ODABRANA POGLAVLJA FIZIKE ČVRSTOG STANJA

OSNOVE FIZIKE ČVRSTOG STANJA

- ZBIRKA RIJEŠENIH ZADATAKA -

v1.0

Danko Radić, 2025.

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Rješenja zadataka

Literatura:

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2. V. Šips, "Uvod u fiziku čvrstog stanja" (Školska knjiga, Zagreb, 2003.)

3. I. Kupčić, "Fizika čvrstog stanja – zbirka riješenih zadataka" (HINUS, Zagreb, 1998.)

4. C. Kittel, "Introduction to Solid State Physics" (Wiley, 2004.)

Ova zbirka tijesno se oslanja na nastavnu skriptu i gradivo izneseno na predavanjima tako da je oznake nekih korištenih fizikalnih veličina, definicije, postupke itd. uputno tamo pogledati.

1. KRISTALNA STRUKTURA

Z-1.1 Dokaži da u kristalu postoje rotacijske osi simetrije $2\pi/n$ samo za n=1, 2, 3, 4 i 6.

naputak: Translacijski vektor rešetke **T** zakrenut za kut ϕ i vektor -**T** zakrenut za $-\phi$ moraju određivati vektor koji je kolinearan i sumjerljiv s **T** (opet mora biti translacijski vektor rešetke). Otud slijedi da kut zakreta $\phi=2\pi/n$, ne može rezultirati s osi reda n=5, 7 i više.

Z-1.2 Dokaži identitet $\Omega\Omega^*=(2\pi)^3$, gdje su Ω i Ω^* volumen elementarne ćelije direktnog, odnosno recipročnog prostora trodimenzionalnog kristala.

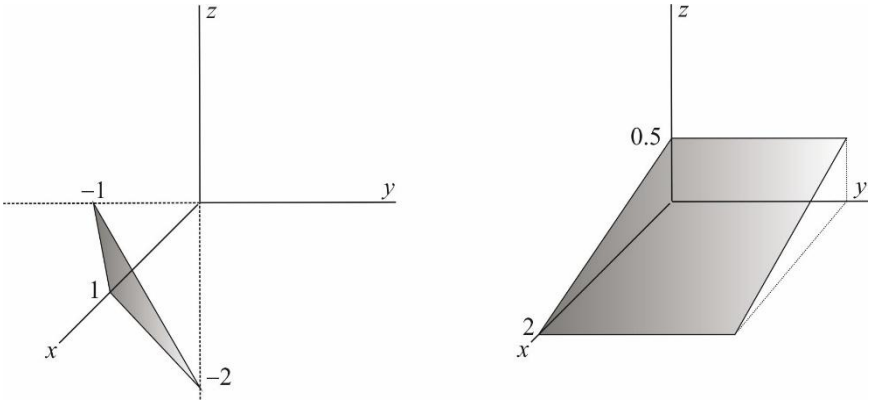
naputak: Koristi pravilo za dvojni vektorski produkt $\mathbf{A}\times(\mathbf{B}\times\mathbf{C})=\mathbf{B}(\mathbf{A}\cdot\mathbf{C})-\mathbf{C}(\mathbf{A}\cdot\mathbf{B})$, definiciju volumena i vektora recipročne rešetke - dobiva se $\Omega^*=(2\pi)^3/\Omega$.

Z-1.3 Dokaži da je rešetka recipročna recipročnoj rešetci, polazna realna rešetka.

Z-1.4 Izvedi izraze za osnovne vektore recipročnog prostora za rešetke:
a) SC
b) BCC
c) FCC
d) heksagonalna rešetka
e) 2D saćasta ("*honeycomb*") rešetka (grafen).

rj:
a) SC:
$\mathbf{a}_1=a\ (1,0,0)$, $\mathbf{a}_2=a\ (0,1,0)$, $\mathbf{a}_3=a\ (0,0,1)$ =>
$\mathbf{b}_1=(2\pi/a)\ (1,0,0)$, $\mathbf{b}_2=(2\pi/a)\ (0,1,0)$, $\mathbf{b}_3=(2\pi/a)\ (0,0,1)$
b) BCC:
$\mathbf{a}_1=(a/2)\ (1,1,-1)$, $\mathbf{a}_2=(a/2)\ (-1,1,1)$, $\mathbf{a}_3=(a/2)\ (1,-1,1)$ =>
$\mathbf{b}_1=(2\pi/a)\ (1,1,0)$, $\mathbf{b}_2=(2\pi/a)\ (0,1,1)$, $\mathbf{b}_3=(2\pi/a)\ (1,0,1)$
c) FCC:
$\mathbf{a}_1=(a/2)\ (0,1,1)$, $\mathbf{a}_2=(a/2)\ (1,0,1)$, $\mathbf{a}_3=(a/2)\ (1,1,0)$ =>
$\mathbf{b}_1=(2\pi/a)\ (-1,1,1)$, $\mathbf{b}_2=(2\pi/a)\ (1,-1,1)$, $\mathbf{b}_3=(2\pi/a)\ (1,1,-1)$
d) $\mathbf{a}_1=a\ (1,0,0)$, $\mathbf{a}_2=(a/2)\ (-1,\sqrt{3},0)$, $\mathbf{a}_3=c\ (0,0,1)$ =>
$\mathbf{b}_1=(2\pi/a)\ (1,1/\sqrt{3},0)$, $\mathbf{b}_2=(2\pi/a)\ (0,\ 2/\sqrt{3},0)$, $\mathbf{b}_3=(2\pi/c)\ (0,0,1)$
e) $\mathbf{a}_1=(a/2)\ (3,\ -\sqrt{3})$, $\mathbf{a}_2=(a/2)\ (3,\ \sqrt{3})$ =>
$\mathbf{b}_1=(2\pi/3a)\ (1,-\sqrt{3})$, $\mathbf{b}_2=(2\pi/3a)\ (1,\sqrt{3})$

Z-1.5 Millerovi indeksi:
a) Napiši Millerove indekse zadanih ravnina:



b) Skiciraj ravnine sa zadanim Millerovim indeksima: {2 2 1}, {0 4 0}.

Z-1.6 Odredi gustoću pakiranja atoma u kristalnoj ravnini $\eta=S_{\circ}/S_{\square}$, gdje je $S_{\circ}$ površina atoma presječenih ravninom, a $S_{\square}$ ukupna površina ravnine, za:
(1) SC {1 0 0}
(2) BCC {1 0 0}
(3) FCC {1 0 0}
(4) SC {1 1 1}
(5) BCC {1 1 0}
(6) FCC {1 1 0}

rj:
(1) $\eta=\pi/4$
(2) $\eta= 3\pi/16=0.589$
(3) $\eta= \pi/4$
(4) $\eta= \pi/4\sqrt{3}=0.454$
(5) $\eta= 3\pi/8\sqrt{2}=0.833$
(6) $\eta= \pi/4\sqrt{2}=0.555$

Z-1.7 Pod kojim kutevima se javljaju prva dva difrakcijska maksimuma pri raspršenju X-zraka valne duljine 1.5Å na površini kristala čije su odgovarajuće kristalne ravnine udaljene za 2Å?

rj: $\Theta_1=22.02^{\circ}$, $\Theta_2=48.59^{\circ}$

Z-1.8 U Kartezijevom koordinatnom sustavu izvedi izraz za udaljenost od ishodišta *n*-te paralelne kristalne ravnine u kubičnoj rešetci indeksirane istim Millerovim indeksima {h k l}.

