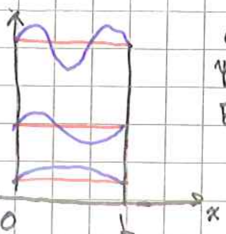
③ 24/1 2013

Frielektronmodellen (FEM)

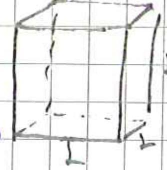


$V(x)=0$
$\Psi(x)\sim\sin(x)$
$E=\frac{\hbar^2k^2}{2m}$

Fixa RV.
$k=\frac{2\pi}{\lambda}=\frac{\pi}{L}n,$
$n=1,2,3\ldots$

Annan representation:

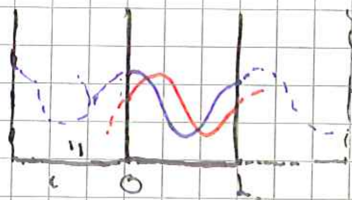
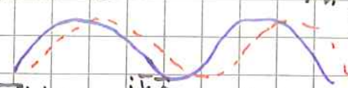
3D:



$k_i=\frac{\pi}{L}n_i$
$\Psi(x,y,z)\sim\sin(k_xx)\sin(k_yy)\sin(k_zz)$
$E=\frac{\hbar^2}{2m}(k_x^2+k_y^2+k_z^2)=$
$=\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}(n_x^2+n_y^2+n_z^2)$
$(n_x,n_y,n_z,\text{spinn})$
~10^{-15} eV om L=1cm
jmf. $kT\sim25$ meV@RT

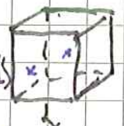
$L=1$cm, $n\sim10^{28}\,m^{-3}\rightarrow$ antal e^- $10^{28}\cdot(10^{-2})^3=10^{22}$ st.
⟹ Tillståndstäthet.

Fixa RV: stående vågor $\Psi(x,t)\sim\sin(kx)e^{-iE/\hbar\cdot t}$
periodiska RV → gående vågor $\Psi(x,t)\sim e^{i(kx-\omega t)}$ $\omega=E/\hbar$

3D: $\phi(\bar r)\sim e^{i\bar k\bar r}$ $k=(k_x,k_y,k_z)$
$E=\frac{\hbar^2k^2}{2m}$ $k^2=\bar k\cdot\bar k=(k_x^2,k_y^2,k_z^2)$

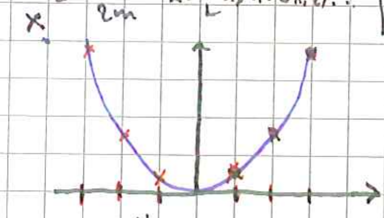
$\phi(x,y,z)=\phi(x+L,y,z)=\phi(x,y+L,z)=\phi(x,y,z+L)$



$\phi(\bar r)\sim e^{i(k_xx,k_yy,k_zz)}$
x-led: $e^{ik_xx}=e^{ik_x(x+L)}\Rightarrow e^{ik_xL}=1.\Rightarrow k_xL=2\pi\cdot n.$
∴ $k_x=\frac{2\pi}{L}\cdot n_x,\ n_x=0,\pm1,\pm2,\ldots$

e^{ik_xx} & e^{-ik_xx} samma E, olika riktning.

Fixa RV	Periodiska RV.
$\Psi\sim\sin(kx)$	$\Psi\sim e^{ikx}$
$E=\frac{\hbar^2k^2}{2m}$ $k=\frac{\pi}{L}n,\ n=0,1,2,\ldots$	$E=\frac{\hbar^2k^2}{2m}$ $k=\frac{2\pi}{L}n,\ n=0,\pm1,\pm2,\ldots$



operator i kin. energi:
$H=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$
rörelsemängd:
$P=-i\hbar\frac{d}{dx}$

Ψ	e^{ikx}	$\sin(kx)$
H	$\frac{\hbar^2k^2}{2m}$ ✓	$\frac{\hbar^2k^2}{2m}$ ✓
P	$\hbar k$ ✓	✗

Energi och rörelsemängd väldef.

p för $\sin(kx)$?
$\langle p\rangle=0$
$\sin(kx)=\frac{1}{2i}(e^{ikx}-e^{-ikx})$

$|e^{ikx}|=1.$ Exakt rörelsemängd ⟹ Obestämd position
$\Delta x\cdot\Delta p\geq\hbar$

Fria elektroner e^{ikx} $p=\hbar k$ $(=mv)$.

