Semiconductor Bloch equations

- Hamiltonian $\quad H = H_{EL} + H_{EL\text{-}EL} + H_{EL\text{-}L}$

$$H_{EL} = \sum_k \left(\varepsilon_k^c\, c_k^+ c_k + \varepsilon_k^v\, v_k^+ v_k \right)$$

$$H_{EL\text{-}EL} = \frac{1}{2} \sum_{kk'q\neq 0} v(q) \left[c_{k+q}^+ c_{k'-q}^+ c_{k'} c_k + v_{k+q}^+ v_{k'-q}^+ v_{k'} v_k + 2\, c_{k+q}^+ v_{k'-q}^+ v_{k'} c_k \right]$$

$$H_{EL\text{-}L} = -\sum_k \left(dE\, c_k^+ v_k + d^* E^*\, v_k^+ c_k \right)$$

unterschl. Vorz. für ee, hh und eh-I
nach Übergang cv-Bild → eh-Bi
⇒ im 2. Summanden 4x tauschen
⇒ im 3. Summanden 1x v^+v taus

- Heisenberg equation of motion

$$\frac{d}{dt} A(t) = \frac{i}{\hbar} \left[H, A(t) \right] \qquad \left[a_k, a_{k'} \right]_+ = \left[a_k^+, a_{k'}^+ \right]_+ = 0$$

$$\left[a_k, a_{k'}^+ \right]_+ = \delta_{kk'} \qquad a = c, v$$

free-carrier Hamiltonian

$$\left[H_{EL}, c_k \right] = \sum_{k'} \varepsilon_{k'}^c \left(c_{k'}^+ c_{k'} c_k - \underline{c_k c_{k'}^+} c_{k'} \right) = \sum_{k'} \varepsilon_{k'}^c \left(c_{k'}^+ c_{k'} c_k - \delta_{kk'} c_{k'} + c_{k'}^+ c \right.$$

$$= -\varepsilon_k^c\, c_k$$

$$\left[H_{EL}, v_k \right] = -\varepsilon_k^v\, v_k \qquad\qquad c_k c_{k'}^+ = \delta_{kk'} - c_{k'}^+ c_k$$

H_{EL} ist symmetrisch in c und v

carrier-field interaction

$$\left[H_{EL\text{-}L}, c_k \right] = -dE \sum_{k'} \left(c_{k'}^+ v_{k'} c_k - c_k \underline{c_{k'}^+} v_{k'} \right) = -dE \sum_{k'} \left(c_{k'}^+ v_{k'} c_k - \delta_{kk'} v_{k'} + c_{k'}^+ \underline{c_k} v \right.$$

$$= dE\, v_k$$

$$\left[H_{EL\text{-}L}, v_k \right] = d^* E^*\, c_k$$

$H_{EL\text{-}L}$: $v \leftrightarrow c$, $dE \leftrightarrow d^* E^*$

coulomb interaction

$$\delta_{k,k'+q} \quad -\delta_{k,k''-q}$$

$$\left[H_{EL\text{-}EL}^{I}, c_k \right] = \frac{1}{2} \sum_{k',k'',q} v(q) \left(c_{k'+q}^+ c_{k''-q}^+ c_{k''} c_{k'} c_k - c_k c_{k'+q}^+ c_{k''-q}^+ c_{k''} c_{k'} \right)$$

sign sign

$$= \frac{1}{2} \sum_{k',q} v(q) \left(-c_{k'-q}^+ c_{k'} c_{k-q} + c_{k'+q}^+ c_{k+q} c_{k'} \right)$$

$$= -\sum_{k',q} v(q)\, c_{k'-q}^+ c_{k'} c_{k-q}$$

$$\delta_{k,k'+q}$$

$$\left[H_{EL\text{-}EL}^{II}, c_k \right] = \sum_{k'k''q} v(q) \left(c_{k'+q}^+ v_{k''-q}^+ v_{k''} c_{k'} c_k - c_k c_{k'+q}^+ v_{k''-q}^+ v_{k''} c_{k'} \right)$$

sign sign sign

$$= -\sum v(q)\, v_{k'-q}^+ v_{k'} c_{k-q}$$

$$\left[H^{II}_{EL-EL}, v_k\right] = -\sum_{k',q} V(q)\, v^+_{k'-q} v_{k'} v_{k-q}$$

H_{EL-EL} ist symmetr. in cu $c \leftrightarrow v$

$$\left[H^{III}_{EL-EL}, v_k\right] = -\sum_{k',q} V(q)\, c^+_{k'-q} c_{k'} v_{k-q}$$