rj: $d_{h,k,l} = 2\pi \dfrac{n}{\left|\vec{G}_{h,k,l}\right|}$

Z-1.9 Promatramo problem difrakcije X-zraka valne duljine λ=1.5Å na površini kristala konstante rešetke a=3.6Å, čije su odgovarajuće kristalne ravnine udaljene za 2.5Å, i svi atomi su istog strukturnog faktora f. Koristit ćemo Kartezijev koordinatni sustav s jediničnim vektorima u smjeru x, y, i z osi, a BCC odnosno FCC ćeliju opisati kao SC+baza.

a) Za kristal BCC tipa s dva karakteristična atoma u bazi na pozicijama $\rho_1=(0,0,0)$ i $\rho_2=a(1/2,1/2,1/2)$, pokaži da pripadni Millerovi indeksi ravnine moraju zadovoljavati uvjet $h+k+l$ je paran broj, te odredi najmanji Braggov kut pod kojim se javlja difrakcijski maksimum raspršenog zračenja (konstruktivna interferencija).

b) Za kristal FCC tipa s četiri karakteristična atoma u bazi na pozicijama $\rho_1=(0,0,0)$, $\rho_2=a(1/2,1/2,0)$, $\rho_3=a(1/2,0,1/2)$ i $\rho_4=a(0,1/2,1/2)$ pokaži da refleksija (difrakcijski maksimum) X-zraka iščezava sa svake kristalne ravnine čiji su Millerovi indeksi kombinacija parnih i neparnih brojeva.

rj:

a) Geometrijski strukturni faktor BCC baze je $F_{h,k,l} = f\left(1+e^{i\pi(h+k+l)}\right)$, pa je $F_{h,k,l}\neq 0$ za $h+k+l$ paran, te $F_{h,k,l}=0$ za $h+k+l$ neparan. Dakle nužan uvjet maksimuma je $h+k+l$ paran. Iz Laueove formule dobivamo kuteve konstruktivne interferencije izabranu $\{h\ k\ l\}$ ravninu, $\sin(\Theta/2)=(\lambda/2a)(h^2+k^2+l^2)^{1/2}$, gdje je traženi Braggov kut $\phi=\Theta/2$. Od strukturnim faktorom dozvoljenih parnih kombinacija $h+k+l$, npr. {1 1 0}, {2 0 0}, {2 2 0}, {4 0 0} i srodnih kombinacija, tražimo onu s minimalnim $h^2+k^2+l^2$, a to je {1 1 0} (i ostale uređene trojke s dvije jedinice i nulom). Minimalni Braggov kut je $\phi = \arcsin\left(\frac{\lambda}{\sqrt{2}a}\right) = 17.1°$.

b) Geometrijski strukturni faktor FCC baze $F_{h,k,l} = f\left(1+e^{i\pi(h+k)}+e^{i\pi(h+l)}+e^{i\pi(k+l)}\right)$ =0 za bilo koju ravninu $\{h\ k\ l\}$ za koju trojka h, k i l čini kombinaciju parnih i neparnih brojeva (može se pokazati tablicom).

Z-1.10 a) Izvedi izraz za broj Schottkyevih defekata u kristalu.
b) Izvedi izraz za broj Frenkelovih defekata u kristalu.

naputak:

a) Pošavši od termodinamičke vjerojatosti $B = \binom{N}{N_S}$, $N>>N_S>>1$ (N-broj atoma u kristalu, N_S-broj Schottkyevih defekata), uz korištenje Stirlingove formule $\ln(x!)\approx x\ln(x)-x$, pokazuje se da je $N_S=N\exp(-E_S/k_BT)$, gdje je E_S energija aktivacije jednog Schottkyevog defekta.

b) Pošavši od termodinamičke vjerojatosti $B = \binom{N}{N_F}\binom{N'}{N_F}$, $N>>N_F>>N'>>1$ (N-broj atoma u kristalu, N_F-broj Frenkelovih defekata, N'-broj raspoloživih intersticijskih mjesta), uz korištenje Stirlingove formule $\ln(x!)\approx x\ln(x)-x$, pokazuje se da je $N_F=\sqrt{(NN')}\exp(-E_F/2k_BT)$, gdje je E_F energija aktivacije jednog Frenkelovog defekta.

2. MEĐUATOMSKE INTERAKCIJE U KRISTALIMA

Z-2.1 Polazeći od problema 2 točkasta naboja $+q$ i $-q$ udaljena za d i kulonske sile kojom međudjeluju, izvedi izraze za:
a) potencijal dipola na udaljenosti $r>>d$
b) potencijalnu energiju dipola u vanjskom električnom polju točkastog naboja Q na udaljenosti $r>>d$
c) električno polje dipola na položaju **r** u odnosu na centar dipola.

rj:

a) $\Phi(\vec{r}) = \dfrac{\vec{p}\cdot\vec{r}}{4\pi\varepsilon_0 r^3}, \quad \vec{p} \equiv q\vec{d}$

b) $U = -\vec{p}\cdot\vec{E}, \quad \vec{E} = -\vec{\nabla}\Phi(\vec{r}), \quad \left(\Phi(\vec{r}) = \dfrac{Q}{4\pi\varepsilon_0 r}\right)$

c) $\vec{E}(\vec{r}) = \dfrac{1}{4\pi\varepsilon_0}\dfrac{3\vec{r}(\vec{p}\cdot\vec{r}) - r^2\vec{p}}{r^5}$

Z-2.2 Razmatrajući međudjelovanje dvaju atoma plemenitih plinova na udaljenostima koje su mnogo veće od linearnih dimenzija atoma, odredi uzajamnu potencijalnu energiju.

rj: $U \approx -\dfrac{B}{r^6}, \quad B \equiv \dfrac{\alpha p^2}{4\pi^2\varepsilon_0}$ (α - polarizabilnost, p - dipolni moment atoma)

Z-2.3 Ako je potencijalna energija interakcije dvaju atoma, ovisno o njihovoj udaljenosti r, predstavljena dvjema potencijskim funkcijama u kompeticiji, $E_p = -\dfrac{a}{r^n} + \dfrac{b}{r^{n'}}$, odredi uvjet stabilnosti sustava.

rj: $n'>n$

Z-2.4 Interakcijska potencijalna energija dana je izrazom $U(r) = -\dfrac{A}{r^n} + Be^{-\frac{r}{a}}$, gdje su A, B, a i n parametri, a r udaljenost susjednih čestica. Odredi energiju sustava u ravnotežnom stanju (ravnotežnoj udaljenosti r_0).

rj: $U(r_0) = -\dfrac{A}{r_0^n}\left(1 - \dfrac{na}{r_0}\right)$

Z-2.5 Odredi Madelungovu konstantu ionskog kristala sastavljenog od $+q$ i $-q$ naboja
a) za 1D kristal egzaktno i Evjen-Frankovom metodom (uzmi 5 ćelija)
b) za 3D NaCl kristal Evjen-Frankovom metodom (uzmi 2 ćelije)

rj:
Evjen-Frankova metoda temelji se na organiziranju sume alternirajućeg reda u Madelungovoj konstanti na način da se sumira po doprinosima elektrostatski neutralnih ćelija.
a) $\alpha_M=2\ln 2=1.38629$ (egzaktno), $\alpha_M=1.367$ (Evjen-Frank)
b) $\alpha_M=1.76$

Z-2.6 Odredi energiju rešetke 1D linearnog ionskog kristala sastavljenog od N iona naboja $\pm q$ ako je repulzivna Paulijeva interakcija među susjedima oblika A/R^n, n je prirodan broj.

