1. DRUDE-SOMMERFELDova teória kovov

A) Základné aproximácie:

1. Aproximácia voľných elektrónov $\Longleftrightarrow$ model želé
2. Aproximácia nezávislých elektrónov $\Longleftrightarrow$ zanedbať e-e zrážky
3. Aproximácia relaxačného času:
   - okamžité zrážky
   - stredný voľný čas τ
   - po zrážke je elektrón termalizovaný

B) Elektrónový plyn pri $T=0$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \varepsilon\psi$$

Born - von Kármán:

$$\psi(x,y,z+L) = \psi(x,y,z)$$
$$\psi(x,y+L,z) = \psi(x,y,z)$$
$$\psi(x+L,y,z) = \psi(x,y,z)$$

kocka s objemom $\Omega = L^3$

vl. funkcie $\psi_k(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}}$ $\qquad k = \frac{2\pi}{L}(\underbrace{m,n,l}_{\text{celé čísla}})$

$$1 = \int d^3r\,|\psi_k(r)|^2$$

$$\vec{p}\,\psi_k = \hbar\vec{k}\,\psi_k \qquad \vec{v} = \frac{\hbar\vec{k}}{m} \qquad \varepsilon_k = \frac{\hbar^2\vec{k}^2}{2m} = \frac{1}{2}m\vec{v}^2$$

Počet častíc $\quad N = 2\sum_{k<k_F} 1 = 2\left(\frac{L}{2\pi}\right)^3 \int_{k<k_F} d^3k = \frac{2}{8\pi^3}\,\frac{4\pi}{3}k_F^3\,\Omega$

Fermiho plocha

$$\boxed{n = \frac{N}{\Omega} = \frac{k_F^3}{3\pi^2}} \longrightarrow \boxed{k_F = (3\pi^2 n)^{1/3}}$$

Energia

$$E = 2\left(\frac{L}{2\pi}\right)^3 \int d^3k\,\frac{\hbar^2k^2}{2m} = \frac{\Omega}{5\pi^2}\,\frac{\hbar^2}{2m}\,k_F^5$$

$$\boxed{\frac{E}{N} = \frac{3}{5}\varepsilon_F} \qquad \boxed{\varepsilon_F = \frac{\hbar^2k_F^2}{2m}}$$

• Tlak $\quad p = -\dfrac{\partial E(N,\Omega)}{\partial \Omega} \qquad E = \dfrac{3}{5}\left(3\pi^2\right)^{2/3}\dfrac{\hbar^2}{2m}\dfrac{N^{5/3}}{\Omega^{2/3}}$

$$p = \frac{2}{3}\frac{E}{\Omega} = \frac{2}{3}\cdot\frac{3}{5} n\varepsilon_F \qquad \boxed{p = \frac{2}{5} n \varepsilon_F}$$

• Hustota stavov (počet stavov v jednotkovom objeme so spinom σ)

počet stavov s energiou $< \varepsilon$: $\quad G(\varepsilon) = \dfrac{1}{\Omega}\left(\dfrac{L}{2\pi}\right)^3 \int d^3k = \dfrac{1}{8\pi^3}\dfrac{4\pi}{3}k^3$

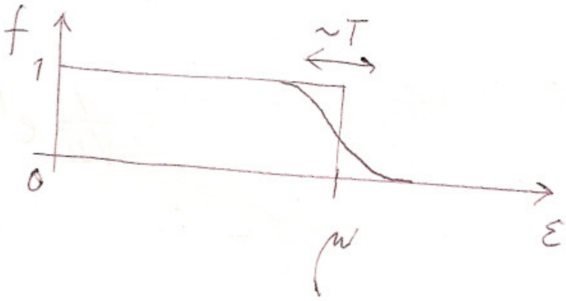
$$G(\varepsilon) = \frac{1}{6\pi^2}\left(\frac{2m\varepsilon}{\hbar^2}\right)^{3/2} \qquad N(\varepsilon) = \frac{dG}{d\varepsilon} \qquad \boxed{N(\varepsilon) = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}}$$

c) Elektrónový plyn pri $T>0$

$$\begin{cases} E = 2\sum_k \varepsilon_k f_k \\ N = 2\sum_k f_k \end{cases} \qquad \boxed{f_k = \frac{1}{e^{\frac{\varepsilon_k-\mu}{T}}+1}} \quad \text{Fermi-Dirac}$$

možno písať:

$$\boxed{\begin{aligned} \frac{E(T)}{\Omega} &= 2\int_0^\infty d\varepsilon\, N(\varepsilon) f(\varepsilon)\,\varepsilon \\ \frac{N}{\Omega} &= 2\int_0^\infty d\varepsilon\, N(\varepsilon) f(\varepsilon) \end{aligned}}$$



Sommerfeldov ~~rozvoj~~ rozvoj:

$$\boxed{\int_0^\infty d\varepsilon\, H(\varepsilon) f(\varepsilon) = \int^{\mu} d\varepsilon\, H(\varepsilon) + \frac{\pi^2}{6}T^2 H'(\mu) + \frac{7\pi^4}{360}T^4 H'''(\mu) + \dots}$$

Dôkaz.