$\swarrow$ 1 Teil Coulomb

$$i\hbar \frac{d}{dt} c_k = \underbrace{\varepsilon^c_k c_k}_{\psi_k\,(2)} - \underbrace{dE\, v_k}_{f^v_k\,(1)} + \sum_{k',q\neq 0} V(q) \underbrace{\left[c^+_{k'-q} c_{k'} + v^+_{k'-q} v_{k'}\right] c_{k-q}}_{(3)}$$

$$i\hbar \frac{d}{dt} c^+_k = -\varepsilon^c_k c^+_k + d^* E^* v^+_k - \sum_{k',q\neq 0} V(q)\, c^+_{k-q} \left[c^+_{k'} c_{k'-q} + v^+_{k'} v_{k'-q}\right]$$

$$i\hbar \frac{d}{dt} v_k = \varepsilon^v_k v_k - d^* E^* c_k + \sum_{k',q\neq 0} V(q) \left[c^+_{k'-q} c_{k'} + v^+_{k'-q} v_{k'}\right] v_{k-q}$$

$$i\hbar \frac{d}{dt} v^+_k = -\underbrace{\varepsilon^v_k v^+_k}_{\psi^*\,(2)} + \underbrace{dE\, c^+_k}_{f^c_k\,(1)} - \sum_{k',q\neq 0} V(q)\, \underbrace{v^+_{k-q} \left[c^+_{k'} c_{k'-q} + v^+_{k'} v_{k'-q}\right]}_{(3)} c_k$$

$\llcorner$ 2 Teil Coulomb (3)

- Equation of motion for density-matrix elements

$$\begin{pmatrix} f^c_k & \psi_k \\ \psi^*_k & f^v_k \end{pmatrix} = \begin{pmatrix} \langle c^+_k c_k \rangle & \langle v^+_k c_k \rangle \\ \langle c^+_k v_k \rangle & \langle v^+_k v_k \rangle \end{pmatrix}$$

$\swarrow$ Reihenfolge wichtig?

$$\frac{d}{dt}\psi_k = \langle \dot v^+_k c_k \rangle + \langle v^+_k \dot c_k \rangle$$

$$i\hbar \frac{d}{dt}\psi_k = \underbrace{(\varepsilon^c_k - \varepsilon^v_k)\,\psi_k}_{(2)} + \underbrace{dE\,(f^c_k - f^v_k)}_{(1)\ \checkmark}$$

$$+ \sum_{k',q} V(q) \left[\langle v^+_k (c^+_{k'-q} c_{k'} + v^+_{k'-q} v_{k'})\, c_{k-q} \rangle \right.$$

$$\left. - \langle v^+_{k-q} (c^+_{k'} c_{k'-q} + v^+_{k'} v_{k'-q})\, c_k \rangle \right] \quad (3)$$

$$\frac{d}{dt} f^c_k = \langle \dot c^+_k c_k \rangle + \langle c^+_k \dot c_k \rangle = \langle \dot c^+_k c_k \rangle + \text{c.c.}$$

$$i\hbar \frac{d}{dt} f^c_k = d^* E^* \psi_k$$

$$+ \sum_{k',q} V(q) \left[\langle c^+_k (c^+_{k'-q} c_{k'} + v^+_{k'-q} v_{k'})\, c_{k-q} \rangle \right.$$

$$- \text{c.c.}$$

- **Hartree-Fock decoupling** — factorization of ⟨4 operators⟩ in product of macroscopic expectation values

$$\langle a_k^+ b_l^+ c_m d_n \rangle = \langle a_k^+ d_k\rangle\langle b_l^+ c_l\rangle\, \delta_{kn}\,\delta_{lm} + \ldots$$
$$\qquad - \langle a_k^+ c_k\rangle\langle b_l^+ d_l\rangle\, \delta_{km}\,\delta_{ln} - \ldots$$

Anzuwenden auf ③

$$\left[i\hbar \frac{d}{dt}\psi_k\right]_{HF} = -\sum_q V(q)\,\Big(\psi_k f^c_{k-q} + f^v_k \psi_{k-q}$$
$$\qquad - \underbrace{\psi_{k-q} f^c_k}_{ⓑ} - \underbrace{f^v_{k-q}\psi_k}_{ⓐ} \Big)$$

$$\left[i\hbar \frac{d}{dt} f^c_k\right]_{HF} = -\sum_q V(q)\,\Big(f^c_k f^c_{k-q} + \psi_k^* \psi_{k-q}\Big) - \text{c.c.}$$

ⓐ / ⓑ : $k-q=k'$

- **Hartree-Fock equations**

$$i\hbar\frac{d}{dt}\psi_k = \Big[\underbrace{\varepsilon^c_k - \varepsilon^v_k}_{②} - \sum_{k'} V_{k-k'}\,(\underbrace{f^c_{k'} - \overbrace{f^v_{k'} + \underbrace{1}_{\text{woher?}}}^{f^h_{k'}}}_{ⓐ})\Big]\psi_k$$

wird zu $\hat{\varepsilon}^c_k + \hat{\varepsilon}^h_k$

$$\quad + \underbrace{(f^c_k - f^v_k)}_{-(1-f^h_k-f^e_k)}\,\underbrace{\Big(\underbrace{dE}_{①} + \underbrace{\sum_{k'} V_{k-k'}\psi_{k'}}_{ⓑ}\Big)}_{:=\hat{\Omega}}$$