rj: $E=-N\dfrac{q^2\ln 2}{2\pi\varepsilon_0 R_0}\left(1-\dfrac{1}{n}\right)$

3. DINAMIKA KRISTALNE REŠETKE

Z-3.1 Za beskonačnu jednodimenzionalnu kristalnu rešetku konstante a, sastavljenu od atoma mase m, odredi disperzijsku relaciju fonona $\omega(k)$ ako uzmemo u obzir međudjelovanje svakog atoma sa svojih prvih 5 susjeda, pri čemu su β_n su konstante elastične sile ovisno o rednom broju susjeda n=1, 2, ..., 5 u harmoničkoj aproksimaciji.

rj: $\omega^2(k) = \frac{4}{m}\sum_n \beta_n \sin^2\frac{kna}{2}$, n=1, 2,.., 5

Z-3.2 Odredi disperzijsku relaciju $\omega(k)$ titranja beskonačnog jednodimenzionalnog lanca s 2 atoma mase m_1 u m_2 u bazi jedinične ćelije konstante rešetke a i konstante elastične sile β u harmoničkoj aproksimaciji. Odredi vrijednosti $\omega_\pm(0)$ i $\omega_\pm(\pi/a)$.

rj:

$$\omega_\pm^2(k) = \frac{\beta}{\mu}\left(1 \pm \sqrt{1 - \frac{4\mu^2}{m_1 m_2}\sin^2\frac{ka}{2}}\right); \quad \mu \equiv \frac{m_1 m_2}{m_1 + m_2}$$

$\omega_-(0)=0$; $\omega_+(0)=(2\beta/\mu)^{1/2}$; $\omega_-(\pi/a)=(2\beta/m_1)^{1/2}$; $\omega_+(\pi/a)=(2\beta/m_2)^{1/2}$

Z-3.3 Za jednodimenzionalnu kristalnu rešetku izgrađenu od jednakih atoma mase m, pri čemu su ravnotežni razmaci među susjednim atomima $c, d, c, d, ...$, s pripadnim konstantama elastične sile među susjedima $\beta, \gamma, \beta, \gamma, ...$ u harmoničkoj aproksimaciji, odredi disperzijsku relaciju $\omega(k)$ sustava u aproksimaciji prvih susjeda, uzevši da je duljina $c+d \equiv a$. Posebno izvedi $\omega(k)$ u granici konačnog $k \to 0$. Kakav je odnos amplituda titranja u granici k=0.

rj:

$$\omega_\pm^2(k) = \frac{1}{m}\left(\beta + \gamma \pm \sqrt{\beta^2 + \gamma^2 + 2\beta\gamma\cos(ka)}\right)$$

$$\omega_\pm^2(k \to 0) = \frac{\beta+\gamma}{m}\left[1 \pm \left(1 - \frac{1}{2}\frac{\beta\gamma}{(\beta+\gamma)^2}(ka)^2\right)\right] \quad \Rightarrow \quad \omega_\pm(k \to 0) = \begin{cases} \sqrt{\frac{\beta\gamma}{2m(\beta+\gamma)}}\,|ka|; & A \\ \sqrt{\frac{2(\beta+\gamma)}{m}}; & O \end{cases}$$

s odnosom amplituda $A_-=B_-$ za akustičko (A) i $A_+=-B_+$ za optičko titranje (O), pri čemu je $a=c+d$.

Z-3.4 Odredi valni vektor i frekvenciju titranja lokaliziranog fononskog stanja lake susptitucijske primjese mase m u beskonačnom jednodimenzionalnom lancu atoma mase M ($m<M$) s konstantom rešetke a i konstantom elastične sile β u harmoničkoj aproksimaciji.

rj: $\omega = \sqrt{\frac{2\beta}{m}\left(1 + \frac{m}{2M}\right)}$; $k = \pm\frac{\pi}{a}$, $m < M$

Z-3.5 Odredi Debyevu temperaturu za Ca i Cu uz pretpostavku da je brzina zvuka $v_s=3\cdot10^3$m/s u oba krisala jednaka. Parametri jedinične ćelije su a(Ca)=0.558nm, a(Cu)=0.361nm, a struktura je FCC tipa.

rj: $\Theta_D = \frac{\hbar v_s}{k_B a}\sqrt[3]{24\pi^2} = \begin{cases} 250K, & Ca \\ 390K, & Cu \end{cases}$

Z-3.6 U okviru Debyeva modela izračunajte energiju osnovnog stanja akustičkih oscilatora (modova fonona) u molu kristala ako je Debyeva temperatura Θ_D=300K.

rj: $U=(9/8)N_A k_B \Theta_D$ = 2.8 kJ/mol

Z-3.7 Izračunaj broj akustičkih fonona N u uzorku zlata od $\mathcal{N}$ elementarnih ćelija, pri temperaturi T=20K, u Debyevoj aproksimaciji, ako je Debyeva temperatura zlata Θ_D=170K.

rj: $\frac{N}{\mathcal{N}} = 18\zeta(3)\left(\frac{T}{\Theta_D}\right)^3 = 0.035$

Z-3.8 Izačunaj broj atoma u kristalu u kojem svaka primitivna ćelija sadrži 1 atom, ako je za njega izmjeren toplinski kapacitet kristalne rešetke C_V=0.8J/K pri temperaturi T=30K, u Debyeovoj aproksimaciji ako je Debyeva temperatura Θ_D=320K.

rj: $N = \frac{5C_V}{12\pi^4 k_B}\left(\frac{\Theta_D}{T}\right)^3 = 3\cdot10^{23}$

Z-3.9 Izračunaj toplinski kapacitet 1D kristalne rešetke s jednim atomom po primitivnoj ćeliji na temperaturi puno nižoj od Debyeve.

rj: $C_V = \frac{\pi L k_B^2}{\hbar v_s} T$

Z-3.10 Izračunaj toplinski kapacitet kristala s jednim atomom po primitivnoj ćeliji, koji se sastoji od ravnina atoma s potpuno krutom (vibracijski neaktivnom) vezom među ravninama, u Debyevoj aproksimaciji na temperaturi $T<<\Theta_D$.

rj: $C_V = \frac{6L^2 k_B^3 \zeta(3)}{\pi v_s^2 \hbar^2} T^2$ (L je linearna dimenzija kristala)

4. SOMMERFELDOV MODEL METALA

Z-4.1 Odredi koncentraciju jako degeneriranog elektronskog plina pri temperaturi T=0 ako je prosječan valni broj elektrona k=1.5·10^{10}m^{-1}.

rj: $n = \frac{1}{3\pi^2}\left(\frac{4}{3}k\right)^3 = 2.7\cdot 10^{29}\, m^{-3}$

Z-4.2 Odredi relaciju koja povezuje tlak i volumen slobodnog elektronskog plina na T=0.

rj: $P = \frac{2}{3}\frac{U}{V}$, U je unutrašnja energija

Z-4.3 Izračunaj tlak slobodnog elektronskog plina na temperaturi T=0 ako je elektronska koncentracija n=5.6·10^{28}m^{-3}.

rj: $P = \frac{\hbar^2 (3\pi^2)^{2/3} n^{5/3}}{5m} = 1.9\cdot 10^{10}\, Pa$

Z-4.4 Za dvodimenzionalni slobodni elektronski plin odredi kemijski potencijal μ na temperaturi T izrazivši ga u vidu temperaturno ovisne korekcije na Fermijevu energiju E_F, tj. u obliku μ(T)=E_F+h(T) gdje je h(T) tražena korekcija.

