Elektron szemiklasszikus dinamikája:

(1) $\hbar \dot{\underline{k}} = -e\left[\underline{E}(\underline{r},t) + \underline{v}_n(\underline{k}) \times \underline{B}(\underline{r},t)\right]$

(2) $\dot{\underline{r}} = \underline{v}_n(\underline{k}) = \frac{1}{\hbar}\frac{\partial E_n(\underline{k})}{\partial \underline{k}}$ $\quad n$: sávindex

példa: $\varepsilon(\underline{k}) = -\varepsilon_0\left(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right)$

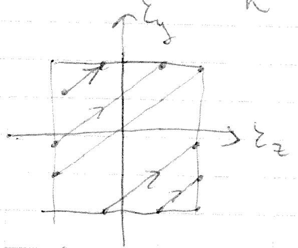
$$\underline{v} = \frac{1}{\hbar}\,\mathrm{grad}_{\underline{k}}\,\varepsilon(\underline{k}) = \frac{\varepsilon_0 a}{\hbar}\begin{pmatrix}\sin(k_x a)\\ \sin(k_y a)\\ \sin(k_z a)\end{pmatrix} = -\frac{\varepsilon_0 a}{\hbar}\begin{pmatrix}\sin\left(\frac{eE_x a t}{\hbar}\right)\\ \sin\left(\frac{eE_y a t}{\hbar}\right)\\ \sin\left(\frac{eE_z a t}{\hbar}\right)\end{pmatrix}$$

$$\dot{\underline{r}} = \underline{v} = \frac{\varepsilon_0 a}{\hbar}\begin{pmatrix}\sin(k_x a)\\ \sin(k_y a)\\ \sin(k_z a)\end{pmatrix}$$

$$\left.\begin{array}{l}\underline{E} = \mathrm{const}\\ \underline{B} = 0\end{array}\right\} \Rightarrow \hbar\dot{\underline{k}} = -e\underline{E}$$

$$\underline{k}(t) = -\frac{e\underline{E}}{\hbar}t$$

$$\dot{x}(t) = -\frac{\varepsilon_0 a}{\hbar}\sin\left(\frac{eE_x a}{\hbar}t\right) \Rightarrow x(t) = \frac{\varepsilon_0 a}{\hbar}\frac{\hbar}{E_x e}\cos\left(\frac{eE_x a t}{\hbar}\right) = \frac{\varepsilon_0}{eE_x}\cos\left(\frac{eE_x a}{\hbar}t\right)$$



Vezetési jelenségek fémekben, szemiklassz. leírás

$g_n(\underline{r},\underline{k},t)\,d^3\underline{r}\,\frac{d^3\underline{k}}{(2\pi)^3}$ az n-edik sávban lévő elektronok száma t időpillanatban a fázistér $d^3\underline{k}\cdot d^3\underline{r}$ térfogatában az $(\underline{r},\underline{k})$ pontban

egyensúlyban:

$$g_n^{(0)} = f(\varepsilon_n(\underline{k})) \Rightarrow f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

Külső térben

$$\hbar\dot{\underline{k}} = -e(\underline{E} + \underline{v}\times\underline{B})$$

$$\underline{v}_n = \frac{1}{\hbar}\,\mathrm{grad}_{\underline{k}}\,\varepsilon_n(\underline{k})$$

ütközés → relaxációs közelítés

$$dg = \frac{dt}{\tau(\underline{r},\underline{k})}\,g_n^{(0)}(\underline{r},\underline{k})$$

$$g(\underline{k},t) = g^0(\underline{k}) + \int_{-\infty}^{t} dt' \, e^{-\frac{t-t'}{\tau(\varepsilon(\underline{k}))}} \left(-\frac{\partial g^0}{\partial \varepsilon}\right) \underline{v}(\underline{k}(t')) \Big[-e\underline{E}(t') - \operatorname{grad}_{\underline{r}} \mu(t') - \frac{\varepsilon(\underline{k})-\mu}{T} \operatorname{grad}_{\underline{r}} T(t') \Big]$$

- $\underline{B}$ explicitem nincs benne, de mozgásegyenleten keresztül $\underline{r}(t)\,\underline{k}(t)$ megoldásban
- gyenge E, kicsi grad T közelítés
- $\tau = \tau(\varepsilon(\underline{k}))$ közelítés

spec. eset. $B = 0 \Rightarrow \underline{k}(t') = \underline{k}$

$\underline{E}$ sztatikus

grad T nem függ t-től

$$g(\underline{k}) = g^0(\underline{k}) - e\underline{E}\cdot\underline{v}(\underline{k})\cdot\tau(\varepsilon(\underline{k}))\left(-\frac{\partial g^0}{\partial \varepsilon}\right)$$