③ wird zu ⓐ+ⓑ

↳ Das ist der Valenzband beitrag, Doppelzählung vermeiden, denn wir haben diesen Beitrag (und besser als Hartree Fock) schon in Bandstruktur / effektiv Masse Näherung

$$i\hbar\frac{d}{dt} f^c_k = -i\hbar\frac{d}{dt} f^v_k$$
$$= \Big(d^*E^* + \sum_{k'} V_{k-k'}\psi^*_{k'}\Big)\psi_k - \text{c.c.}$$

- **electron-hole picture** $f^e_k = f^c_k \quad f^h_k = (1-f^v_k)$

$$\varepsilon^e_k = \varepsilon^c_k \qquad \varepsilon^h_k = -\varepsilon^v_k$$

$$\boxed{\begin{aligned}
i\hbar\frac{d}{dt}\psi_k &= (\tilde{\varepsilon}^e_k + \tilde{\varepsilon}^h_k)\,\psi_k - (1-f^e_k-f^h_k)\,\Omega_k\\
i\hbar\frac{d}{dt} f^e_k &= \Omega^*_k\psi_k - \Omega_k\psi^*_k = i\hbar\frac{d}{dt} f^h_k\\
\tilde{\varepsilon}^{e,h}_k &= \varepsilon^{e,h}_k - \sum_{k'} V_{k-k'} f^{e,h}_{k'}\\
\Omega_k &= dE + \sum_{k'} V_{k-k'}\psi_{k'}
\end{aligned}}$$

HF ⇒ coherent part: no dephasing, scattering, screening

- simplest approx. for the incoherent part ← phänomenologisch

$$\left[i\hbar \frac{\partial}{\partial t} \psi_k \right]_{inc} = -i \frac{\hbar}{T_2} \psi_k = -i \Gamma \psi_k$$

T_2: Lebenszeit; Γ: Linienbreite

$$\left[i\hbar \frac{\partial}{\partial t} f_k \right]_{inc} = 0 \qquad (T_1 \gg T_2)$$

- rotating frame for a monochromatic field

$$E(t) = \tilde{E}(t)\, e^{-i\omega_0 t}$$

$$\Rightarrow \psi(t) = \tilde{\psi}(t)\, e^{-i\omega_0 t}$$

$$\dot{\psi}(t) = \dot{\tilde{\psi}}(t)\, e^{-i\omega_0 t} - i\omega_0 \tilde{\psi}(t)\, e^{-i\omega_0 t}$$

eingesetzt

$$\boxed{\begin{aligned} i\hbar \frac{\partial}{\partial t} \tilde{\psi}_k &= (\tilde{\varepsilon}^e_k + \tilde{\varepsilon}^h_k - \hbar\omega_0 - i\Gamma)\, \tilde{\psi}_k - (1 - f^e_k - f^h_k)\, \tilde{\Omega}_k \\ i\hbar \frac{\partial}{\partial t} f^{e,h}_k &= \tilde{\Omega}^*_k \tilde{\psi}_k - \tilde{\Omega}_k \tilde{\psi}^*_k \\ \tilde{\varepsilon}^{e,h}_k &= \varepsilon^{e,h}_k - \sum_{k'} V_{kk'} f^{e,h}_{k'} \\ \tilde{\Omega}_k &= d\tilde{E} + \sum_{k'} V_{kk'} \tilde{\psi}_{k'} \end{aligned}}$$

$-\hbar\omega_0 - i\Gamma$: zusätzliche Terme

- parabolic dispersion   Näherung für System $\hat{\psi} = \hat{\psi} \cdot e^{-\frac{i}{\hbar}(\varepsilon^e_k + \varepsilon^h_k - \hbar\omega)t}$

$$\varepsilon^{e,h}_k = \frac{E_G}{2} + \frac{\hbar^2}{2m_{e,h}} k^2$$

↑ Bandlücke drin

↓ gut am Γ Pkt
→ heißt, dass e^- frei sind

Inhomogeneous exciton equation

Einhüllende

$$\frac{\partial}{\partial t}\tilde{\Psi}_k \ll \frac{1}{T_2}\tilde{\Psi}_k \quad \text{(steady state)}$$

$$f_k^{e,h} \ll 1 \quad \text{(low density)}$$ unangeregt, Grundzustand

$$\boxed{\left(\varepsilon_k^e + \varepsilon_k^h - \hbar\omega_0 - i\Gamma\right)\tilde{\Psi}_k - \sum_{k'} V_{kk'}\tilde{\Psi}_{k'} = d\tilde{E}}$$

Faltung nach $\mathcal{F}$-Trafo

Einheiten umschreiben

- interband suszeptibelity $\chi_k = \frac{\tilde{\Psi}_k}{d\tilde{E}}$
- parabolic band structure $\varepsilon_k^{e,h} = \frac{E_G}{2} + \frac{\hbar^2}{2m_{e,h}}k^2$ $\qquad \frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_h}$

$$\left(\frac{\hbar^2 k^2}{2\mu} + E_G - \hbar\omega_0 - i\Gamma\right)\chi_k - \sum_{k'} V_{kk'}\chi_{k'} = 1$$

