underline{k}}$

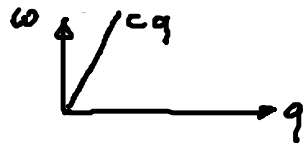
Erwartungswert im Fourierraum:

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

Näherung für opt. Grenzfall:

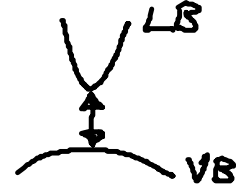


(1) $q \approx 0$ (Impuls der Photonen klein gegen Gesamtimpuls der Elektronen)



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

\Rightarrow nur Interbandübergänge (LB \leftrightarrow VB)



(3) 2-Band-Modell $n = L, V$ und $\mu_{LV}(\underline{k}) \approx \mu_{LV}(0)$

konstantes Dipolmatrixelement

Elektron-Loch-Bild:

Interbandpolarisation (makr.)

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



mikroskop. Interbandpolarisation

eines Zustands \underline{k} :

$$\begin{aligned} p(\underline{k}, t) &= \langle d_{\underline{k}} a_{\underline{k}} \rangle \\ p^*(\underline{k}, t) &= \langle a_{\underline{k}}^+ d_{\underline{k}}^+ \rangle \end{aligned}$$

4.2.2 Elektronen-Feld-WW-Op.

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

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

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

Bandkantenoptik wie in § 4.2.1:

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

4.3 Halbleiter-Bloch-Gleichungen

- 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)

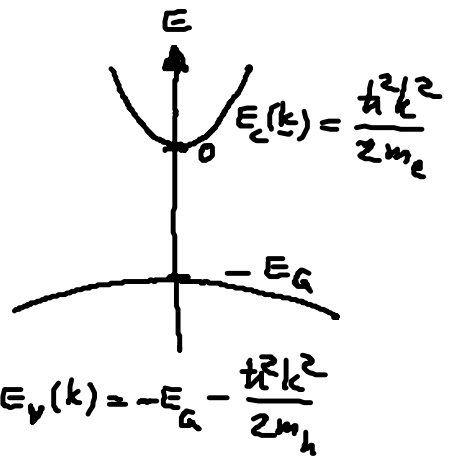
$$\frac{d}{dt} \langle \hat{F} \rangle = \left\langle \frac{i}{\hbar} [\hat{H}, \hat{F}] + \frac{\partial \hat{F}}{\partial t} \right\rangle \quad (\text{bildunabhängig})$$

Berechne Kommutatoren ① $[\hat{H}, a_k^+ a_k]$
 ② $[\hat{H}, a_k^+ d_k^+]$

Ham. op. $\hat{H} = \hat{H}_0 + \hat{H}_{opt}$

Elektron-Loch-Bild

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



Beiträge zum Kommutator ①

$$\begin{aligned} [\hat{H}_0, a_{\underline{l}}^+ a_{\underline{l}}] &= \sum_{\underline{k}} [E_c(\underline{k}) (a_{\underline{k}}^+ a_{\underline{l}} a_{\underline{l}}^+ a_{\underline{k}} - a_{\underline{l}}^+ a_{\underline{l}} a_{\underline{k}}^+ a_{\underline{k}})] - \sum_{\underline{k}} E_v(\underline{k}) (\dots) \\ &= \sum_{\underline{k}} [E_c(\underline{k}) (-\cancel{a_{\underline{k}}^+ a_{\underline{l}} a_{\underline{l}}^+ a_{\underline{k}}} + \cancel{a_{\underline{l}}^+ a_{\underline{l}} a_{\underline{k}}^+ a_{\underline{k}}}) \\ &\quad + \underbrace{\delta_{\underline{k}\underline{l}} a_{\underline{k}}^+ a_{\underline{l}} - \delta_{\underline{k}\underline{l}} a_{\underline{l}}^+ a_{\underline{k}}}] - \sum_{\underline{k}} E_v(\underline{k}) (\dots) \\ &= 0 \end{aligned}$$

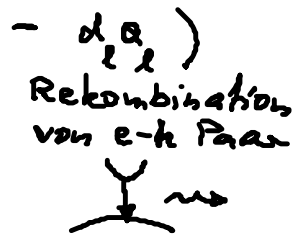
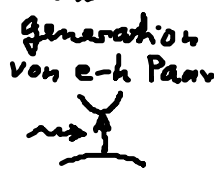
d.h. \hat{H}_0 liefert keine Zeitabh. von f_e und f_h 4x vertauschen

$$\begin{aligned} [\hat{H}_{opt}, a_{\underline{l}}^+ a_{\underline{l}}] &= \sum_{\underline{k}} \{ \mu \cdot E [(a_{\underline{k}}^+ d_{\underline{l}}^+ a_{\underline{l}}^+ a_{\underline{k}} - a_{\underline{l}}^+ a_{\underline{l}} a_{\underline{k}}^+ d_{\underline{k}}^+) + (d_{\underline{k}}^+ a_{\underline{l}}^+ a_{\underline{l}}^+ a_{\underline{k}} - a_{\underline{l}}^+ a_{\underline{l}} a_{\underline{k}}^+ d_{\underline{k}}^+)] \} \\ &= \sum_{\underline{k}} \{ \mu \cdot E [(-\delta_{\underline{k}\underline{l}} a_{\underline{l}}^+ d_{\underline{k}}^+) + \delta_{\underline{k}\underline{l}} d_{\underline{k}}^+ a_{\underline{l}}^+]] \} \\ &= -\mu \cdot E (a_{\underline{l}}^+ d_{\underline{l}}^+ - d_{\underline{l}}^+ a_{\underline{l}}^+) \end{aligned}$$