áramsűrűség $\quad \underline{j} = -e 2 \int \frac{d^3k}{(2\pi)^3} g\,\underline{v}(\underline{k})$

spin

$\underline{j} = \underline{\underline{\sigma}}\,\underline{E}$

$$\underline{\underline{\sigma}}^{(n)} = e^2 \int \frac{d^3k}{4\pi^3} \tau_n(\varepsilon_n(\underline{k}))\, \underline{v}_n(\underline{k}) \circ \underline{v}_n(\underline{k}) \left(-\frac{\partial g^0}{\partial \varepsilon}\right)\Big|_{\varepsilon=\varepsilon_n} \qquad (0)$$

n = sávindex

köbös rács

ha $\underline{j} \parallel \underline{E} \Rightarrow \underline{\underline{\sigma}}$ diagonális

teljesen betöltött sávra $\underline{\underline{\sigma}} = 0$

$\underline{\underline{\sigma}}$ különböző alakjai

a) fémben $T = 0$ közelítés jó

$$-\frac{\partial f}{\partial \varepsilon} = \delta(\varepsilon - \varepsilon_F)$$

$$\sigma_{\alpha\beta} = e^2 \tau(\varepsilon_F) \int \frac{d^3k}{4\pi^3} v_\alpha v_\beta \left(-\frac{\partial f}{\partial \varepsilon}\right)\Big|_{\varepsilon=\varepsilon(k)} = e^2 \tau(\varepsilon_F) \int \frac{d^3k}{4\pi^3} v_\alpha \cdot$$

$$\cdot \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial k_\beta} \frac{-\partial f}{\partial \varepsilon}\Big|_{\varepsilon=\varepsilon_F} =$$

$$= e^2 \tau(\varepsilon_F) \int \frac{d^3k}{4\pi^3} v_\alpha \left(-\frac{1}{\hbar}\frac{\partial f}{\partial k_\beta}\right) \overset{\text{parc. int}}{=}$$

$$= e^2 \tau(\varepsilon_F) \int \frac{d^3k}{4\pi^3} \frac{1}{\hbar} \frac{\partial v_\alpha}{\partial k_\beta} f(\varepsilon(k))$$

$(M^{-1})_{\alpha\beta}$

$$\sigma_{\alpha\beta} = e^2 \tau(\varepsilon_F) \int_{\substack{\text{betöltött}\\ \text{állapotokra}}} \frac{d^3k}{4\pi^3} (M^{-1})_{\alpha\beta} \qquad (a)$$

pl: $\varepsilon(k) = \dfrac{\hbar^2 k^2}{2m^*}$

$$(M^{-1})_{\alpha\beta} = \frac{1}{m^*}\delta_{\alpha\beta}$$

elektron szám-sűrűség

$$\boxed{\sigma_{\alpha\beta} = \frac{e^2 \tau n}{m^*} \delta_{\alpha\beta}} \quad \text{Drude-modell}$$

$$\left(\frac{N}{V} = n = \int \frac{d^3k}{4\pi^3} f(\varepsilon(k)) \right)$$

b) köbös rácsban $\sigma_{\alpha\beta} = \sigma \delta_{\alpha\beta}$

$$v_\alpha v_\beta = c\, \delta_{\alpha\beta}$$

$$v^2 = c \cdot 3 \Rightarrow c = \frac{v^2}{3}$$

$$\sigma = e^2 \frac{1}{3 \cdot 4\pi^3} \frac{\tau}{\hbar} \int d^3k\, |v(k)| \left| \frac{\partial \varepsilon(k)}{\partial k} \right| \left(-\frac{\partial f}{\partial \varepsilon} \right) \Bigg|_{\varepsilon = \varepsilon(k)} = *$$

$dk_\perp$ konst ε-os $\parallel v$

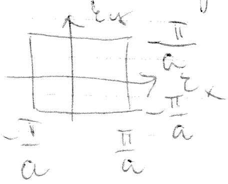
$dS_\varepsilon \to$ felületelem $\qquad d^3k = dS_\varepsilon\, dk_\perp$

$$\frac{\partial \varepsilon}{\partial k} = \frac{\partial \varepsilon}{\partial k_\perp}$$

$$* = \frac{e^2 \tau}{12\pi^3 \hbar} \iint dS_\varepsilon \int dk_\perp |v(k)| \frac{\partial \varepsilon}{\partial k_\perp} \underbrace{\left(-\frac{\partial f}{\partial \varepsilon} \right)}_{\approx \delta(\varepsilon(k) - \varepsilon_F)} =$$

$$\sigma = \frac{e^2 \tau}{12\pi^3 \hbar} \iint_{\substack{\text{Fermi}\\ \text{felület}}} dS_\varepsilon\, |v(k)| \qquad (b)$$