- excitonic units: $E_B = \frac{\hbar^2}{2\mu a_0^2}$

$x = k\cdot a_0$ ... wave number

$\varphi = \frac{\hbar\omega_0 - E_G}{E_B}$ ... detuning

$\gamma = \Gamma / E_B$ ... dephasing

$v_{kk'} = \frac{1}{E_B} V_{kk'}$

$\chi_k = E_B \chi_k$

$$(x^2 - \varphi - i\gamma)\chi_x - \sum_{x'} v_{xx'}\chi_{x'} = 1$$

$k_1 x_1 +$

$$\begin{pmatrix} x_1^2-\varphi-i\gamma-v_{11} & -v_{12} & \cdots \\ -v_{21} & x_2^2-\varphi-i\gamma-v_{22} & \\ \vdots & & \ddots \end{pmatrix}\begin{pmatrix}\chi_1\\ \chi_2 \\ \vdots\end{pmatrix} = \begin{pmatrix}1\\1\\ \vdots \\ 1\end{pmatrix}$$

$$\chi(\omega_0) = \sum_x \chi_x(\omega_0)$$

20/07/17

Spektrum:

$$\frac{\hbar\omega - E_G}{E_B}$$

Suszeptibilität:

$$P_{\substack{(t)\\ \omega}} = \sum_k \Big(\underbrace{d_k^* \psi_{k\substack{(t)\\ \omega}}}_{\langle v_k^\dagger c_k \rangle} + \underbrace{d_k \psi^*_{k\substack{(t)\\ \omega}}}_{\langle c_k^\dagger v_k \rangle} \Big)$$

mit $\psi_k = \psi_k(E)$

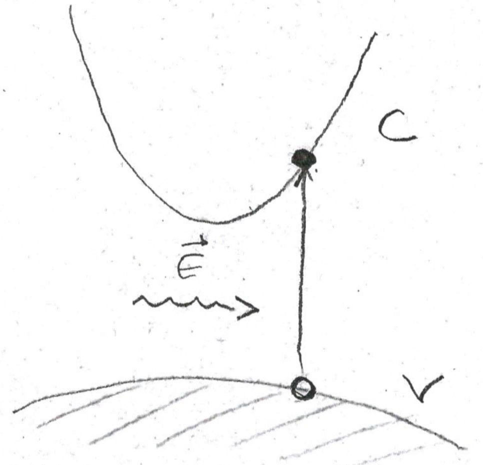
$$\boxed{\chi(\omega) = \frac{P(\omega)}{E(\omega)}}$$

$$\chi_k = \frac{\psi_k}{E}$$

$$\chi = \sum_k \left(d_k^* \chi_k + d_k \chi_k^* \right)$$

Berechnung optischer Eigenschaften von Halbleitern in der Umgebung der fundamentalen Bandlücke

1. Bandstruktur in Effektivmassennäherung



$$\varepsilon^c_k = \frac{E_G}{2} + \frac{\hbar^2}{2m_e} k^2$$

$$\varepsilon^v_k = -\frac{E_G}{2} - \frac{\hbar^2}{2m_h} k^2$$

Bloch-Wellenfunktionen

$$\varphi_{\lambda\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}\, u_{\lambda\vec{k}}(\vec{r})$$

2. Einteilchen-Operator in 2. Quantisierung

$$\langle A(t)\rangle = \sum_{ss'} \int d^3r\, d^3r' \, \langle \vec{r}'s' | A | \vec{r}s\rangle \langle \psi^+_{s'}(\vec{r}',t)\, \psi_s(\vec{r},t)\rangle$$

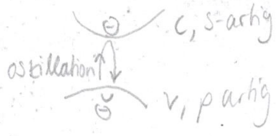
Bsp: a) Teilchendichte:

$$n(t) = \frac{1}{V}\sum_s \int d^3r \, \langle \psi^+_s(\vec{r},t)\, \psi_s(\vec{r},t)\rangle$$

b) Dipoldichte

$$P(t) = \frac{1}{V}\sum_s \int d^3r \, e\vec{r}\, \langle \psi^+_s(\vec{r},t)\, \psi_s(\vec{r},t)\rangle$$

3. Dichtematrix-Elemente in Bloch-Basis



$$\begin{pmatrix} \langle c^+_k c_k\rangle & \langle v^+_k c_k\rangle \\ \langle c^+_k v_k\rangle & \langle v^+_k v_k\rangle \end{pmatrix} = \begin{pmatrix} f^c_k & \psi_k \\ \psi^*_k & f^v_k \end{pmatrix}$$

