English Summary :

4. Quantum Statistics

4.1 Density matrix – statistical operator $\hat{\varrho}$: $\langle \hat{M} \rangle = \mathrm{tr}(\hat{\varrho}\hat{M})$
(mixed state)

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

distrib. fct. of electrons $f_e(\underline{k}) = \langle a_k^+ a_k \rangle$
of holes $f_h(\underline{k}) = \langle d_k^+ d_k \rangle$

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

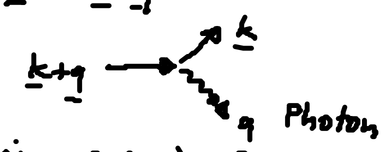
- Blochdarstellung $\hat{\psi}(r,t) = \sum_{n\underline{k}} a_{n\underline{k}} \psi_{n\underline{k}}(\underline{r})$ ← Blochfkt. $e^{i\underline{k}\underline{r}}\, u_{n\underline{k}}(\underline{r})$

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

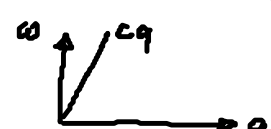
- Fouriertrafo $\hat{\underline{P}}(\underline{q},t) = \int d^3r\, \hat{\underline{P}}(\underline{r},t)\, e^{-i\underline{q}\underline{r}}$
- Def.: el. Dipolmatrixelement $\underline{\mu}_{nn'}(\underline{k}) = \frac{1}{V_{EZ}} \int d^3r\, u_{n\underline{k}}(\underline{r})\, e\underline{r}\, u_{n'\underline{k}}(\underline{r})$
  (oft auch mit $d_{nn'}$ bezeichnet; $e<0$)
- Näherung: schwache $\underline{k}$-Abhängigkeit der Blochfkt. $u_{n\underline{k}}$

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

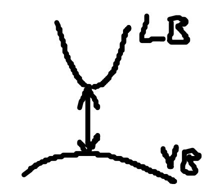
Näherung für opt. Grenzfall :



(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 $\mu_{LV}(\underline{k}) \approx \mu_{LV}(0)$
konstantes Dipolmatrixel.

Elektron-Loch-Bild :

Interbandpolarisation (makr.)

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

$\langle d_{\underline{k}} a_{\underline{k}} \rangle \rightarrow p(\underline{k},t)$ $\qquad$ $\langle a^+_{\underline{k}} d^+_{\underline{k}} \rangle \rightarrow p^*(\underline{k},t)$

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

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

4.2.2 Elektron-Feld-WW-Op.

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

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

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

Bandkantenoptik wie in 4.2.1 :

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

4.3 Halbleiter-Blochgleichungen

- Zeitentwicklung folgender Größen :

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

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

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

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

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

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

Berechne Kommutatoren ① $[\hat H, a_k^+ a_k]$

② $[\hat H, a_k^+ d_k^+]$

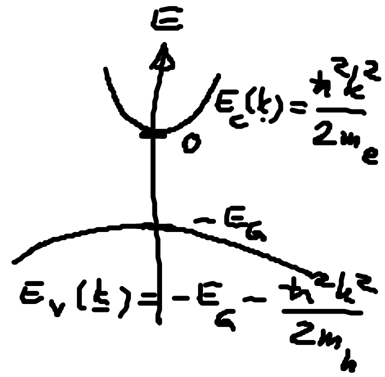
Ham.op. $\hat H = \hat H_0 + \underset{\S 3.6.1}{\hat H_{e-e}} + \underset{\S 3.6.2}{\hat H_{ii}} + \underset{\S 3.7.2}{\hat H_{e-ph}} + \underset{\S 4.2.2}{\hat H_{opt}}$

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:

$$\hat H_0 = \sum_{\underline{k}} E_c(\underline{k})\, a_k^+ a_k - \sum_{\underline{k}} E_v(\underline{k})\, d_k^+ d_k$$



Beiträge zum Kommutator ①:

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

$$= \sum_k \Big[E_c(k)\big(-a_k^+ a_l^+ a_k a_l + a_l^+ a_k^+ a_l a_k + \cancel{\delta_{kl} a_k^+ a_l} - \cancel{\delta_{lk} a_l^+ a_k}\Big] - \sum_k E_v(k)(\dots)$$

$$= 0$$

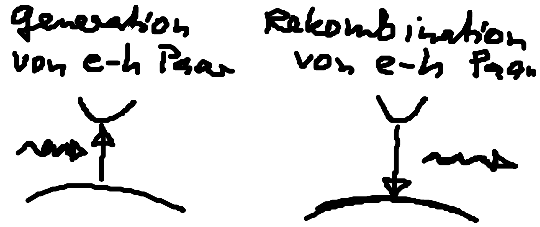
d.h. $\hat H_0$ liefert keine Zeitabh. von f_e und f_h

4x vertauschen

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

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

$$= -\mu\cdot E\,\big(\underbrace{a_l^+ d_l^+}_{} - \underbrace{d_l a_l}_{}\big)$$



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

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:

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

$$= \sum_k \mu \cdot \underline{E} \Big[(a_k^+ a_l d_k^+ d_l - a_l a_k^+ d_l d_k^+) + 0 \Big]$$

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

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

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

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

$$\frac{\hbar}{i} \dot{p}(k,t) = \boxed{\langle [\hat{H}_{opt}, d_k a_k] \rangle = \mu \cdot \underline{E} \left(\underbrace{f_e(k) + f_h(k) - 1}_{= -(1-f_e)(1-f_h) + f_e f_h} \right)}$$

$$\underbrace{\uparrow \text{Absorption} \qquad \downarrow \text{Emission}}$$

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

Polarisation getrieben durch klass. Lichtquelle

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

$$= \sum_{\underline{k}} \left(-E_c(\underline{k}) \delta_{\ell k} d_\ell a_k - (-1) E_v(\underline{k}) \delta_{\ell k} d_k a_\ell \right)$$

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

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. :

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

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

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

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

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