rj: iz $N_{T=0} = N_{T\neq 0}$, te uz korištenje ln(1+x)=ln[x(1+1/x)], dobivamo

$$\mu(T) = E_F + k_B T \ln\left(1 - e^{-\frac{E_F}{k_B T}}\right)$$

Z-4.5 Koristeći Sommerfeldov razvoj $\int_0^\infty F(E) f(E) dE \approx \int_0^\mu F(E) dE + \frac{1}{6}(\pi k_B T)^2 \left.\frac{\partial F}{\partial E}\right|_{E=\mu}$, gdje je $F(E)$ zadana funkcija energije a $f(E)$ Fermijeva funkcija raspodjele, izračunaj do prve neiščezavajuće korekcije u temperaturi:
a) ovisnost kemijskog potencijala μ o temperaturi T
b) toplinski kapacitet C_V
jako degeneriranog fermionskog plina s gustoćom stanja g_F na Fermijevoj energiji E_F.

rj:

a) $\mu(T) = E_F\left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{E_F}\right)^2\right]$

b) $C_V = \frac{\pi^2}{3} g_F k_B^2 T$

Z-4.6 Pri temperaturi T=0.1K izmjeren je toplinski kapacitet elektronskog plina u jediničnom volumenu metala C_V=4JK^{-1}m^{-3}. U Sommerfeldovom modelu odredi koncentraciju vodljivih elektrona u metalu.

rj: $n = \frac{9}{\pi^2}\left(\frac{\hbar^2 C_V}{k_B^2 m T}\right)^3 = 1.5\cdot 10^{28} m^{-3}$

Z-4.7 Pri mjerenjima toplinskog kapaciteta metala na sobnoj temperaturi (T=300K), zanemaruje se doprinos elektronskog plina i zadržava samo doprinos kristalne rešetke. Kvantitativno pokaži zašto je to moguće na primjeru metala s jednim elektronom po primitivnoj ćeliji, Fermijeve energije 1eV i Debyeve temperature 200K.

rj: $\frac{c_v^{el}}{c_v^{ph}} = \frac{\pi^2}{6}\frac{k_B T}{E_F} \sim 10^{-2}$

Z-4.8 Izvedi Dushman-Richardsonovu formulu koja opisuje termoelektronsku emisiju iz metala s izlaznim radom Φ na temperaturi T.

rj: $j = AT^2 e^{-\frac{\Phi}{k_B T}}$

5. ELEKTRON U PERIODIČKOM POTENCIJALU

Z-5.1 Za sustav slobodnih elektrona, izloženih periodičkom potencijalu karakteriziranom vektorom recipročne rešetke **G** i odgovarajućim komponentama potencijala $V_{\mathbf{G}n}$, primjenom prve korekcije u standardnom stacionarnom računu smetnje, odredi valnu funkciju elektrona.

rj: $\Psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \left[1 + \frac{2m}{\hbar^2} \sum_n \frac{V_{\vec{G}_n} e^{i\vec{G}_n\cdot\vec{r}}}{\vec{k}^2 - (\vec{k}+\vec{G}_n)^2} \right]$

Z-5.2 Razvij disperzijsku relaciju (vrpcu) slobodnih elektrona u periodičkom potencijalu karakteriziranom recipročnim vektorom periodičnosti **G**, $E_{\pm}(\vec{k}) = \frac{1}{2}\left[E^0_{\vec{k}} + E^0_{\vec{k}+\vec{G}} \pm \sqrt{\left(E^0_{\vec{k}} - E^0_{\vec{k}+\vec{G}}\right)^2 + 4\left|V_{\vec{G}}\right|^2} \right]$, dobivenu računom smetnje za degenerirane nivoe gdje je $E_{\mathbf{k}}{}^{o}$ slobodnoelektronska energija, a $V_{\mathbf{G}}=\langle\Phi_{\mathbf{k}}|V|\Phi_{\mathbf{k+G}}\rangle$ matrični element periodičkog potencijala $V(\mathbf{r})$, u okolini ruba Brillouinove zone $\mathbf{k}=-(\mathbf{G}/2)+\Delta\mathbf{k}$ ($\Delta\mathbf{k}$ je mali valni vektor u odnosu na rub Brillouinove zone $-\mathbf{G}/2$). Odredi iznos energetskog procijepa Δ između vrpci.

rj:

$$E_{\pm}(\Delta\vec{k}) = \frac{\hbar^2}{2m}\left(\frac{G^2}{4} + (\Delta k)^2 \right) \pm \sqrt{\left(\frac{\hbar^2}{2m}\right)^2 \left(\vec{G}\cdot\Delta\vec{k}\right)^2 + \left|V_{\vec{G}}\right|^2}$$

$$\Delta = E_+ - E_- = 2\left|V_{\vec{G}}\right|$$

Z-5.3 U 1D TBA modelu s vrpcom (disperzijskom relacijom) određenom izrazom $E(k)=E_0+2t\cos(ka/2)$, odredi efektivnu masu i grupnu brzinu elektrona, te rezultat primijeni na dugovalnu granicu $ka<<1$ i komentiraj njegovo značenje.

rj:

$$m^* = -\frac{2\hbar^2}{a^2 t\cos(ka/2)} \approx -\frac{2\hbar^2}{a^2 t}, \quad ka \ll 1$$

$$v = -\frac{at}{\hbar}\sin(ka/2) \approx \frac{\hbar k}{m^*}, \quad ka \ll 1$$

Negativna vrijednost efektivne mase ukazuje na šupljinsku vrpcu oko centra BZ.

Z-5.4 Za 3D TBA elektronsku vrpcu disperzije

$$E(\vec{k}) = E_0\left(\cos\frac{k_x a}{2}\cos\frac{k_y b}{2} + \cos\frac{k_y b}{2}\cos\frac{k_z c}{2} + \cos\frac{k_x a}{2}\cos\frac{k_z c}{2} \right),$$

izvedi elemente tenzora efektivne mase.

rj:

$$\frac{1}{m^*_{xx}} = -\frac{E_0 a^2}{4\hbar^2}\cos\frac{k_x a}{2}\left(\cos\frac{k_y b}{2}+\cos\frac{k_z c}{2}\right)$$

$$\frac{1}{m^*_{yy}} = -\frac{E_0 b^2}{4\hbar^2}\cos\frac{k_y b}{2}\left(\cos\frac{k_x a}{2}+\cos\frac{k_z c}{2}\right)$$

$$\frac{1}{m^*_{zz}} = -\frac{E_0 c^2}{4\hbar^2}\cos\frac{k_z c}{2}\left(\cos\frac{k_x a}{2}+\cos\frac{k_y b}{2}\right)$$

$$\frac{1}{m^*_{xy}} = \frac{1}{m^*_{yx}} = \frac{E_0 ab}{4\hbar^2}\sin\frac{k_x a}{2}\sin\frac{k_y b}{2}$$

$$\frac{1}{m^*_{xz}} = \frac{1}{m^*_{zx}} = \frac{E_0 ac}{4\hbar^2}\sin\frac{k_x a}{2}\sin\frac{k_z c}{2}$$

$$\frac{1}{m^*_{yz}} = \frac{1}{m^*_{zy}} = \frac{E_0 bc}{4\hbar^2}\sin\frac{k_y b}{2}\sin\frac{k_z c}{2}$$

Z-5.5 Zadana je elektronska vrpca u aproksimaciji efektivne mase, $E(\vec{k}) = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x^*}+\frac{k_y^2}{m_y^*}+\frac{k_z^2}{m_z^*}\right)$, gdje su m_x^*, m_y^*, m_z^* redom efektivne mase u smjeru *x*, *y*, *z* osi. Odredi izraz za gustoću stanja.

rj: $g(E) = \frac{1}{\pi^2\hbar^3}\sqrt{2m_x^* m_y^* m_z^* E}$

Z-5.6 Odredi tenzor recipročne efektivne mase za 2D heksagonalnu rešetku s TBA disperzijskom relacijom vrpce $E(\vec{k}) = E_0 - 2t\cos k_y a - 4t\cos\frac{\sqrt{3}k_x a}{2}\cos\frac{k_y a}{2}$ u dugovalnoj granici, koristeći razvoj kosinusa oko dna vrpce.

