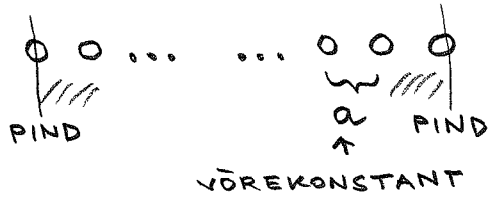
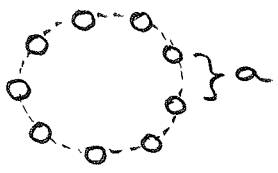
ELEKTRONI FERMI LAINEVEKTOR, KIIRUS JA ENERGIA

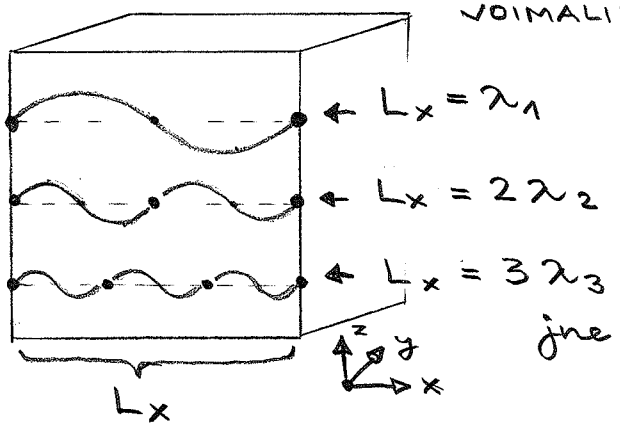
BOHRI MUDELI JUURES KASUTATUD "TSÜKLILINE RAJATINGIMUS":
VAATLEME MITTE POTENTSIAALILOHU SERVADELT TAGASI PEEGELDUVAT VAID RINGORBIIDIL KULGEVAT ELEKTRONILAINET.

TAHKISES: ASENDAME AATOMITEST KOOSNEVA FIKSEERITUD OTSTEGA "KETI"



⇒ SULETUD "KETIGA" (SEOME "OTSAD" MÕTTELISELT KOKKU...)





VÕIMALIKUD ELEKTRONILAINED KUUBIKUDULISES TAHKISE TÜKIS:

$$\lambda_n = \frac{L_x}{n} \;;\; k_x = \frac{2\pi}{\lambda_n} = \frac{2\pi}{L} n$$

(n ↑ KVANTARV)

SEEGA k_x SAAB MUUTUDA

$$\Delta k_x = \frac{2\pi}{L}$$ KAUPA.

SAMA KEHTIB k_y JA k_z KOHTA.

TÕRJUTUSPRINTSIIP (PAULI): ELEKTRONIL ON PERSOONAALNE RUUM, AGA KA PERSOONAALNE FAASIRUUM POORDVÕRES (k-RUUMIS).
ÜKS LUBATUD KAHEELEKTRONILINE (SPINNID ↑↓) OLEK PAIKNEB k-RUUMI "KUUBIS" SERVA PIKKUSEGA $2\pi/L$ JA "RUUMALAGA" "V_1"

$$\left(\frac{2\pi}{L}\right)^3 = \frac{8\pi^3}{V}$$, KUS $V = L^3$ ON TAHKISE "TÜKI" RUUMALA.

OLEKUTE KONTSENTRATSIOON "POORDRUUMIS": "n" $= \frac{"N"}{"V"} = \frac{1}{"V_1"}$ ← 2-EL. OLEKU RUUMALA

SEEGA: "n" $= \frac{V}{8\pi^3}$. OLEKUD "TÄIDAVAD SFÄÄRI" "RAADIUSEGA" k_F (NN. FERMI LAINEVEKTOR) JA "RUUMALAGA" $\frac{4}{3}\pi k_F^3$.