Kohärenzen ~ 100 fs

Besetzung $\sim$ ps–ns
wichtig für Laser

zu 2. Einteilchen-Operator in 2. Quantisierung:

$$\langle A(t)\rangle = \sum_{ss'} \int d^3r\, d^3r' \, \langle \vec{r}s' | A | \vec{r}s\rangle \, \langle \psi^+_{s'}(\vec{r}',t)\, \psi_s(\vec{r},t)\rangle$$

a) Teilchendichte:

$$n(t) = \frac{1}{V}\sum_s \int d^3r \, \langle \psi^+_s(\vec{r},t)\, \psi_s(\vec{r},t)\rangle$$

b) Dipoldichte:

$$P_{tot}(t) = \frac{1}{V}\sum_s \int d^3r \, e\vec{r}\, \langle \psi^+_s(\vec{r},t)\, \psi_s(\vec{r},t)\rangle$$

Bloch-Basis: $\psi_s(\vec{r},t) = \sum_{\lambda\vec{k}} a_{\lambda\vec{k}s}(t)\, \varphi_{\lambda\vec{k}}(\vec{r})$

$$n(t) = \frac{1}{V}\sum_{s\lambda\lambda'}\sum_{\vec{k}\vec{k}'} \langle a^+_{\lambda\vec{k}s}(t)\, a_{\lambda'\vec{k}'s}(t)\rangle \underbrace{\int d^3r\, \varphi^*_{\lambda\vec{k}}(\vec{r})\, \varphi_{\lambda'\vec{k}'}(\vec{r})}_{\delta_{\lambda\lambda'}\delta_{\vec{k}\vec{k}'}}$$

$$= \frac{1}{V}\sum_{\lambda\vec{k}s} \langle a^+_{\lambda\vec{k}s}(t)\, a_{\lambda\vec{k}s}(t)\rangle$$

$$P_{tot}(t) = \frac{1}{V}\sum_{s\lambda\lambda'}\sum_{\vec{k}\vec{k}'} \langle a^+_{\lambda\vec{k}s}(t)\, a_{\lambda'\vec{k}'s}(t)\rangle$$

Unterschied

$$\frac{1}{V}\int d^3r\, e^{-i(\vec{k}-\vec{k}')\vec{r}}\, u^*_{\lambda\vec{k}\approx 0}(\vec{r})\, e\vec{r}\, u_{\lambda'\vec{k}\approx 0}(\vec{r})$$

$$P(t) = \frac{1}{V}\sum_{s\lambda\lambda'}\sum_{\vec{k}\vec{k}'} \langle a^+_{\lambda\vec{k}s}(t)\, a_{\lambda'\vec{k}'s}(t)\rangle\, \delta_{\vec{k}\vec{k}'}\, \vec{d}_{\lambda\lambda'}$$

$$= \frac{1}{V}\sum_{\vec{k},s}\sum_{\lambda\lambda'} \langle a^+_{\lambda\vec{k}s}(t)\, a_{\lambda'\vec{k}s}(t)\rangle\, \vec{d}_{\lambda\lambda'}$$

lineare optische Eigenschaften

- Halbleiter-Blochgleichungen linear im opt. Feld

$$i\hbar \frac{\partial}{\partial t} f^{c,v}_k = 0 \qquad \text{AB: } f^c_k = 0 \quad f^v_k = 1$$

$$i\hbar \frac{\partial}{\partial t} \psi_k = (\varepsilon^c_k - \varepsilon^v_k - i\gamma)\psi_k - dE - \frac{1}{V}\sum_{k'} V_{kk'}\psi_{k'}$$

(1)

- Fourier-Transformation $\psi_k(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t}\psi_k(\omega)$ (2)

$$(\varepsilon^c_k - \varepsilon^v_k - \hbar\omega - i\gamma)\psi_k(\omega) - \frac{1}{V}\sum_{k'} V_{kk'}\psi_{k'}(\omega) = dE(\omega)$$

(1) Ableitung von (2) — Spektralbasis

$$P(\omega) = \frac{1}{V}\sum_{k'} d^* \psi_k(\omega) + c.c. \quad \leftarrow \text{in } k\text{-Basis}$$

Einführung der Suszeptibilität $\chi_k(\omega) = \frac{\psi_k(\omega)}{dE(\omega)}$

$$\boxed{\begin{aligned} &(\varepsilon^c_k - \varepsilon^v_k - \hbar\omega - i\gamma)\chi_k(\omega) - \frac{1}{V}\sum_{k'} V_{kk'}\chi_{k'}(\omega) = 1 \\ &\chi(\omega) = \frac{1}{V}\sum_k |d|^2 \chi_k(\omega) \end{aligned}}$$

- dimensionslose Größen:

$x = k \cdot a_0$ — a_0 ... Bohr-Radius

$\frac{\hbar^2}{2\mu a_0^2} = E_B$ ... Rydberg-Energie

$\frac{\hbar\omega - E_G}{E_B} = \varphi$ ... Verstimmung

$$V_{kk'} = \frac{e^2}{\varepsilon_0}\frac{1}{|\vec{k}-\vec{k}'|^2} \quad \text{mit } \frac{e^2}{\varepsilon_0} = 8\pi a_0 E_B \qquad \Gamma = \frac{\gamma}{E_B}$$

$$\chi_k = \frac{\tilde{\chi}_x}{E_B}$$

$$\boxed{(x^2 - \varphi - i\Gamma)\tilde{\chi}_x - \int dx'\, V(x,x')\tilde{\chi}_{x'} = 1}$$

$$\frac{1}{V}\sum_{k} = \frac{1}{(2\pi)^3}\int d^3k = \frac{1}{(2\pi)^3}\int_0^\infty dk\,k^2 \int_0^\pi d\vartheta \sin\vartheta \int_0^{2\pi} d\varphi$$

$\cos\vartheta = z$

$$= \frac{1}{(2\pi)^3}\int_0^\infty dk\,k^2 \int_{-1}^{1} dz \int_0^{2\pi} d\varphi$$

1. $$\frac{1}{V}\sum_{k'} V_{kk'} f_{k'} = \frac{1}{(2\pi)^3}\int d^3k'\; V(\vec{k}-\vec{k}')\, f_{|\vec{k}'|}$$

$$V(\vec{k}-\vec{k}') = \frac{e^2}{\varepsilon_0}\,\frac{1}{|\vec{k}-\vec{k}'|^2}$$

$$\frac{e^2}{\varepsilon_0} = 8\pi a_0 E_B$$

$$= \frac{E_B}{\pi^2}\int d^3x'\; \frac{1}{|\vec{x}-\vec{x}'|^2}\, f_{x'}$$

$$= \frac{E_B}{\pi^2}\int_0^\infty dx'\, x'^2 f_{x'}\; \underbrace{\int dz\, \frac{1}{x^2+x'^2-2xx'z}}_{\frac{1}{xx'}\ln\left|\frac{x+x'}{x-x'}\right|}\; \underbrace{\int_0^{2\pi} d\varphi}_{2\pi}$$

$$= E_B \int_0^\infty dx'\; V(x,x')\, f_{x'}$$

$$V(x,x') = \frac{2}{\pi}\,\frac{x'}{x}\,\ln\left|\frac{x+x'}{x-x'}\right|$$

2. $$\frac{1}{V}\sum_k \chi_k = \frac{4\pi}{(2\pi)^3}\int dk\,k^2 \chi_k = \frac{1}{2\pi^2}\,\frac{1}{a_0^3}\int dx\, x^2 \chi_x$$

$$\frac{1}{\varepsilon_0}\chi = \frac{|d|^2}{\varepsilon_0 a_0^3 E_B}\,\frac{1}{2\pi^2}\int dx\; x^2 \tilde{\chi}_x$$

woher?

für Energien gilt

$$\varepsilon^c_k - \varepsilon^v_k - \hbar\omega = \frac{\hbar^2}{2m_e}k^2 + \frac{\hbar^2}{2m_h}k^2 + E_G - \hbar\omega$$

$$= \frac{\hbar^2}{2\mu a_0^2}x^2 + E_G - \hbar\omega$$

$x = k a_0$

$$= E_B\left(x^2 - \varphi\right)$$

$$\varphi = \frac{\hbar\omega - E_G}{E_B}$$

4. Bewegungsgleichungen in Hartree-Fock-Näherung: Halbleiter-Blochgleichungen

$$i\hbar \frac{\partial}{\partial t} \psi_k = (\tilde{\varepsilon}_k^c - \tilde{\varepsilon}_k^v - i\gamma)\psi_k + (f_k^c - f_k^v)\,\Omega_k$$

$$i\hbar \frac{\partial}{\partial t} f_k^c = \Omega_k^* \psi_k - \Omega_k \psi_k^* = -i\hbar \frac{\partial}{\partial t} f_k^v$$

$$\tilde{\varepsilon}_k^c = \varepsilon_k^c - \frac{1}{V}\sum_{k'} v_{kk'} f_{k'}^c$$

$$\tilde{\varepsilon}_k^v = \varepsilon_k^v - \frac{1}{V}\sum_{k'} v_{kk'}(f_{k'}^v - 1)$$

renormierte Einteilchen-Energien

$$\Omega_k = \vec{d}\vec{E} + \frac{1}{V}\sum_{k'} v_{kk'} \psi_{k'}$$

renormierte Rabi-Energie

5. makr. Polarisation (Dipoldichte)

$$\vec{P} = \frac{1}{V}\sum_k \vec{d}_k^* \psi_k + c.c.$$

Teilchendichte

$$n^{c,v} = \frac{1}{V}\sum_k f_k^{c,v}$$

Suszeptibilität

$$\vec{P}(t) = \int dt'\, \chi(t-t')\, \vec{E}(t')$$

(im linearen od. stationären Fall:

$$\vec{P}(\omega) = \chi(\omega)\, \vec{E}(\omega)$$

dielektr. Funktion, kompl. Brechungsindex:

$$\varepsilon = n^2 = 1 + \frac{1}{\varepsilon_0}\chi$$

$a^+a(a\psi) = (n-1)a\psi$

$a^+a(a^+\psi) = (n+1)a^+\psi$

Was ist EW von a^+/a?