Definujme $K(\varepsilon) = \displaystyle\int_0^\varepsilon d\varepsilon' H(\varepsilon') \quad \longrightarrow \quad H(\varepsilon) = \dfrac{dK}{d\varepsilon}$

Per partes: $\displaystyle\int_0^\infty d\varepsilon\, H(\varepsilon) f(\varepsilon) = \cancel{\left[K(\varepsilon) f(\varepsilon)\right]_0^\infty} + \int_0^\infty d\varepsilon\, K(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right)$

$0 \to$ zameníme za $-\infty$

$$K(\varepsilon) = K(\mu) + \sum_{n=1}^{\infty} \left.\frac{d^n K(\varepsilon)}{d\varepsilon^n}\right|_{\varepsilon=\mu} \frac{(\varepsilon-\mu)^n}{n!}$$

$$\int_0^\infty d\varepsilon\, H(\varepsilon) f(\varepsilon) = K(\mu) \underbrace{\int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right)}_{=1} + \sum_{n=1}^{\infty} \frac{d^n K(\varepsilon)}{d\varepsilon^n} \frac{1}{n!} \underbrace{\int_{-\infty}^{\infty} d\varepsilon\, (\varepsilon-\mu)^n \left(-\frac{\partial f}{\partial \varepsilon}\right)}_{\frac{1}{4T}\int_{-\infty}^{\infty} \frac{d\varepsilon\,(\varepsilon-\mu)^n}{\cosh^2\left(\frac{\varepsilon-\mu}{2T}\right)}}$$

$$\int_0^\infty d\varepsilon\, H(\varepsilon) f(\varepsilon) = \int_0^\mu d\varepsilon\, H(\varepsilon) + \frac{1}{2} \sum_{n=1}^{\infty} \frac{d^{n-1} H}{d\varepsilon^{n-1}} \frac{(2T)^n}{n!} \underbrace{\int_{-\infty}^{\infty} \frac{dx\, x^n}{\cosh^2 x}}_{\text{iba párne } n}$$

Tieto integrály možno vypočítať a dostaneme Sommerfeldov rozvoj

D) Závislosť $\mu = \mu(T)$

$$\frac{N}{\Omega} = 2\int_0^\infty d\varepsilon\, N(\varepsilon) f(\varepsilon) = 2\int^\mu d\varepsilon\, N(\varepsilon) + \frac{\pi^2}{3} T^2 N'(\mu) + \dots$$

pri $T = 0$:

$$\frac{N}{\Omega} = 2\int^{\varepsilon_F} d\varepsilon\, N(\varepsilon) \longrightarrow \text{Porovnaním dostaneme}$$

$$\int^{\varepsilon_F} d\varepsilon\, N(\varepsilon) \approx \int^{\mu} d\varepsilon\, N(\varepsilon) + \frac{\pi^2}{6} T^2 N'(\mu) \qquad (*)$$

$\mu = \varepsilon_F + \delta\mu$, ukážeme $\delta\mu = O(T^2)$

$$(*) \longrightarrow \delta\mu\, N(\varepsilon_F) + \frac{\pi^2}{6} T^2 N'(\varepsilon_F) = 0 \longrightarrow \boxed{\delta\mu = -\frac{\pi^2}{6} T^2 \frac{N'(\varepsilon_F)}{N(\varepsilon_F)}}$$

$$\boxed{\mu = \varepsilon_F - \frac{\pi^2}{6} T^2 \frac{N'(\varepsilon_F)}{N(\varepsilon_F)}}$$

korekcia rádu $\frac{T^2}{\varepsilon_F} \ll \varepsilon_F$

E) Merné teplo

$$c_V = \frac{1}{\Omega}\left(\frac{\partial E}{\partial T}\right)_\Omega \qquad \frac{E(T)}{\Omega} = 2\int^{\mu} d\varepsilon\, N(\varepsilon)\varepsilon + \frac{\pi^2}{3}T^2\left[N(\varepsilon)\varepsilon\right]'_{\varepsilon=\mu}$$