KUI UURITAVAS TAHKISE "TÜKIS" ON N JUHTIVUSELEKTRONI, (KONTS. $n = \frac{N}{V}$)

SIIS: $N = \underset{(\uparrow\downarrow)}{2} \cdot \underbrace{\frac{V}{8\pi^3}}_{"n"} \cdot \underbrace{\frac{4}{3}\pi k_F^3}_{"V"} = \frac{V}{3\pi^2} k_F^3$ JA $\frac{3\pi^2 N}{V} = k_F^3$

SEEGA: $\boxed{k_F = (3\pi^2 n)^{1/3}}$, $v_F = \frac{p_F}{m} = \frac{\hbar k_F}{m} = \boxed{\frac{\hbar}{m}(3\pi^2 n)^{1/3}}$ ← IMPULSS

FERMI LAINEVEKTOR ↑ ELEKTRONI FERMI KIIRUS

JA FERMI ENERGIA: $E_F = \frac{(\hbar k_F)^2}{2m} = \boxed{\frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}}$

ELEKTRONOLEKUTE TIHEDUS

$$\mathcal{D}(E) = \frac{d^2 z}{dE\, dV}$$ "NÄITAB OLEKUTE ARVU z ÜHIKULISE ENERGIAVAHEMIKU KOHTA JA ÜHIKULISE RUUMALAGA V AINETÜKIS.

KUI ÜKS 2-ELEKTRONILINE $(\uparrow\downarrow)$ OLEK VÕTAB k-RUUMIS ENDA ALLA "RUUMALA" $\frac{8\pi^3}{V}$, SIIS p-RUUMIS TA VÕTAB $\hbar^3 \cdot \frac{8\pi^3}{V} = \frac{h^3}{V}$.

OLEKUTE KONTSENTRATSIOON p-RUUMIS: $n_p = \frac{1}{\text{"}V_1\text{"}} = \frac{V}{h^3} = \frac{V}{8\pi^3 \hbar^3}$

p-RUUMI "SFAARI" KIHIS PAKSUSEGA dp JA "RAADIUSEGA" p $\Rightarrow$ SEEGA "RUUMALAGA" $4\pi p^2 dp$

ON $dz = 2 \cdot \underbrace{\frac{V}{8\pi^3 \hbar^3}}_{n_p} \cdot \underbrace{4\pi p^2 dp}_{\text{"RUUMALA"}}$ ÜHEELEKTRONILIST OLEKUT.

$(\uparrow\downarrow)$

ARV = KONTS. × "RUUMALA"

ARVESTAME, ET:

$$E = \frac{p^2}{2m} \Rightarrow p = (2mE)^{1/2}$$

$$\frac{dE}{dp} = \frac{2p}{2m} = v \quad \text{(DISPERSIOONISEOS)},$$

MILLEST $dp = \frac{m}{p} dE$ (*)

NÜÜD SIIS:

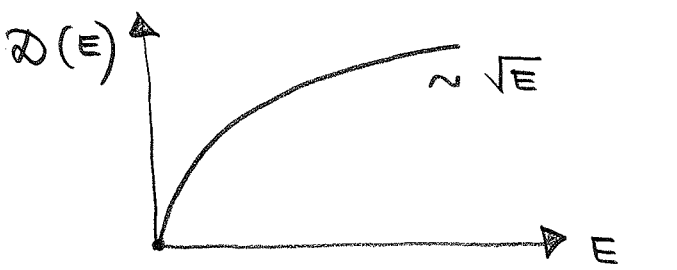
$$dz = 2 \underbrace{\frac{V}{8\pi^3 \hbar^3}}_{n_p} 4\pi \underbrace{2mE}_{p^2} \cdot \underbrace{m (2mE)^{-1/2}}_{m/p} dE = \ldots$$

dp (*)

$$\ldots = (2m)^2 \frac{V}{2\pi^2 \hbar^3} (2m)^{-1/2} E^{1-1/2} dE$$

$$\mathcal{D}(E) = \frac{d^2 z}{dE\, dV} = \frac{1}{2\pi^2} \frac{(2m)^{3/2}}{(\hbar^2)^{3/2}} E^{1/2} = \underbrace{\frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2}}_{\text{const}} E^{1/2}$$

$$\mathcal{D}(E) = \text{const} \cdot \sqrt{E}$$



ELEKTRONOLEKUTE TIHEDUS LUBATUD ENERGIATSOONI "ÄÄRE LÄHEDUSES:

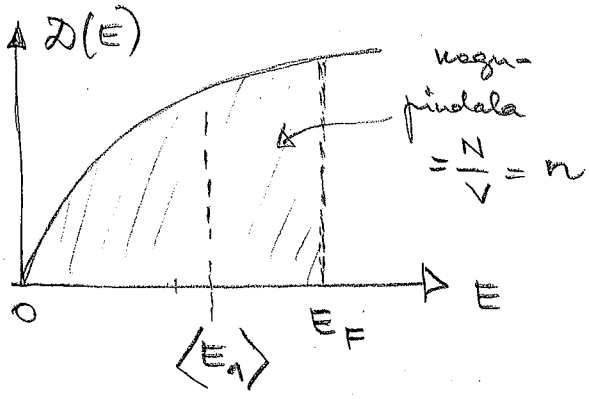
$\left(E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}, \text{ NII ET } m = \text{const}\right)$

... ENERGIATASEMED

ÜHE JUHTIVUSELEKTRONI KESKMINE ENERGIA

$\langle E_1 \rangle = \frac{E_{kogu}}{N}$ — <u>kõigi elektronide koguenergia</u> / elektronide arv

$$E_{kogu} = \cancel{N}^{*} \cdot \langle E_1 \rangle = \int_0^{E_F} \int_0^{V} \mathcal{D}(E) \cdot E \, dV \, dE =$$



$$= \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \cdot V \int_0^{E_F} E^{1+\frac{1}{2}} \, dE =$$

$$= \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \cdot V \cdot \frac{E_F^{5/2}}{5/2} =$$

$$= \frac{1}{\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \cdot V \cdot \frac{1}{5} \cdot \underbrace{\left[\frac{\hbar^2}{2m} \cdot \left(3\pi^2 n \right)^{2/3} \right]^{3/2}}_{E_F} \cdot E_F =$$

$$= \frac{1}{5\pi^2} \cancel{\left(\frac{2m}{\hbar^2} \right)^{3/2}} \cdot V \cdot \cancel{\left(\frac{\hbar^2}{2m} \right)^{3/2}} \cdot 3\pi^2 n \cdot E_F = \frac{3}{5} \overset{*}{N} E_F$$

$[V \cdot n = N]$

Seega $\boxed{\langle E_1 \rangle = \frac{3}{5} E_F}$

Kui valitsus $\mathcal{D}(E) \sim E$, siis oleks $\langle E_1 \rangle = \frac{1}{2} E_F$

Aga meie $\mathcal{D}(E) \sim \sqrt{E}$, siis $\langle E_1 \rangle = \frac{3}{5} E_F$ (rohkem!)

Cu (ühevalentnise eeldusel):

$$n = \rho \frac{N_A}{M} = 8{,}9 \frac{g}{cm^3} \frac{6 \cdot 10^{23} \frac{1}{mol}}{63{,}5 \frac{g}{mol}} =$$

$$= 8{,}5 \cdot 10^{22} \, cm^{-3} = 8{,}5 \cdot 10^{28} \, m^{-3}$$

$$k_F = \left(3\pi^2 n \right)^{1/3} =$$

$$= \left(3\pi^2 \cdot 8{,}5 \cdot 10^{28} \right)^{1/3} m^{-1} =$$

$$= \left(2{,}55 \cdot 10^{30} \right)^{1/3} m^{-1} \cong 1{,}37 \cdot 10^{10} \, m^{-1}$$ ← Fermi lainevektor

$$\lambda_F = \frac{2\pi}{k_F} = \frac{6{,}28}{1{,}37 \cdot 10^{10} \, m^{-1}} \cong 4{,}87 \cdot 10^{-10} \, m \cong 4{,}9 \, \text{Å}$$

Fermi lainepikkus

Võrevõntant on $3{,}61$ Å $\Rightarrow$ Fermi

ääre ja 1. Brillouini tsoon on ligikaudu ühesuurused.

Fermi kiirus $v_F = \frac{\hbar k_F}{m} = \frac{1{,}05 \cdot 10^{-34} \, J \cdot s \cdot 1{,}37 \cdot 10^{10} \, m^{-1}}{9{,}1 \cdot 10^{-31} \, kg} \cong 1{,}4 \cdot 10^{6} \, m/s$

vrd. $2{,}2 \cdot 10^{6}$ m/s Bohri kiirus.

Fermi energia $E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\left(1{,}05 \cdot 10^{-34} \right)^2 \cdot \left(1{,}37 \cdot 10^{10} \right)^2}{2 \cdot 9{,}1 \cdot 10^{-31} \cdot 1{,}6 \cdot 10^{-19}} \, eV \approx 6 \, eV$

$\frac{1}{2} kT \cong 0{,}04 \, eV \cong 230 \, kT$ (RT)