$a^+\psi = \lambda\psi \quad a^+a\psi = \mu\lambda\psi = n\psi$

$a\psi = \mu\psi \quad a^+aa^+\psi = (n+1)a^+\psi$

$\underbrace{a^+a^+a}_{aa^++1}\psi = a^+n\psi = na^+\psi = n\cdot\mu a^+\psi$

$a^+a^+a\psi = [a^+a+1]a^+\psi_n = \mu_n[a^+a+1]\psi_n$
$= \mu_n(n+1)\psi_n$

$a^+a^+a\psi = a^+n\psi_n = na^+\psi_n = n\mu_n\psi_{n+1}$

$\mu_n(n+1)\psi_n = n\mu_n$

$$P(\omega) = \chi(\omega)E(\omega)$$

$$\cancel{P = \langle er\rangle = \sum_S \int d^3r \langle \hat{\psi}^+_S(r,t)\,|er|\,\underbrace{\hat{\psi}_S(r,t)}_{\sum_{\lambda\vec{k}} \hat{a}_{\lambda\vec{k}s}\varphi_{\lambda\vec{k}}(\vec{r})}\rangle}$$

$$n(t) = \sum_{\substack{s,\lambda\lambda'\\ kk'}} \int d^3r \langle a^+_{\lambda'\vec{k}'s}|a_{\lambda\vec{k}s}\rangle\, \varphi^*_{\lambda\vec{k}}(\vec{r})\,\varphi_{\lambda'\vec{k}'}(\vec{r}) \quad \to s$$

$$= \sum_{s,\lambda,k} \langle a^+_{\lambda\vec{k}s}|a_{\lambda\vec{k}s}\rangle$$

$$\boxed{\langle er\rangle = \sum_{ss'} \int d^3r \int d^3r' \underbrace{\langle r's'|e\hat{r}|r's\rangle}_{er\,\delta_{rr'}\delta_{ss'}} \langle \hat{\psi}^+_{s'}(\vec{r},t)\,\hat{\psi}_s(\vec{r},t)\rangle}$$

1T. Operator in 2. Quantisierung

$$= \sum_S \int d^3r\, er \langle \underbrace{\hat{\psi}^+_S(\vec{r},t)}_{\sum_{\lambda',\vec{k}'} \hat{a}^+_{s\lambda'\vec{k}'}\varphi_{\lambda'\vec{k}'}(\vec{r})} \hat{\psi}_s(\vec{r},t)\rangle$$

$$= \sum_S \int d^3r\, er \sum_{\lambda\lambda',kk'} \langle \hat{a}^+_{s\lambda'\vec{k}'}\varphi_{\lambda'k'}(\vec{r})\,|\,\hat{a}_{s\lambda\vec{k}}\varphi_{\lambda\vec{k}}(\vec{r})\rangle$$

$$P(t) = \sum_{s,\vec{k}}\sum_{\lambda\lambda'} d_{\lambda\lambda'}\psi$$

$$= \sum_{\substack{s\lambda\lambda'\\ kk'}} \langle \hat{a}^+_{s\lambda'\vec{k}'}|\hat{a}_{s\lambda\vec{k}}\rangle \underbrace{\int d^3r\, er\, \varphi^*_{\lambda'k'}(\vec{r})\varphi_{\lambda k}(\vec{r})}_{\delta_{kk'}d_{\lambda\lambda'}} = \sum_{\substack{s\lambda\lambda'\\ k}} d_{\lambda\lambda'} \underbrace{\langle \hat{a}^+_{s\lambda'k}\,\hat{a}_{sk\lambda}\rangle}_{\text{im }(\cdot)\text{-Bild: } \psi/\psi^*}$$

Haug Koch CH 5

$H = \hbar\omega_c [a^+a + \frac{1}{2}]$

$\Psi_{nn'} = \frac{(a^+)^n (b^+)}{\sqrt{n!n'!}} \Psi_{00}$

$H\Psi_{00} = \frac{\hbar\omega_c}{2}\Psi_{00}$

$H a_+ \Psi_{00} = \hbar\omega_c [\underbrace{a^+ a a_+}_{(\hat{n}+1)a^+} \Psi_0 + \frac{1}{2}\Psi] = \frac{3}{2}\hbar\omega_c$

$a^+\Psi \,?$

$a^+a\Psi_n \to n$

$a^+aa^+\Psi_n \to n+1$

$L_z^e = -L_z^h$

$L_z^h = -(a^+a - b^+b)$

$= b^+b - a^+a$

$\frac{\rho^2}{4} - \Delta + L_z^e = a^+a + \frac{1}{2}$

$\frac{\rho^2}{4} - \Delta + \cancel{a^+a} - b^+b = \cancel{a^+a} + \frac{1}{2}$

$\frac{\rho^2}{4} - \Delta = b^+b + \frac{1}{2}$

$H^h = \underline{b^+b + \frac{1}{2}} - (a^+a - b^+b)$

$= a^+a$

$\frac{\rho^2}{4} - \Delta + L_z^e = a^+a + \frac{1}{2}$

$\Leftrightarrow \frac{\rho^2}{4} - \Delta + \cancel{a^+a} - b^+b = \cancel{a^+a} + \frac{1}{2}$

