8. Übungsblatt: $\boxed{13.6.2016}$

Quantenmechanischer Strom

Überblick: (1.) Herleiten der Leitfähigkeitsformel

$$\langle j \rangle = \frac{q}{V}\sum_{k} c_{k}(t)\, \nabla_{k} \frac{\epsilon_k}{\hbar}$$

(2.) Kinetik der Blochelektronen
Heisenberg-Bwgl.

(3.) Dissipation (mit Phononen)
Bloch-Grüneisen-Verhalten

$$\rho(r,t) = |\psi(r,t)|^2 = \psi^*\psi$$

$$\dot\rho = \frac{d}{dt}(\psi^*\psi) = \dot\psi^*\psi + \psi^*\dot\psi$$

$$i\hbar\frac{d}{dt}\psi = H\psi$$

$$-i\hbar\frac{d}{dt}\psi^* = \psi^* H^\dagger = \psi^* H$$

$$= \frac{1}{-i\hbar}(\psi^* H)\psi + \psi^*\frac{1}{i\hbar}(H\psi)$$

$$H = -\frac{\hbar^2}{2m}\Delta + U$$

$$= \frac{\hbar}{2mi}\left[(\psi^*\Delta)\psi - \psi^*(\Delta\psi)\right]$$

$$\Delta = \nabla\cdot\nabla$$

$$\left[\begin{aligned} &\nabla\cdot\left(f\nabla g - (\nabla f)g\right) = \\ &= \cancel{\nabla f\cdot\nabla g} + f(\Delta g) - \cancel{\nabla f\cdot\nabla g} - (\Delta f)g \end{aligned}\right]$$

$$= \frac{\hbar}{2mi}\left[(\psi^*\nabla\cdot\nabla)\psi + (\psi^*\nabla)\cdot(\nabla\psi) - (\psi^*\nabla)\cdot(\nabla\psi) - \psi^*(\Delta\psi)\right]$$

$$= \frac{\hbar}{2mi}\nabla\cdot\Big[\underbrace{(\psi^*\nabla)\psi}_{=-\psi(\nabla\psi^*)} - \psi^*(\nabla\psi)\Big]$$

$$\dot\rho = -\frac{1}{2}\nabla\cdot\left[\psi\left(\frac{\hbar}{i}\nabla\right)/m\,\psi + \psi^*\frac{p}{m}\psi\right]$$

NR: zu zeigen $\overleftarrow{\nabla} = -\overrightarrow{\nabla}$

$$\langle p\rangle = \langle p^\dagger\rangle = \langle p\rangle^*$$

$$\langle\psi|\overleftarrow{p}|\psi\rangle = \left(\langle\psi|\overrightarrow{p}|\psi\rangle\right)^*$$

$$\dot{\rho} + \nabla \cdot \underline{j} = 0$$

$$\underline{j} = \frac{1}{2}\left(\psi \frac{\underline{p}}{m} \psi^* + \psi^* \frac{\underline{p}}{m} \psi\right)$$

$= \langle \psi^* | p^+ | \psi \rangle = \langle \psi^* | p | \psi \rangle$

$\hookrightarrow$ partielle Integration

$\longrightarrow$ Korrespondenzprinzip $\frac{\underline{p}}{m} = \underline{v}$

$\longrightarrow$ Wahrscheinlichkeitsstrom

$$j_{el} = \frac{q}{2m}\left(\hat{\psi}^*(\underline{r},t)\, \underline{p}\, \hat{\psi}(\underline{r},t) + h.a.\right)$$

$$\underline{p} \longrightarrow \hat{p} - q A(\underline{r},t)$$

$$A(\underline{r},t) = 0$$

$$\hat{\psi}(\underline{r},t) = \sum_{\lambda_1 \underline{k}_1} \varphi_{\underline{k}_1 \lambda_1}(\underline{r})\, a^+_{\underline{k}_1 \lambda_1}(t)$$

$\uparrow$ trägt alle Ortsabhängigkeit

$$j_{el} = \frac{q}{2m} \sum_{\substack{\lambda_1 \lambda_2 \\ \underline{k}_1 \underline{k}_2}} \underbrace{\varphi^*_{\underline{k}_1 \lambda_1}(\underline{r})\, \hat{\underline{p}}\, \varphi_{\underline{k}_2 \lambda_2}(\underline{r})}_{\text{Übungsaufgabe (Blatt 8)}}\; \underbrace{a^+_{\underline{k}_1 \lambda_1} a_{\underline{k}_2 \lambda_2}}_{\text{quantenkinetisch ausrechnen}} + h.a.$$

alle Eigenschaften des FK gehen dort ein

$$\langle j_{el} \rangle_{qm} = \frac{q}{2m} \sum_{\substack{\lambda_1 \lambda_2 \\ \underline{k}_1 \underline{k}_2}} \varphi^*_{\underline{k}_1 \lambda_1}(\underline{r})\, \hat{\underline{p}}\, \varphi_{\underline{k}_2 \lambda_2}(\underline{r}) \langle a^+_{\underline{k}_1 \lambda_1} a_{\underline{k}_2 \lambda_2} \rangle + h.a.$$