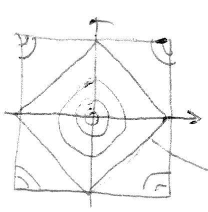
Példa: tight-binding, négyzetrácsos



$$\varepsilon(k) = \varepsilon_0 - 2\lambda \cos k_x a - 2\lambda \cos k_y a$$

1 elektron / elemi cella

$$\cos k_x a \approx 1 - \frac{(k_x a)^2}{2}$$



$$(k_x a)^2 + (k_y a)^2 = a^2 (k_x^2 + k_y^2) = a^2 k^2$$

→ konst felület → Fermi-felület ha 1 e^- cellánként $\qquad \varepsilon_F = \varepsilon_0$

a) $\sigma_{xx} = \sigma_{yy} = \sigma$

$$\underline{v} = \frac{1}{\hbar} \operatorname{grad} \varepsilon(\underline{k}) = \frac{1}{\hbar} 2\lambda a \begin{pmatrix} \sin(k_x a) \\ \sin(k_y a) \end{pmatrix}$$

$$(b) \Rightarrow \sigma_{xx} = \frac{e^2}{2\pi^2} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} dk_x\, dk_y \left(\frac{2\lambda a}{\hbar}\right)^2 \sin^2(k_x a)\, \delta(\varepsilon(k) - \varepsilon_F) =$$

$$= \frac{e^2 \tau}{2\pi^2} \left(\frac{2\lambda a}{\hbar}\right)^2 4 \iint_0^{\pi/a} \sin^2(k_x a)\, \delta(\underbrace{2\lambda \cos(k_x a) + 2\lambda \cos(k_y a)}_{f(k_x)}) =$$

$$\delta(f(x)) = \sum_{f(x_i)=0} \frac{\delta(x - x_i)}{|f'(x_i)|}$$

$f'(k_x) = -2\lambda a \sin(k_x a)$

$\Rightarrow \delta\left(k_x - \left(\frac{\pi}{a} - k_y\right)\right)$

$$= \frac{e^2 \tau}{2\pi^2} 4 \left(\frac{2\lambda a}{\hbar}\right)^2 \iint_0^{\pi/a} \sin^2(k_x a) \frac{1}{2\lambda a \sin(k_x a)} \delta\left(k_x + k_y - \frac{\pi}{a}\right) dk_x\, dk_y$$

$$= \frac{4 e^2 \tau \lambda a}{\pi^2 \hbar^2} \underbrace{\int_0^{\pi/a} \sin\left(\frac{\pi}{a} - k_y\right) a\, dk_y}_{2/a} =$$

$$= \frac{8 e^2 \tau \lambda}{\pi^2 \hbar} = \frac{2e^2}{4} \frac{16 \lambda \tau}{h}$$

$$(a) \Rightarrow (M^{-1})_{xx} = \frac{1}{\hbar} \frac{\partial v_x}{\partial k_x} = \ldots = \frac{2\lambda a^2}{\hbar^2} \cos k_x a$$

$$\sigma_{xx} = \frac{e^2 \tau}{2\pi} \int dk_x\, dk_y \frac{2\lambda a^2}{\hbar^2} \cos(k_x a) = 4 \frac{e^2 \tau}{2\pi^2} \frac{2\lambda a^2}{\hbar^2} \int_0^{\pi/a} dk_y \underbrace{\int_0^{\frac{\pi}{a} - k_y} dk_x \cos(k_x a)}_{\frac{1}{a} \sin\left(\frac{\pi}{a} - k_y a\right)}$$

$$= \frac{8 e^2 \tau \lambda}{\pi^2 \hbar^2}$$

$$(b) \Rightarrow \sigma = \frac{e^2 \tau}{4\pi^2 \hbar} \int_{\text{Fermi}} dS_{\varepsilon_F}\, |v(k)| =$$

felület $\to$ vonal $\to$ $dS_{\varepsilon_F} = \sqrt{2}\, dk_x$

$$= \frac{e^2 \tau}{4\pi^2 \hbar} \sqrt{2}\, 4 \int_0^{\pi/a} dk_x\, |v| = \frac{e^2 \tau \sqrt{2}}{4\pi^2 \hbar} 4 \int_0^{\pi/a} dk_x \frac{2\lambda a}{\hbar} \underbrace{\sqrt{\sin^2(k_x a) + \sin^2(k_y a)}}_{\sqrt{2 \sin^2 k_x a}} =$$

$$= \frac{e^2 \tau \sqrt{2}}{4\pi^2 \hbar} 4\sqrt{2} \frac{2\lambda a}{\hbar} \underbrace{\int_0^{\pi/a} \sin(k_x a)\, dk_x}_{2/a} =$$

$$= \frac{e^2 \tau \, 8 A}{\pi^2 \hbar^2}$$