rj: $\left[\mathbf{m}^*\right]^{-1} = \frac{3ta^2}{\hbar^2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$

Z-5.7 U aproksimaciji čvrste veze (TBA) izvedi Blochove energije i Blochove valne funkcije za 1D lanac od *N* atoma s jednim stanjem energije E^0 i valne funkcije $\phi(\mathbf{r}-\mathbf{R})$, u aproksimaciji prvih susjeda ako je preklapanje orbitala parametrizirano integralom elektronskog preskoka *t*.

rj:

$$E(k) = E^0 - 2t\cos(ka)$$

$$\Psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_j e^{i\vec{k}\cdot\vec{R}_j}\phi(\vec{r}-\vec{R}_j)$$

gdje je: E^0 – sredina vrpce (atomska energija), $\mathbf{R}_j$ – koordinata j-tog čvora rešetke, $\mathbf{k}$ – Blochov valni vektor, $\phi(\mathbf{r}-\mathbf{R}_j)$ – atomska valna funkcija na čvoru j, N – broj atoma u kristalu

Z-5.8 Izračunaj kohezivnu energiju 1D kristala konstante rešetke a u aproksimaciji čvrste veze (TBA) prvih susjeda s integralom elektronskog preskoka t, i prikaži ju kao funkciju popunjenja vrpce parametriziranim Fermijevim valnim brojem k_F.

rj: $E_{coh}^{1at.} = \frac{4t}{\pi}\sin(k_F a)$

Z-5.9 Izračunaj gustoću stanja 1D kristala konstante rešetke a u aproksimaciji čvrste veze (TBA) prvih susjeda s integralom elektronskog preskoka t, a zatim iz nje izračunaj kohezivnu energiju kao funkciju popunjenja vrpce parametriziranim Fermijevom energijom E_F.

rj:

$$g(E) = \frac{2L}{\pi a}\frac{1}{\sqrt{4t^2 - E^2}}$$

$$E_{coh}^{1at.} = \frac{2}{\pi}\sqrt{4t^2 - E_F^2}$$

Z-5.10 Za 2D volumno centriranu pravokutnu rešetku stranica jedinične ćelije a i b, u okviru aproksimacije čvrste veze prvih susjeda s integralom elektronskog preskoka t, odredi:
a) elektronsku vrpcu i razvoj oko njezinog dna,
b) gustoću stanja pri dnu vrpce.

rj:
a) Dno vrpce nalazi se u ishodištu (centru) BZ pa su egzaktni i aproksimativni izraz oko (0,0):

$$E(\vec{k}) = E^0 - 4t\cos\frac{k_x a}{2}\cos\frac{k_y b}{2}$$

$$E(\vec{k}) \approx E^0 - 4t + \frac{t}{2}\left[(k_x a)^2 + (k_y b)^2\right]$$

b) Koristeći definicijski izraz $g(E)=\Sigma_n\delta(E-E_n)$ dobivamo

$g(E) = \frac{L^2}{\pi abt}\Theta\left(E - E^0 + 4t\right)$, gdje je L^2 površina uzorka

6. ELEKTRIČNI I TOPLINSKI TRANSPORT

Z-6.1 Izvedi Ohmov zakon u (krajnje) simplificiranom modelu djelovanja konstantnog električnog polja **E** na (nabijeni) slobodni elektron u kristalu metala pri čemu je pretpostavka da na elektron djeluje također i sila trenja proporcionalna njegovoj brzini.

rj:

$\vec{v}(t) = \vec{C}e^{-t/\tau} - \frac{e\vec{E}\tau}{m}$ - opće rješenje diferencijalne jednadžbe za brzinu elektrona (**C** je konstanta određena početnim uvjetom) koje u stacionarnoj granici daje $\vec{j} = \frac{e^2 n\tau}{m}\vec{E}$, gdje je τ - relaksacijsko vrijeme, n - koncentracija elektrona, m - masa elektrona, a $-e$ njegov naboj

Z-6.2 Izvedi izraz za vodljivost metala u vremenski oscilirajućem električnom polju $\mathbf{E}=\mathbf{E}_0\exp(-i\omega t)$ polazeći od modela slobodnog elektrona na koji djeluje sila trenja proporcionalna njegovoj brzini. Zatim izvedi vodljivost u granicama $\omega\tau<<1$ i $\omega\tau>>1$, gdje je τ relaksacijsko vrijeme. Skiciraj rezultat grafički.

rj:

$$\sigma(\omega) = \sigma_0 \frac{1+i\omega\tau}{1+(\omega\tau)^2}, \quad \sigma_0 \equiv \frac{e^2 n\tau}{m}$$

$$\omega\tau \ll 1: \quad \sigma(\omega) \approx \sigma_0(1+i\omega\tau)$$

$$\omega\tau \gg 1: \quad \sigma(\omega) \approx \sigma_0\left(\frac{1}{(\omega\tau)^2} + \frac{i}{\omega\tau}\right)$$

Z-6.3 Izvedi izraz za tenzor magnetovodljivosti **M** u magnetskom polju $\mathbf{B}=(0,0,B)$ za česticu naboja q.

rj:

$$\mathbf{M} = \frac{\sigma_0}{1+(\tilde{\omega}_c\tau)^2}\begin{pmatrix} 1 & \tilde{\omega}_c\tau & 0 \\ -\tilde{\omega}_c\tau & 1 & 0 \\ 0 & 0 & 1+(\tilde{\omega}_c\tau)^2 \end{pmatrix}, \quad \sigma_0 \equiv \frac{q^2 n\tau}{m}, \quad \tilde{\omega}_c \equiv \frac{qB}{m} = \mathrm{sgn}(q)\frac{|q|B}{m}$$

gdje veličina $\tilde{\omega}_c$ označava ciklotronsku frekvenciju koja nosi i predznak naboja, a s "pravom" ciklotronskom frekvencijom $\omega_c=|q|B/m$ povezana je na način: $\tilde{\omega}_c = -\omega_c,\ q<0; \quad \tilde{\omega}_c = \omega_c,\ q>0$

Z-6.4 Iz izraza za tenzor magnetovodljivosti za česticu naboja q

$$\mathbf{M} = \frac{\sigma_0}{1+(\tilde{\omega}_c\tau)^2}\begin{pmatrix} 1 & \tilde{\omega}_c\tau & 0 \\ -\tilde{\omega}_c\tau & 1 & 0 \\ 0 & 0 & 1+(\tilde{\omega}_c\tau)^2 \end{pmatrix}, \quad \sigma_0 \equiv \frac{q^2 n\tau}{m}, \quad \tilde{\omega}_c \equiv \frac{qB}{m} = \mathrm{sgn}(q)\frac{|q|B}{m}$$

izračunaj Hallovu konstantu (magnetsko polje je u z-smjeru).

rj: $R_H = \frac{1}{nq}$

Z-6.5 Izvedi izraze za Hallovu vodljivost i Hallovu konstantu u aproksimaciji slabog magnetskog polja **B**=(0,0,*B*) ako su nosioci naboja i elektroni i šupljine.

rj:

Pošavši od tenzora **M**, zanemarenjem članova ~B^2, dobiva se $R_H = \frac{n_h\mu_h^2 - n_e\mu_e^2}{e(n_h\mu_h - n_e\mu_e)^2}$, gdje su $\mu_e = e\tau_e/m_e$ i $\mu_h = e\tau_h/m_h$ pokretljivosti elektrona i šupljina, a n_e i n_h pripadne koncentracije.