um Strom durch den FK auszurechnen, noch über Beobachtungsebene mitteln

$$\langle \langle j_{el} \rangle_{qm} \rangle_{\mathbb{R}} = \frac{q}{2m} \frac{1}{V} \int_{FK} d^3r \, \langle j_{el} \rangle_{qm}(\underline{r})$$

$$= \sum_{\underline{R}_n} \frac{1}{N \Omega_{EZ}} \int_{\Omega_{EZ}} d^3r' \, \langle j_{el} \rangle_{qm}(\underline{r}' + \underline{R}_n)$$

$$\varphi_{\lambda,k_1}(\underline{r}) = u_{\lambda k_1}(\underline{r})\, e^{i k_1 \cdot \underline{r}}$$

ÜBS: $(k_1 - k_2)\cdot \underline{r}' \ll 1$

$$\langle\langle j_{el}\rangle\rangle_{\mathrm{qm}\,\|\,R} = \frac{q}{2}\sum_{\underline{k}} \underbrace{\langle a^{+}_{\underline{k}}(t) a_{\underline{k}}(t)\rangle}_{\text{Ladungsdichte}} \nabla_{\underline{k}} \frac{\varepsilon_k}{\hbar}$$

Geschwindigkeit abhängig von der eff. Masse

für eine parabolische Bandstruktur ergibt sich also $\hbar^{-1}\nabla_{\underline{k}}\,\varepsilon_{\underline{k}} = \hbar^{-1}\nabla_{\underline{k}}\frac{\hbar^2 \underline{k}\cdot\underline{k}}{2m^*}$

$$= \frac{\hbar}{2m^*}\sum_i \underline{e}_i \partial_{k_i}\sum_j k_j^2 = \frac{\hbar}{2m^*}\sum_i 2k_i\underline{e}_i = \frac{\hbar}{m^*}\underline{k}$$

$\Longrightarrow$ alles ist gegeben außer Quantenkinetik

$$\frac{d}{dt}\langle a^{+}_{k} a_{k}\rangle = \ldots = \frac{i}{\hbar}\langle [H, a^{+}_{k} a_{k}]\rangle + \cancel{\partial\langle\rangle}$$

$$-i\hbar\frac{d}{dt} a^{+}_{k} a_{k} = \Big[\sum_q \varepsilon_q a^{+}_{q} a_{q} - i q \underline{E}_L\cdot\sum_q \nabla_q a^{+}_{q} a_{q}, a^{+}_{k} a_{k}\Big]$$

$$= \sum_q \varepsilon_q \underbrace{[a^{+}_{q} a_{q}, a^{+}_{k} a_{k}]}_{=0} - i q \underline{E}_L\cdot\sum_q \nabla_q [a^{+}_{q} a_{q}, a^{+}_{k} a_{k}]$$

$$\sum_q \nabla_q a^{+}_{q} a_{q}\, a^{+}_{k} a_{k} = \sum_q a^{+}_{q} \lim_{\delta q\to 0}\frac{a_{q+\delta q} - a_q}{\delta q} a^{+}_{k} a_{k}$$

$$= \sum_q a^{+}_{q}\left(\frac{a_{q+\delta q}\, a^{+}_{k} - a_q\, a^{+}_{k}}{\delta q}\right) a_k =$$

$$= \sum_q a^{+}_{q}\left(\frac{\delta_{q+\delta q,k} - a^{+}_{k} a_{q+\delta q} - \delta_{q,k} + a^{+}_{k} a_q}{\delta q}\right) a_k$$

$$= \sum_q \lim_{\delta q \to 0} \frac{1}{\delta q}\left(\delta_{q+\delta q, k}\, a_q^\dagger a_k - \delta_{q,k}\, a_q^\dagger a_k\right)$$

$$+ \sum_q \lim_{\delta q \to 0} \frac{1}{\delta q}\left(- a_k^\dagger a_{q+\delta q}\, \delta_{q,k} + a_k^\dagger a_q\, \delta_{q,k}\right)$$

$$+ \sum_q \underbrace{\lim_{\delta q \to 0} \frac{1}{\delta q}\, a_k^\dagger a_k \left(a_q^\dagger a_{q+\delta q} - a_q^\dagger a_q\right)}_{\to\, D_q\, a_q^\dagger a_q}$$

$$= \lim_{\delta q \to 0} \frac{1}{\delta q}\left(a_{k-\delta q}^\dagger a_k - a_k^\dagger a_k - a_k^\dagger a_{k+\delta q} + a_k^\dagger a_k\right)$$

$$+ \underset{\sim\sim\sim}{i\, q}\, \underline{E}_L \cdot \sum_q a_k^\dagger a_k D_q\, a_q^\dagger a_q$$

$$= - D_k\, a_k^\dagger a_k$$

$$+ \underbrace{\lim_{\delta q \to 0} \frac{a_{k-\delta q}^\dagger a_k - a_k^\dagger a_k}{(-)(-)\delta q}}_{-D_k\, a_k^\dagger a_k} \qquad + i\, q \ldots$$

$$\Rightarrow \left[\sum_q D_q\, a_q^\dagger a_q,\, a_k^\dagger a_k\right] = - D_k \left(a_k^\dagger a_k\right)$$

$$- i\hbar\left(\frac{d}{dt} + \frac{q}{\hbar}\, \underline{E}_L \cdot \underline{D}_k\right) a_k^\dagger a_k = 0 \quad \text{(ohne Phononen)}$$