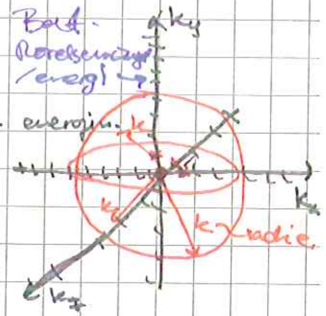
Tillståndstäthet

$Z(E)=\frac{dS(E)}{dE}$ S(E): antal tillstånd m. energi ≤E.

$dS(E)=Z(E)dE$: antal tillstånd mellan E och E+dE

$E=\frac{\hbar^2}{2m}(k_x^2+k_y^2+k_z^2)$ $k_i=\frac{2\pi}{L}n_i$

avstånd till vilken vågor når om energi...



$E=\frac{\hbar^2k^2}{2m}.$

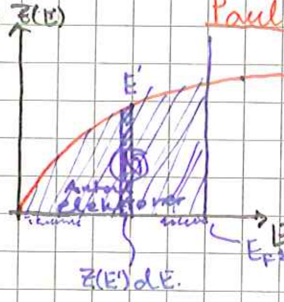
$S(k)=\frac{4\pi k^3}{3}\cdot2$ / Volymen per k-punkt.

$S(k)=\frac{4\pi k^3}{3}\cdot2\left(\frac{L}{2\pi}\right)^3$
$E=\frac{\hbar^2k^2}{2m}$
$S(E)=\frac{2L^3}{(2\pi)^3}\frac{4\pi}{3}\left(\frac{2m}{\hbar^2}\right)^{3/2}$ [illegible]
$Z(E)=\frac{dS(E)}{dE}=4\pi L^3\left(\frac{2m}{h^2}\right)^{3/2}\sqrt{E}$
$=C\sqrt{E}$

Tillståndstäthet för FEM (3D)

$\left(\frac{2\pi}{L}\right)^3$

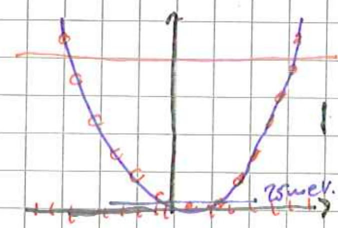
Lägger i e^- i tillstånden
el. konc. n. $N=n\cdot L^3$ st e^-
Om T=0K: alla e^- ligger så lågt de kan.
Pauliprincipen.



$N=nL^3=\int_0^{E_F}Z(E)dE=$ (T=0)
$=\int_0^{E_F}C\sqrt{E}dE=C\cdot\frac{2}{3}(E_F)^{3/2}\Rightarrow$
$\Rightarrow\frac{h^2}{2m}\left(\frac{3n}{8\pi}\right)^{2/3}=E_F$

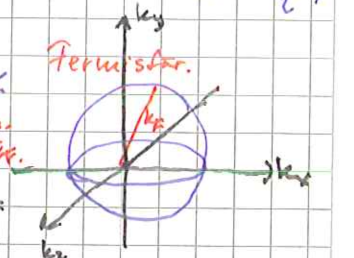
∴ Fermienergin i en metall beror endast på elektronkoncentrationen.

Metaller: $n\sim10^{28}\,m^{-3}\Rightarrow E_F\sim5-10$ eV

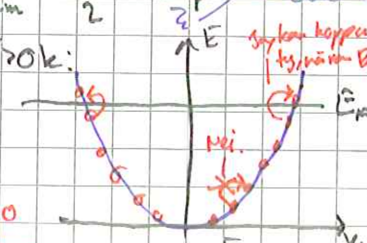


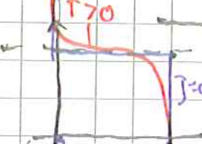
$E_{medel}=\frac{3}{2}kT$
metaller $kT\ll E_F$, $\frac{1}{40}$ eV ≈ 25 meV @RT. (kap 2)

$E_F=\frac{\hbar^2k_F^2}{2m}=\frac{mv_F^2}{2}=kT_F$ ~ 50000 K



Om T>0K:





$E_F(T)$ = Ferminivå (T>0)

← FERMI-DIRAC FÖRDELNING.

$F(E)=\frac{1}{e^{(E-E_F)/kT}+1}$ $F(E_F)=\frac{1}{2}$