Z-6.6 Izvedi izraze za Hallovu vodljivost i Hallovu konstantu u aproksimaciji jakog magnetskog polja **B**=(0,0,*B*) ako su nosioci naboja i elektroni i šupljine.

rj:
Pošavši od tenzora **M**, zanemarenjem članova ~$1/B^2$, dobiva se
$\sigma_{xy} = \frac{e}{B}(n_h - n_e)$, $R_H = \frac{1}{e(n_h - n_e)}$, gdje su n_e i n_h koncentracije elektrona i šupljina.

Z-6.7 Odredi ciklotronsku frekvenciju elektrona s elipsoidnom ekvienergetskom plohom danom disperzijskom relacijom vrpce $E(\vec{k}) = \hbar^2\left(\frac{k_x^2 + k_y^2}{2m_t} + \frac{k_z^2}{2m_l}\right)$ gdje su m_t i m_l transverzalna i longitudinalna efektivna masa. Magnetsko polje usmjereno je u smjeru x-osi tj. **B**=(*B*,0,0).

rj: $\omega_c = \frac{eB}{\sqrt{m_l m_t}}$

Z-6.8 Provjeri valjanost Wiedermann-Franzovog zakona u režimima $T<<<\Theta_D$, $T<<\Theta_D$, $T>>\Theta_D$ argumentiravši temperaturnu ovisnost konkretnim izrazima.

rj:

$$\frac{\kappa_e\rho}{T} \sim \frac{l_0 C_V^{el.}\rho}{T} \sim \begin{cases} const, & T <<< \Theta_D \\ T^2, & T << \Theta_D \\ const, & T >> \Theta_D \end{cases}$$

7. POLUVODIČI

Z-7.1 Za intrinsični poluvodič s fenomenološkom ovisnošću procijepa o temperaturi $E_g(T)=E_g(T)-\alpha T^2/(T+T_0)$, odredi parametar T_0 ako je $\alpha=3.2\cdot10^{-4}$eV/K, a poluvodiču se zagrijavanjem od T=0 do T=300K energijski procijep smanji za 0.08eV.

rj: $T_0 = T\left(\frac{\alpha T}{E_g(0)-E_g(T)}-1\right)=60K$

Z-7.2 Pošavši od izraza za koncentracije efektivnih nosilaca naboja N_e i N_h izvedi izraz za položaj Fermijevog nivoa u intrinsičnom poluvodiču na temperaturi T ako su efektivne mase elektrona i šupljima m_e i m_h.

rj: $E_F = \frac{E_C+E_V}{2}-\frac{3}{4}k_BT\ln\frac{m_e^*}{m_h^*}$, gdje su E_C i E_V energije dna vodljive i vrha valentne vrpce

Z-7.3 Izvedi zakon akcije (djelovanja) masa (ZAM) za intrinsični poluvodič.

rj: $n_i = \frac{2}{h^3}(2\pi k_BT)^{3/2}(m_e^*m_h^*)^{3/4}e^{-\frac{E_g}{2k_BT}}$

Z-7.4 Izračunaj postotak povećanja intrinsične koncentracije nosilaca u siliciju pri povišenju temperature za 1K u odnosu na sobnu (300K) ako je za silicij E_g=1.1eV pri 300K.
($k_B=8.62\cdot10^{-5}$eV/K)

rj: $\xi=(n_i(T_2)-n_i(T_1))/n_i(T_1)=7.86\%$

Z-7.5 Siliciju na sobnoj temperaturi (T=300K, $n_i=1.45\cdot10^{10}$cm^{-3}) dodana je koncentracija $N_D=5\cdot10^{14}$cm^{-3} donorskih i $N_A=3\cdot10^{14}$cm^{-3} akceptorskih primjesa. Odredi tip poluvodiča i koncentracije manjinskih i većinskih nosilaca naboja u njemu.

rj:
$n=2\cdot10^{14}$cm^{-3} - većinski, $p=1.05\cdot10^{6}$cm^{-3} - manjinski; poluvodič je n-tipa

Z-7.6 Odredi položaj Fermijevog nivoa na T=300K za germanij ($n_i=2.4\cdot10^{13}$cm^{-3} na 300K) koji sadrži $N_D=5\cdot10^{16}$cm^{-3} atoma fosfora (donori) i $N_A=8\cdot10^{16}$cm^{-3} atoma bora (akceptori).

rj: $|E_F-Ei|=k_BT\ln(p/n_i)=0.185$eV

Z-7.7 Odredi položaj Fermijevog nivoa za silicij (E_g=1.1eV, $n_i=1.45\cdot10^{10}$cm^{-3} na 300K) dopiran s $N_D=10^{14}$cm^{-3} donorskih primjesa na T=400K.

rj: $|E_F - Ei| = 0.11\text{eV}$

Z-7.8 Fermijev nivo n-tipa silicija (E_g=1.1eV, C=$2.32 \cdot 10^{31}\text{cm}^{-6}\text{K}^{-3}$) na 370K udaljen je za 0.37eV od dna vodljive vrpce. Odredi koncentraciju primjesa bora, koji treba dodati u taj poluvodič, da se Fermijev nivo pomake za 0.08eV prema sredini zabranjenog pojasa. (k_B=$8.62 \cdot 10^{-5}$eV/K)

rj: $\Delta p = 4.48 \cdot 10^{10}\text{cm}^{-3}$

8. DIELEKTRIČNI ODZIV

Z-8.1 Vodič vodljivosti $\sigma(\omega)$ nalazi se u oscilirajućem električnom polju $\mathbf{E}=\mathbf{E}_0\exp(-i\omega t)$. Izvedi izraz za ukupnu relativnu permitivnost kristala ε_r induciranu protjecanjem električne struje, pošavši od Maxwellovih jednadžbi i Ohmovog zakona, pod pretpostavkom da polje ne vrši polarizaciju rešetke tj. da je "intrinsična" relativna permitivnost kristala $\varepsilon_r'=1$. Usporedbom dobivenog izraza s relativnom permitivnošću elektronske plazme, $\varepsilon_{pl}(\omega)=1-\omega_p^2/(\omega^2+i\omega\tau^{-1})$, gdje je ω_p frekvencija elektronske plazme a τ relaksacijsko vrijeme, odredi izraz za vodljivost $\sigma(\omega)$.

rj: $\varepsilon_r(\omega)=1+i\dfrac{\sigma(\omega)}{\varepsilon_0\omega}$, $\quad\sigma(\omega)=\dfrac{\sigma_0}{1-i\omega\tau}$, $\quad\sigma_0=\dfrac{e^2n\tau}{m}$

Z-8.2 Polazeći od općenitog izraza za dielektričnu funkciju elektronskog plina u "jellium modelu"

$$\varepsilon_r(\vec{q},\omega)=1-\frac{e^2}{\varepsilon_0 q^2}\sum_{\vec{k},s}\frac{f(E_{\vec{k}})-f(E_{\vec{k}+\vec{q}})}{\hbar\omega+E_{\vec{k}}-E_{\vec{k}+\vec{q}}}$$

a) izvedi izraz za $\varepsilon_r(\mathbf{q})$ u Thomas-Fermijevoj aproksimaciji ($\omega=0$, $q<<k_F$) na $T=0$,
b) izvedi izraz za $\varepsilon_r(\omega)$ u dinamičkoj granici ($\omega\neq0$, $q<<k_F$) na $T=0$.

rj:

a) $\varepsilon_r(q)=1+\dfrac{e^2g_F}{\varepsilon_0q^2}$, gdje je g_F gustoća stanja na Fermijevom nivou ($k_{TF}=\sqrt{\dfrac{e^2g_F}{\varepsilon_0}}$ - Thomas-Fermijev valni broj)

b) $\varepsilon_r(\omega)=1-\dfrac{e^2n}{\varepsilon_0m\omega^2}$, gdje su n i m koncentracija i masa elektrona ($\omega_p=\sqrt{\dfrac{e^2n}{\varepsilon_0m}}$ - frekvencija titranja elektronske plazme)