$\frac{\rho^2}{4} - \Delta = b^+b + \frac{1}{2}$

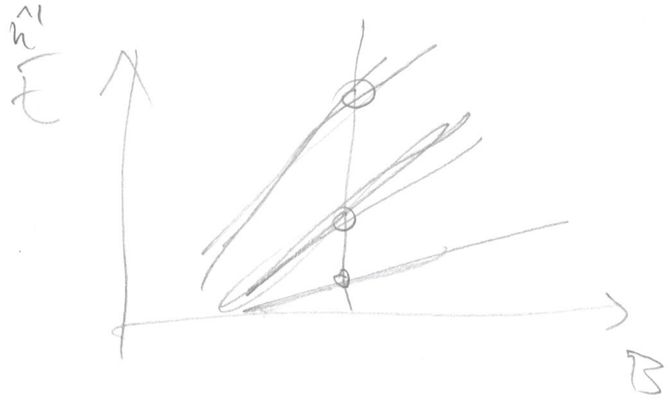
das ändert doch nicht!

$b^+b + \frac{1}{2} + a^+a - b^+b = a^+a + \frac{1}{2}$

$-a^+a + b^+b = \cancel{2b^+b}\, n = 2b^+b - a^+a$

$b^+b - a^+a$

$\hbar\omega(\hat{n}+\frac{1}{2})\phi_n = E_n\phi_n \quad \leftarrow e^-$



$$\boxed{P(t) = \frac{1}{V}\sum_k \alpha_k^{+} \Psi_k(t) + \alpha \Psi_k^{*}(t)}$$

$$f(\vec{r}) = \frac{1}{V}\sum_k e^{i\vec{k}\vec{r}} \tilde{f}_{\vec{k}}$$

$$\tilde{f}_{\vec{k}} = \int d^3r \, e^{-i\vec{k}\vec{r}} f(\vec{r})$$

$$\frac{1}{V}\sum_k \tilde{f}_{\vec{k}} = \int d^3r \underbrace{\frac{1}{V}\sum_k e^{-i\vec{k}\cdot\vec{r}}}_{\delta(\vec{r}=0)} f(\vec{r})$$

$$= f(\vec{r}=0)$$

$$\tilde{f}(\omega) = \int dt \, e^{i\omega t} f(t)$$

$$f(t) = \frac{1}{2\pi}\int d\omega \, e^{-i\omega t} \tilde{f}(\omega) / \delta(t)$$

$$\frac{1}{2\pi}\int d\omega \, \tilde{f}(\omega) = \int dt \underbrace{\frac{1}{2\pi}\int d\omega \, e^{i\omega t}} f(t) \quad = f(t=0)$$

$$\begin{pmatrix} \underset{f^c}{\langle c^+ c \rangle} & \underset{\psi}{\langle c^+ v \rangle} \\ \underset{\psi^*}{\langle v^+ c \rangle} & \underset{f^v}{\langle v^+ v \rangle} \end{pmatrix} \leftrightarrow \underbrace{\begin{pmatrix} \psi d^* & 0 \\ 0 & \psi^* d \end{pmatrix}}_{\rho_0 d}$$

$$d = \begin{pmatrix} 0 & d_{cv} \\ d_{vc} & 0 \end{pmatrix} = \begin{pmatrix} 0 & d \\ d^* & 0 \end{pmatrix}$$

$$\langle d \rangle = \operatorname{tr}(\rho_0 d)$$

$$\operatorname{tr} = \sum \langle i | \cdot | i \rangle$$

$$\langle d \rangle = \iint \hat{\psi}^*_{r'} \, d \, \hat{\psi}_r \, dr \, dr'$$

$$\langle \psi | d | \psi \rangle$$

$$\hat{\psi} = \sum a \cdot \psi$$

$$e^{-r} \qquad \sum_{n=0}^{\infty} \frac{(-r)^n}{n!} \cdot \underbrace{\mathcal{H}_n \mathcal{H}_{n'}}_{d\sigma^*}$$

$$\phi_{00} = \alpha e_0^{-\frac{x^2+y^2}{4}}$$

$$\phi_{nn'} = A_n H_{n'} \, e_0^{-\frac{x^2+y^2}{4}}$$

$$|\psi\rangle = \sum_{i,\beta} |i\rangle \langle i | \psi \rangle$$

$$|i\rangle \quad \phi_\alpha \quad \rho_{\alpha\beta}$$

$$\langle \phi_{nn'} | \phi_\mu \rangle_{nn'} \qquad \langle n | n' \rangle$$