Beschleunigung der Elektronen im internen Feld

Dissipation

Betrachte nun Phononen (aber im einfachsten nicht trivialen Limit)
Boltzmanngl., Phononen in Ratengl.

$$\underbrace{\frac{d}{dt}\langle a_k^\dagger a_k\rangle}_{=:\sigma_k}\Big|_{el-ph} = -\sum_q W_{k\to k+q}\underbrace{\left(1-\langle a_{k+q}^\dagger a_{k+q}\rangle\right)}_{\hat{=}\,\text{Pauliblocking}}\langle a_k^\dagger a_k\rangle$$

$$+\sum_q \omega_{k+q\to k}\langle a_{k+q}^\dagger a_{k+q}\rangle\left(1-\langle a_k^\dagger a_k\rangle\right)$$

$\longrightarrow$ Näherungen sind nötig

Bandkante, also $\langle a_k^\dagger a_k\rangle \ll 1$

$$\frac{d}{dt}\sigma_k = -\sum_q W_{k\to k+q}\,\sigma_k + \sum_q W_{k+q\to k}\,\sigma_{k+q}$$

... siehe VL $\sigma_k^{(0)}+\sigma_k^{(1)}+\ldots=\sigma_k$

$$\frac{d}{dt}\sigma_k^{(1)} = -\underbrace{\sum_q \omega_{k\to k+q}\frac{\cos\vartheta}{k}q}_{=\gamma_k}\,\sigma_k^{(1)}$$

$$\gamma_k = \int d^3q\;|D_q|^2\,n_q\;\delta\left(\varepsilon_{\underline{k}+\underline{q}}-\varepsilon_{\underline{k}}+\hbar\omega_q\right)\frac{q}{k}\cos\vartheta$$

$$\varepsilon_{\underline{k}} = -\frac{\hbar^2}{2m}\underline{k}^2\,,\quad \varepsilon_{\underline{k}+\underline{q}} = -\frac{\hbar^2}{2m}(\underline{k}+\underline{q})^2$$

$$= -\frac{\hbar^2}{2m}\left(k^2+q^2+2|k||q|\cos\vartheta\right)$$

$$\varepsilon_{\underline{k}+\underline{q}}-\varepsilon_k+\underbrace{\cancel{\hbar\omega_q}}_{\ll\varepsilon_k} = \delta\left(-\frac{\hbar^2q^2}{2m}-\frac{\hbar^2}{m}k\,q\cos\vartheta\right)$$

$$\overset{\delta(x)=\delta(-x)}{=} \delta\left(\frac{\hbar^2q^2}{2m}+\frac{\hbar^2kq}{m}\cos\vartheta\right) \overset{\delta(\alpha x)=\frac{1}{|\alpha|}\delta(x)}{=}$$

$$= \frac{m}{\hbar^2kq}\,\delta\left(\frac{q}{2k}+\cos\vartheta\right)$$

$|D_q|^2 \sim q$

$$\gamma_k = 2\pi \int_0^\infty dq\, q^2 \frac{2m}{\hbar^2 k^3} n_q\, q \underbrace{\int_0^\pi d\vartheta \sin\vartheta \cos\vartheta\, \delta\left(\frac{q}{2k}+\cos\vartheta\right)}_{x=\cos\vartheta,\ dx=-d\vartheta \sin\vartheta}$$

$$\overbrace{\qquad\qquad}= \int_{-1}^{1} dx\, x\, \delta\left(\frac{q}{2k}+x\right)$$

$$= 2\pi \frac{2m}{\hbar^2 k^2} \int_0^\infty dq\, q^3 n_q \frac{q}{2k}$$

$$\sim \int_0^\infty dq\, q^4 n_q \quad , \quad n_q = \frac{1}{\exp\left[\frac{\hbar\omega_q}{k_B T}\right]-1}$$

$$= \int_0^\infty dq\, q^4 \frac{1}{\exp\left[\left(\frac{\alpha}{k_B T}\right) q\right]-1} \quad \Bigg| \quad \begin{array}{l} \omega_q = \alpha q \\ \text{Variablensubstitution} \\ x = \alpha \frac{q}{k_B T} \\ dx = \frac{\alpha}{k_B T} dq \end{array}$$

$$\gamma_k \sim \int_0^\infty dx \left(\frac{k_B T}{\alpha}\right)^5 x^4 \frac{1}{e^x-1}$$

d.h. ist proportional zu T^5
Tieftemperaturverhalten
Grüneisen-Bloch-Verhalten