Z-8.3 Nađi električno polje u središtu homogeno polarizirane dielektrične kugle čija polarizacija iznosi P, a radijus R.
(Uzmi da je površinska polarizacija gustoće naboja određena s P i iznos $P\cos(\theta)$, gdje je θ kut otklona radijvektora iz središta u odnosu na pol maksimalne polarizacije.)

rj: $E_x=\dfrac{P}{3\varepsilon_0}$, $\quad E_y=E_z=0$

Z-8.4 a) Odredi renormaliziranu frekvenciju ω_T u odnosu na izvornu frekvenciju fononskih modova ionske rešetke ω_0 iz zahtjeva da se polarizacija može napisati kao $\vec{P}=n\alpha(\omega)\big|_{\omega_T}\vec{E}$ i kao $\vec{P}=\dfrac{n\alpha(\omega)\big|_{\omega_0}}{1-\frac{1}{3\varepsilon_0}n\alpha(\omega)\big|_{\omega_0}}\vec{E}$, gdje je polarizabilnost ćelije $\alpha(\omega)\big|_{\bar{\omega}}\equiv\dfrac{q^2}{M_r}\dfrac{1}{\bar{\omega}^2-\omega^2}$ određena njezinom reduciranom masom M_r i razdvojenim nabojem q unutar nje.

b) Pošavši od izraza za dielektričnu funkciju $\varepsilon_r(\omega) = \varepsilon^{(\infty)} + \frac{\varepsilon^{(0)} - \varepsilon^{(\infty)}}{1 - \omega^2 / \omega_T^2}$, pokaži da se ista može napisati u obliku $\varepsilon_r(\omega) = \varepsilon^{(\infty)} \frac{\omega_L^2 - \omega^2}{\omega_T^2 - \omega^2}$.

rj: a) $\omega_T^2 = \omega_0^2 - \frac{nq^2}{3\varepsilon_0 M_r}$, gdje je *n* - koncentracija dipola, *q* - naboj iona, M_r - reducirana masa elementarne ćelije

Z-8.5 Izvedi disperzijsku relaciju polaritona pošavši od izraza $\omega(k) = \frac{c}{\sqrt{\varepsilon_r(\omega)}} k$, uz zadanu $\varepsilon_r(\omega) = \varepsilon^{(\infty)} + \frac{\varepsilon^{(0)} - \varepsilon^{(\infty)}}{1 - \omega^2 / \omega_T^2}$, te diskutiraj obje grane $\omega_{\pm}(k)$ u granicama $k \to 0$ i $k \to \infty$.

rj:

$$\omega_{\pm}^2(k) = \frac{1}{2\varepsilon^{(\infty)}} \left[\omega_T^2 \varepsilon^{(0)} + c^2 k^2 \pm \sqrt{(\omega_T^2 \varepsilon^{(0)} + c^2 k^2)^2 - 4\varepsilon^{(\infty)} \omega_T^2 c^2 k^2} \right]$$

$$\omega_+(k \to 0) = \sqrt{\omega_L^2 + \left(1 - \frac{\omega_T^2}{\omega_L^2}\right) \frac{c^2}{\varepsilon^{(\infty)}} k^2}; \quad \omega_+(0) = \omega_L$$

$$\omega_-(k \to 0) = \frac{c}{\sqrt{\varepsilon^{(0)}}} k; \quad \omega_-(0) = 0$$

$$\omega_+(k \to \infty) = \frac{c}{\sqrt{\varepsilon^{(\infty)}}} k$$

$$\omega_-(k \to \infty) = \omega_T$$

napomena: Kod računanja graničnih slučajeva vodi računa da u prvom članu pod kvadratnim korijenom u egzaktnom rezultatu uzmeš u obzir članove *istog reda* kao drugi član pod korijenom!

Z-8.6 Promotri sustav s koncentracijom *n* elektrona, od kojih je svaki vezan u matičnom atomu, koji je izložen oscilirajućem električnom polju $\mathbf{E}=\mathbf{E}_0\exp(-i\omega t)$. Pretpostavljajući da svaki elektron zadovoljava jednadžbu gibanja $m(\ddot{x} + \omega_0^2 x) = -eE - m\gamma\dot{x}$, gdje je *m* masa elektrona, ω_0 vlastita frekvencija koja parametrizira povratnu silu vezanja elektrona u atomu, γ fenomenološka konstanta sile trenja, a *x* koordinata u smjeru električnog polja, izvedi izraz za relativnu permitivnost sustava.

rj: $\varepsilon_r(\omega) = 1 + \frac{ne^2}{\varepsilon_0 m(\omega_0^2 - \omega^2 - i\gamma\omega)}$

Z-8.7 Izvedi relaciju koja u najnižoj aproksimaciji određuje ovisnost indeksa loma η(λ) o valnoj duljini λ, uzevši u obzir samo atomsku polarizabilnost dielektrika opisanu relativnom permitivnošću $\varepsilon_r(\omega) = 1 + \frac{\omega_p^2}{\omega_{at}^2 - \omega^2}$, gdje ω_p ima značenje frekvencije elektronske plazme, a ω_{at} frekvenciju koja karakterizira jakost sile kojom je elektron vezan u atomu.

rj:

$$\eta(\lambda) = \eta_0 + \left(\frac{\lambda_0}{\lambda}\right)^2, \text{ gdje su } \eta_0 \equiv \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2}} \quad \text{i} \quad \lambda_0^2 \equiv 2\pi^2 c^2 \frac{\omega_p^2}{\omega_{at}^4} \Bigg/ \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2}}$$

9. MAGNETSKA SVOJSTVA TVARI

Z-9.1 Izračunaj molarnu dijamagnetsku susceptibilnost plina vodikovih atoma u osnovnom stanju ako je pripadna kvantnomehanička valna funkcija elektrona $\Psi(r)=\frac{1}{\sqrt{\pi a_0^3}}\exp\left(-\frac{r}{a_0}\right)$, gdje je $a_0=\frac{\varepsilon_0 h^2}{\pi m e^2}$ Bohrov radijus.

rj: $\chi_d=-\frac{N_A\mu_0\varepsilon_0^2h^4}{2\pi^2m^3e^2}=-2.99\cdot10^{-11}\,m^3mol^{-1}$

Z-9.2 Konstruiravši particijsku funkciju sustava jednakih magnetskih dipola u vanjskom magnetskom polju *B*, pokaži da je magnetizacija sustava *M* jednaka negativnoj derivaciji slobodne energije *F* po magnetskom polju *B* tj. $M=-\frac{\partial F}{\partial B}$.

Z-9.3 Pokaži da se orbitalni magnetski moment točkastog naboja *q*, koji se giba jednoliko po zatvorenoj petlji proizvoljnog oblika u ravnini, može napisati kao $\vec{\mu}=\frac{1}{2}\int\vec{r}\times\vec{j}\,dV$ i $\vec{\mu}=\frac{q}{2m}\vec{L}$, gdje je **L** mehanički angularni moment.