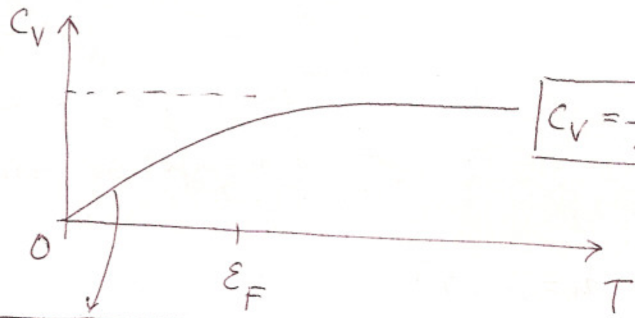
s presnosťou do rádu T^2:

$$\frac{E(T)}{\Omega} = 2\int^{\varepsilon_F} d\varepsilon\, N(\varepsilon)\varepsilon + 2\delta\mu\, N(\varepsilon_F)\varepsilon_F + \frac{\pi^2}{3}T^2\left[N'(\varepsilon_F)\varepsilon_F + N(\varepsilon_F)\right]$$

súčet $= 0$

$$E(T) = E(0) + \frac{\pi^2}{3}T^2 N(\varepsilon_F)\Omega \longrightarrow \boxed{c_V = \frac{2\pi^2}{3}N(\varepsilon_F)\,T}$$

$$N(\varepsilon_F) = \frac{3}{4}\frac{n}{\varepsilon_F} \longrightarrow$$

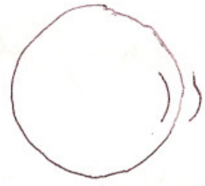


$\boxed{c_V = \frac{3}{2}n}$ klasická štatistika $T \gg \varepsilon_F$

$\boxed{c_V = \frac{\pi^2}{2}\frac{T}{\varepsilon_F}n}$ kvant. štatistika, $T \ll \varepsilon_F$

$c_V \to 0$ pri $T \to 0$ (3. veta termodynamická)

fyzikálny zmysel: vo fermiónovom systéme sú excitované len stavy okolo ε_F:



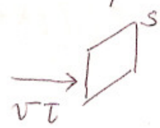
počet stavov $\sim N(\varepsilon_F)T$

) Drudeho transportná teória

- **vodivosť**: hneď po zrážke: $\langle \vec{v} \rangle = 0$

urýchlenie počas τ: $\langle \vec{v} \rangle = \dfrac{e\vec{E}\tau}{m}$

prúd cez plochu S za čas τ



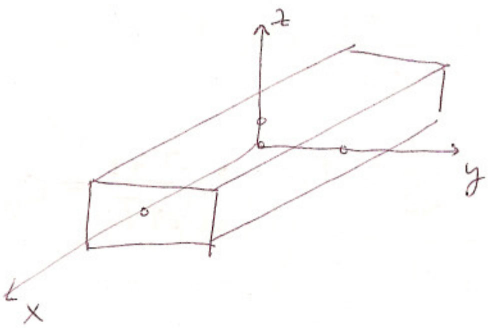
$$I = \frac{Q}{\tau} = \frac{e n \langle v \rangle \tau S}{\tau} = e n \langle v \rangle S$$

$$\vec{j} = e n \langle \vec{v} \rangle = \sigma_0 \vec{E} \qquad \boxed{\sigma_0 = \frac{n e^2 \tau}{m}}$$ merná vodivosť

$$\boxed{e = -|e|}$$

nezávisí od znamienka e !

- **Hallov jav** $\quad m\left(\dot{\vec{v}} + \dfrac{\vec{v}}{\tau}\right) = e\left(\vec{E} + \vec{v} \times \vec{B}\right)$



$$\vec{B} = (0, 0, B)$$

v ustálenom stave:

$$\vec{v} = \frac{e\tau}{m}\left(\vec{E} + \vec{v} \times \vec{B}\right)$$

$$\begin{cases} v_x = \dfrac{e\tau}{m}\left(E_x + v_y B\right) \\ v_y = \dfrac{e\tau}{m}\left(E_y - v_x B\right) \end{cases}$$

$\vec{j} = ne\vec{v}$

$$\begin{pmatrix} 1 & -\omega_c \tau \\ \omega_c \tau & 1 \end{pmatrix} \begin{pmatrix} j_x \\ j_y \end{pmatrix} = \sigma_0 \begin{pmatrix} E_x \\ E_y \end{pmatrix} \qquad \boxed{\omega_c = \frac{eB}{m}}$$ cyklotrónová frekvencia

- **Tenzor odporu** $\quad E_i = \rho_{ik} j_k \qquad \rho_{ik} = \dfrac{1}{\sigma_0}\begin{pmatrix} 1, & -\omega_c \tau \\ \omega_c \tau, & 1 \end{pmatrix}$

