English Summary:

4. Quantum Statistics in Nonequilibrium

4.1 Density matrix – statistical operator

pure states: $\boxed{\text{class. mech.}} \xrightarrow{\text{qm. uncertainty}} \boxed{\text{quantum mech.}}$

macrosc. obs. ↓   ↓ incomplete information on microstates

mixture: $\boxed{\text{class. statistics}}$ $\boxed{\text{quantum statistics}}$

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

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

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

distribution fct. of electrons $f_e(k) = \langle a_k^+ a_k \rangle = \mathrm{tr}(\hat{\rho}\, a_k^+ a_k)$

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

4.2.1 Polarisation des Halbleiters

qm. Dipol<u>dichte</u> (vgl. klass el. Dipolmomentdichte)

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

Erzeugungsop. $\hat{\psi}^+(\underline{r}) := \sum_\lambda \psi_\lambda^*(\underline{r})\, a_\lambda^+$

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

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

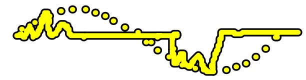
Teilchen<u>dichte</u>op. $\hat{n}(\underline{r}) = \hat{\psi}^+(\underline{r})\hat{\psi}(\underline{r})$

Def. <u>makroskop. Polarisation</u> $\underline{P}$ als Erwartungswert des Dipoldichteop. $\hat{\underline{P}}$

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

reelle Größe

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



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

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

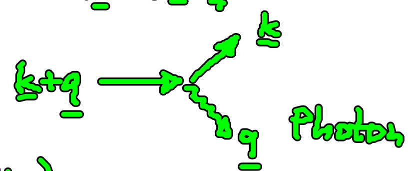
• Def.: el. Dipolmatrixelement $\underline{\mu}_{nn'}(\underline{k})=\frac{1}{V_{EZ}}\int d^3r\,u_{n\underline{k}}(\underline{r})\,e\underline{r}\,u_{n'\underline{k}}(\underline{r})$

(oft auch mit $d_{nn'}$ bezeichnet, $e<0$)

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

Erwartungswert im Fourierraum:

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

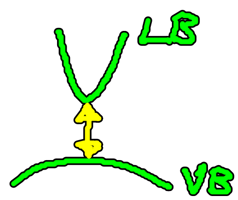


Näherung für opt. Grenzfall:

(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 $\underline{\mu}_{LV}(\underline{k})\approx\underline{\mu}_{LV}(0)$

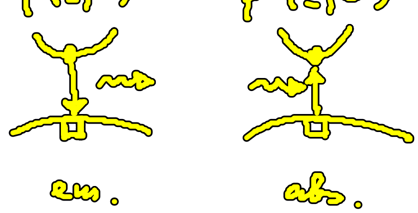
konstantes Dipolmatrixelement

Elektron-Loch-Bild:

Interbandpolarisation (makr.)

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

$p(\underline{k},t)$ $\quad$ $p^*(\underline{k},t)$



mikroskop. Interbandpolarisation eines Zustands $\underline{k}$:

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

4.2.2 Elektron-Feld-WW-Op.

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

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

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

Bandkantenoptik wie in § 4.2.1:

$$\boxed{\hat{H}_{opt} = \sum_{\underline{k}} \underline{\mu}\cdot\underline{E}(t)\left(a^+_{\underline{k}} d^+_{\underline{k}} + d_{\underline{k}} a_{\underline{k}}\right)}$$

4.3 Halbleiter-Bloch-Gleichungen

- Zeitentwicklung folgender Größen:

  Verteilungsfkt. $f_e(\underline{k},t) = \langle a^+_k a_k \rangle$

  $f_h(\underline{k},t) = \langle d^+_k d_k \rangle$

  mikr. Polarisation $p(\underline{k},t) = \langle d_k a_k \rangle$

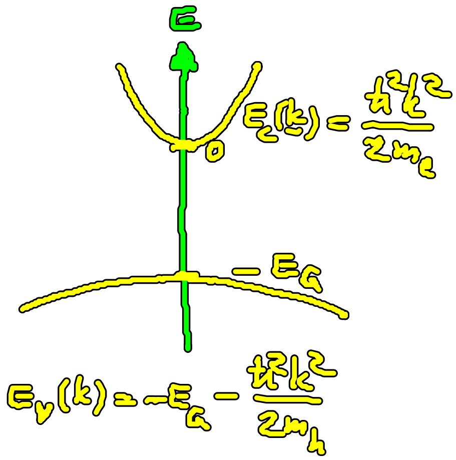
  $p^*(\underline{k},t) = \langle a^+_k d^+_k \rangle$