⊛ $a_{\underline{l}}^+ a_{\underline{l}} a_{\underline{k}}^+ d_{\underline{k}}^+$

$$= -\cancel{a_{\underline{l}}^+ a_{\underline{l}} a_{\underline{k}}^+ d_{\underline{k}}^+} + \delta_{\underline{k}\underline{l}} a_{\underline{l}}^+ d_{\underline{k}}^+$$

$$= a_{\underline{k}}^+ a_{\underline{l}} a_{\underline{l}}^+ d_{\underline{k}}^+ + \dots = \cancel{a_{\underline{k}}^+ d_{\underline{l}}^+ a_{\underline{l}}^+ a_{\underline{k}}^+} + \delta_{\underline{k}\underline{l}} a_{\underline{l}}^+ d_{\underline{k}}^+$$



$$\Rightarrow \langle [\hat{H}_{opt}, a_{\underline{l}}^+ a_{\underline{l}}] \rangle = -\mu \cdot E (p^*(\underline{l}, t) - p(\underline{l}, t)) = \frac{\hbar}{i} \dot{f}_e$$

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

② Dynamik der Polarisation

$$\frac{\partial}{\partial t} p(k, t) = \frac{i}{\hbar} \langle [\hat{H}, d_k a_k] \rangle$$

Beiträge zum Kommutator:

$$\begin{aligned} [\hat{H}_{\text{opt}}, d_l a_l] &= \sum_k \mu \cdot \underline{\underline{E}} \left[\overbrace{(a_k^+ d_k^+ d_l a_l - d_l a_l a_k^+ d_k^+)} + \overbrace{(d_k a_l d_l a_l - d_l a_l d_k a_k^+)} \right] \\ &= \sum_k \mu \cdot \underline{\underline{E}} \left[\overbrace{(a_k^+ a_l d_l^+ d_l - a_l^+ a_l d_l^+ d_l)} + 0 \right] \\ &= \sum_k \mu \cdot \underline{\underline{E}} \left(\overbrace{a_k^+ a_l d_l^+ d_l} + \overbrace{a_l^+ a_l d_l^+ d_l} - \delta_{lk} d_l^+ d_l \right) \\ &= \sum_k \mu \cdot \underline{\underline{E}} \left(\overbrace{a_k^+ a_l d_l^+ d_l} - \overbrace{a_l^+ a_l d_l^+ d_l} + \delta_{lk} a_l^+ a_l - \delta_{lk} d_l^+ d_l \right) \\ &= \sum_k \mu \cdot \underline{\underline{E}} \left(+\delta_{lk} a_l^+ a_l + \delta_{lk} d_l^+ d_l - \delta_{lk} \delta_{lk} \right) \\ &= \mu \cdot \underline{\underline{E}} \left(a_l^+ a_l + d_l^+ d_l - 1 \right) \end{aligned}$$

$$\begin{aligned} \langle [\hat{H}_{\text{opt}}, d_k a_k] \rangle &= \mu \cdot \underline{\underline{E}} \left(f_e(k) + f_h(k) - 1 \right) \\ &= - (1 - f_e) (1 - f_h) + f_e f_h \\ &\quad \uparrow \text{Absorption} \quad \downarrow \text{Em.} \end{aligned}$$

Inversion $f_e - (1 - f_h)$

Polarisation getrieben durch klass. Lichtquelle

$$\begin{aligned} [\hat{H}_0, d_l a_l] &= \sum_k \left\{ E_c(k) \overbrace{(a_k^+ a_l d_l^+ d_l - d_l a_l a_k^+ d_k^+)} - E_v(k) (\dots) \right\} \\ &= \sum_k \left(-E_c(k) \delta_{lk} d_l a_l - (-1) E_v(k) \delta_{lk} d_l a_l \right) \end{aligned}$$

$$= - \underbrace{(\epsilon_c(\underline{k}) - \epsilon_v(\underline{k})) d_{2p}}_{\hbar \omega_p(\underline{k})} \text{ freie Dse. der komplexen Polarisation}$$

opt. Übergangsfrequenz $\omega_p(\underline{k}) = \frac{1}{\hbar} (\epsilon_c(\underline{k}) - \epsilon_v(\underline{k}))$

Halbleiter-Bloch-gln.:

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

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

(3) $\frac{\partial}{\partial t} f_h(\underline{k}, t) = \frac{\partial}{\partial t} f_e(\underline{k}, t)$

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

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

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