- **Tenzor vodivosti** $\quad j_i = \sigma_{ik} E_k$

$$\sigma_{ik} = \frac{\sigma_0}{1 + (\omega_c \tau)^2}\begin{pmatrix} 1 & \omega_c \tau \\ -\omega_c \tau & 1 \end{pmatrix}$$

- **Geometria experimentu:**

$\vec{j} = (j_x, 0) \longrightarrow \boxed{E_x = \dfrac{1}{\sigma_0} j_x}$ pozdĺžne napätie $\qquad \boxed{E_y = \dfrac{B}{ne} \cdot j_x}$ Hallovo napätie (znamienko e !)

Tepelná vodivosť

$$\vec{j}_Q = -\varkappa \vec{\nabla} T$$

jednoduchý 1D model:

$$j_Q(\rightarrow) = \frac{n}{2} v\, \varepsilon(T[x - v\tau])$$

počet elektrónov doprava

energia/častica v mieste $x - v\tau$

$$j_Q(\leftarrow) = -\frac{n}{2} v\, \varepsilon(T[x + v\tau])$$

$$j_Q = \frac{1}{2} n v \left[\varepsilon(T[x - v\tau]) - \varepsilon(T[x + v\tau])\right] = n v \frac{d\varepsilon}{dT}\left(-\frac{dT}{dx}\right) v\tau$$

$$j_Q = n v^2 \tau \frac{d\varepsilon}{dT}\left(-\frac{dT}{dx}\right)$$

v 3D: $v^2 \rightarrow v_x^2 = \frac{1}{3} v^2$

$$\vec{j}_Q = -\frac{1}{3} n v^2 \tau \frac{d\varepsilon}{dT} \vec{\nabla} T$$

$$\varkappa = \frac{1}{3} v^2 \tau \frac{d n\varepsilon}{dT}$$

$$n\varepsilon = \frac{1}{\Omega} E(T) \rightarrow \frac{d n\varepsilon}{dT} = C_V$$

$v \rightarrow v_F$

$$\boxed{\varkappa = \frac{1}{3} v_F^2 \tau C_V}$$

Wiedemann-Franz:

$$\boxed{\frac{\varkappa}{\sigma T} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2}$$

... dobrý súlad teórie s experimentom

Termonapätie

$\vec{\nabla} T$

$\vec{E}$

aby netiekol prúd, $\vec{\nabla} T$ indukuje $\vec{E}$

$$\vec{E} = S \vec{\nabla} T$$

S = Seebeckov koef.

prítomnosť $\vec{E}$ spôsobuje .. $\vec{v}_E = \frac{e\vec{E}\tau}{m}$

prítomnosť $\vec{\nabla} T \Rightarrow$

1D model: $v_Q = \frac{1}{2}\left[v(x - v\tau) - v(x + v\tau)\right]$

$$v_Q = -\tau \frac{d}{dx}\left(\frac{v^2}{2}\right)$$

3D model: $\vec{v}_Q = -\frac{\tau}{3} \vec{\nabla}\left(\frac{v^2}{2}\right) = -\frac{\tau}{3} \frac{d(v^2/2)}{dT} \vec{\nabla} T$

žiadame $\vec{v}_E + \vec{v}_Q = 0 \rightarrow$ $E = \frac{1}{3e} \frac{d}{dT}\left(\frac{1}{2} m v^2\right) \vec{\nabla} T$ $\rightarrow$ $\boxed{S = \frac{C_V}{3ne}}$

o) Problémy Drude-Sommerfeldovej teórie:

- **Hallova konštanta** $R_H = \frac{E_y}{B j_x} = \frac{1}{ne} = -\frac{1}{n|e|} < 0$, nezávisí od T, B

experiment: R_H závisí od T, B, R_H môže byť kladné! (napr. Al)

- **Seebeckov koeficient** $S = -\frac{c_V}{3n|e|} < 0$ ... opäť môže byť kladný!

- **Čo mení počet voľných elektrónov?**

C ... $1s^2 2s^2 2p^2$ izolant (diamant); polokov (grafit)

Si ... $[Ne] 3s^2 3p^2$ polovodič (diamant)

Ge ... $[Ar] 3d^{10} 4s^2 4p^2$ polovodič (diamant)

Sn ... $[Kr] 4d^{10} 5s^2 5p^2$ kov (biely cín, bct); polovodič (sivý cín, diamant)

Pb ... $[Xe] 4f^{14} 5d^{10} 6s^2 6p^2$ kov (fcc)