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

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

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

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

Beiträge zum Kommutator ①

$$[\hat{H}_0, a_l^+ a_l] = \sum_k \left[E_c(k)\left(a_k^+ a_k a_l^+ a_l - a_l^+ a_l a_k^+ a_k\right)\right] - \sum_k E_v(k)(\dots)$$

$$= \sum_k \Big[E_c(k)\Big(-\cancel{a_k^+ a_l^+ a_k a_l} + \cancel{a_l^+ a_k^+ a_l a_k}$$

$$\underbrace{+\delta_{kl} a_k^+ a_l - \delta_{kl} a_l^+ a_k}_{0}\Big] - \sum_k E_v(k)(\dots)$$

$$= 0$$

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

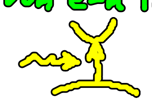
4x vertauschen

$$[\hat{H}_{opt}, a_l^+ a_l] = \sum_k \Big\{\mu \cdot \underline{E}\Big[\big(\cancel{a_k^+ d_k^+} a_l^+ a_l - a_l^+ a_l a_k^+ d_k^+\big) + \big(d_k a_k a_l^+ a_l - \cancel{a_l^+ a_l d_k a_k}\big)\Big]\Big\}$$ ⊛

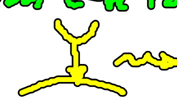
$$= \sum_k \Big\{\mu \cdot \underline{E}\Big[\big(-\delta_{kl} a_l^+ d_k^+\big) + \delta_{kl} d_k a_l\Big]\Big\}$$

$$= -\mu \cdot \underline{E}\left(a_l^+ d_l^+ - d_l a_l\right)$$

Generation von e-h Paar



Rekombination von e-h Paar



⊛ $a_l^+ a_l a_k^+ d_k^+$

$= -a_l^+ a_k^+ a_l d_k^+ + \delta_{kl} a_l^+ d_k^+$

$= a_k^+ a_l^+ a_l d_k^+ \quad + \quad '' \quad = a_k^+ d_k^+ \cancel{a_l^+ a_l} + \delta_{kl} a_l^+ d_k^+$

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

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:

$$[\hat H_{opt}, d_l a_l] = \sum_k \mu\cdot E\left[\left(a_k^+ d_k^+ d_l a_l - d_l a_l a_k^+ d_k^+\right) + \left(d_k a_k d_l a_l - d_l a_l d_k a_k\right)\right]$$

$$= \sum_k \mu\cdot E\left[\left(a_k^+ a_l d_k^+ d_l - a_l a_k^+ d_l d_k^+\right) + 0\right]$$

$$= \sum_k \mu\cdot E\left(a_k^+ a_l d_k^+ d_l + a_k^+ a_l d_l d_k^+ - \delta_{lk} d_l d_k^+\right)$$

$$= \sum_k \mu\cdot E\left(\cancel{a_k^+ a_l d_k^+ d_l} - \cancel{a_k^+ a_l d_k^+ d_l} + \delta_{lk} a_k^+ a_k - \delta_{lk} d_l d_k^+\right)$$

$$= \sum_k \mu\cdot E\left(+\delta_{lk} a_k^+ a_k + \delta_{lk} d_k^+ d_l - \delta_{lk}\delta_{lk}\right)$$

$$= \mu\cdot E\left(a_l^+ a_l + d_l^+ d_l - 1\right)$$

$$\boxed{\langle[\hat H_{opt}, d_k a_k]\rangle = \mu\cdot E\left(\underbrace{f_e(k) + f_h(k) - 1}_{= -(1-f_e)(1-f_h) + f_e f_h}\right)}$$

↑ Absorption ↓ Em.

<u>Inversion</u> $f_e - (1-f_h)$

Polarisation getrieben durch klass. Lichtquelle

$$[\hat H_0, d_l a_l] = \sum_k \left\{E_c(k)\left(a_k^+ a_k d_l a_l - d_l a_l a_k^+ a_k\right) - E_v(k)\left(\cdots\right)\right\}$$

$$= \sum_k\left(-E_c(k)\delta_{lk} d_l a_k - (-1)E_v(k)\delta_{lk} d_k a_l\right)$$

$$= -\underbrace{(E_c(k) - E_v(k))}_{\hbar\omega_p(k)} d_k a_k$$

$\hbar\omega_p(k)$ freie Osz. der komplexen Polarisation

opt. Übergangsfrequenz $\omega_p(k) = \frac{1}{\hbar}(E_c(k) - E_v(k))$

<u>Halbleiter-Bloch-Gln.:</u>

$$\boxed{\begin{aligned}
&(1)\ \frac{\partial}{\partial t} f_e(k,t) = \frac{1}{i}\Omega_p\left(p^*(k,t) - p(k,t)\right)\\
&(2)\ \frac{\partial}{\partial t} p(k,t) = \frac{1}{i}\omega_p(k)\, p(k,t) - \frac{1}{i}\Omega_p\,(\underbrace{f_e + f_h - 1}_{\text{Inversion}})\\
&(3)\ \frac{\partial}{\partial t} f_h(k,t) = \frac{\partial}{\partial t} f_e(k,t)
\end{aligned}}$$

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

<u>Bem.</u>: Kohärente Dynamik eines Ensembles unabh. durch klass. Lichtquelle getriebener 2-Niveau-Systeme (<u>Opt. Blochgln.</u>)

<u>Also</u>: Ladungsträgergeneration (e-h Paar) als kohärenter 2-Stufen-Prozess beschreibbar

$$E \xrightarrow[\text{erzeugt}]{(2)} p \xrightarrow[\substack{\text{generiert}\\ \text{durch WW}\\ \text{Ladungsträger}}]{(1)} f_e, f_h$$