Z-9.4 Odredi magnetizaciju paramagnetskog sustava jednakih magnetskih dipola ako projekcija dipola na smjer magnetskog polja **B** može poprimiti vrijednosti μ, 0, -μ. Primjenom dobivenog rezultata izvedi izraz za magnetsku susceptibilnost u granici $k_BT>>\mu B$.
Usporedi izraz s "kvantnim rezultatom" $M=ng\mu_B j\mathscr{B}_j(x)$, gdje je: *n* koncentracija dipola, *g* Landeov faktor, μ_B Bohrov magneton, $j=J/\hbar$ totalni angularni moment, $\mathscr{B}_j(x)$ Brillouinova funkcija, te $x\equiv g\mu_B jB/k_BT$, za paramagnetizam atoma s predavanja ($j=l=1$, $s=0$, $\mu=\mu_B$).

rj: $\chi=\frac{2}{3}\frac{n\mu_0\mu^2}{k_BT}$

Z-9.5 Izvedi izraz za atomsku paramagnetsku susceptibilnost na temperaturi *T* uz pretpostavku da kut između magnetskog polja **B** i magnetskog dipola **μ** pripada kontinuumu vrijednosti između 0 i π. Potom iz dobivenog rezultata izvedi izraz u granici $k_BT>>\mu B$.

rj:

$$M=n\mu L\left(\frac{\mu B}{k_BT}\right),\quad L(x)\equiv\mathrm{cth}(x)-\frac{1}{x}$$

$$\chi\approx\frac{n\mu_0\mu^2}{3k_BT},\quad \mu B\ll k_BT$$

Z-9.6 Izračunaj totalni angularni moment *j* (kvantni broj) za atom:
a) C^{6}; b) Fe^{26}; c) Co^{27}.

rj: a) $j=0$; b) $j=4$; c) $j=7/2$

Z-9.7 Polazeći od hamiltonijana atomskog elektronskog spina **S** i angularnog momenta **L** u vanjskom magnetskom polju **B**; $H=\frac{e}{2m}\left(\vec{L}+2\vec{S}\right)+\alpha\vec{L}\cdot\vec{S}$, gdje je $\alpha<<1$ konstanta vezanja spin-staza (L-S vezanje), odredi njegovu energiju u granici slabog i u granici jakog magnetskog polja.

rj:
a) Za slabo polje **B**, član L-S vezanja je nezanemariv i uzrokuje precesiju **L** i **S** oko **J**; problem možemo riješiti tako da **L** i **S** prvo proiciramo na **J**, a potom na os kvantizacije određenu s **B** - to je tzv. Zeemanov efekt:

$E=\mu_B g_j j_z B, \quad g_j=1+\frac{j(j+1)-l(l+1)+s(s+1)}{2j(j+1)}$ (Landeov faktor).

b) Za jako polje **B**, član L-S je zanemariv; L i S se ponašaju nevezano i svaki za sebe se direktno proicira na os kvantizacije određenu s **B** - to je Paschen-Bachov efekt:

$E=\mu_B\left(l_z+2s_z\right)B$

Z-9.8 U okviru klasične Weissove teorije feromagnetizma, polazeći od izraza za magnetizaciju paramagneta sa spinovima ±1/2, koncentracije dipola *n*, na temperaturi *T* i u vanjskom magnetskom polju *B*, $M=n\mu_B\tanh\frac{\mu_B B}{k_B T}$, izvedi:

a) uvjet nastajanja spontane magnetizacije,
b) izraz za ovisnost magnetizacije o temperaturi u blizini kritične temperature,
c) izraz za susceptibilnost u paramagnetskoj fazi (Curie-Weiss) u granici visokih temperatura (u odnosu na magnetske pojave).

rj:

a) Dobiva se transcedentna jednadžba $x=\tanh\left(\frac{T_C}{T}x\right)$, $x\equiv\frac{M}{n\mu_B}$, $T_C\equiv\frac{\mu_0\mu_B^2\lambda n}{k_B}$ koja ima neiščezavajuća rješenja za $x\sim M$ ako je $T<T_C$ tj. $T<\frac{\mu_0\mu_B^2 n\lambda}{k_B}$ (λ je Weissova konst.).

b) $M\sim\sqrt{T-T_C}$

c) $\chi_p=\frac{C}{T-T_C}, \quad C\equiv\frac{n\mu_0\mu_B^2}{k_B}$

Z-9.9 Izvedi izraz za spinski paramagnetizam vodljivih elektrona (Pauli) u metalu na $T=0$, koristeći razvoj Fermi-Diracove raspodjele pri $\mu_B B<<E_F$.

rj: $\chi_P=\mu_0\mu_B^2 g_F$

Z-9.10 Izvedi izraz za spinsku susceptibilnost slobodnog elektronskog plina ako u Paulijev paramagnetizam uključimo i odbojnu kulonsku interakciju elektrona suprotnog spina na istom čvoru rešetke (kratkodosežna interakcija) parametriziranu na način $E_{\text{int}}=Un_{\uparrow}n_{\downarrow}$ (U je konstanta interakcije, $n_{\uparrow}$, $n_{\downarrow}$ su koncentracije spina ↑, ↓). Koji uvjet je potrebno ispuniti da se elektronski spinovi spontano urede feromagnetski? Neka je g_{F} gustoća stanja elektrona na Fermijevoj energiji.

rj: $\chi = \dfrac{g_F \mu_0 \mu_B^2}{1 - \dfrac{g_F U}{2}}$

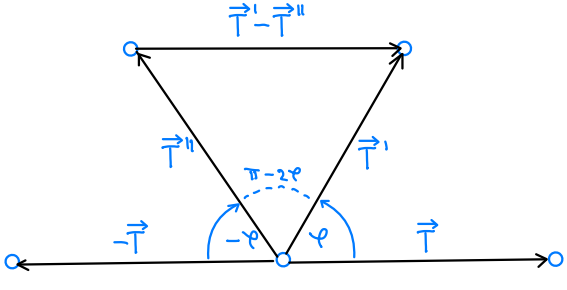
Odatle slijedi uvjet spontane magnetizacije (feromagnetizam): $1 - \dfrac{g_F U}{2} = 0$ (Stonerov kriterij).

RJEŠENJA ZADATAKA

I. KRISTALNA STRUKTURA

Z-1.1

Kristal mora istovremeno zadovoljavati translacijsku i rotacijsku simetriju, dakle svaka operacija mora čvor rešetke preslikati na čvor da bi sustav na nju bio invarijantan. Definiramo vektor translacije rešetke $\vec{T}$ koji povezuje 2 čvora rešetke. Tada i $-\vec{T}$ također povezuje 2 čvora rešetke. Ako $\vec{T}$ zarotiramo za kut φ u vektor $\vec{T}'$, a $-\vec{T}$ zarotiramo za kut $-\varphi$ u vektor $\vec{T}''$, gdje je $\varphi = \frac{2\pi}{n}$, n je red osi rotacije, tada vektor $\vec{T}'-\vec{T}''$ mora opet povezivati dva čvora rešetke, te biti kolinearan i sumjerljiv s $\vec{T}$.



$$\vec{T}'-\vec{T}'' = m\vec{T} \quad \Big|^2, \quad m \in \mathbb{Z}$$

$$|\vec{T}'|^2+|\vec{T}''|^2-2|\vec{T}'||\vec{T}''|\underbrace{\cos(\pi-2\varphi)}_{=-\cos 2\varphi} = m|\vec{T}|^2 \quad \Big| : |\vec{T}|^2$$

$$\Downarrow \quad (|\vec{T}'| = |\vec{T}''| = |\vec{T}|)$$

$$1 + 1 + 2\cos 2\varphi = m^2$$

$$4\cos^2\varphi = m^2$$

$$\Downarrow$$

$$2\cos\frac{2\pi}{n} = m, \quad m \in \mathbb{Z} \ \& \ n \in \mathbb{N}_0$$

n	$2\cos\frac{2\pi}{n}$	$\stackrel{?}{\in}\mathbb{Z}$
1	2	✓
2	−2	✓
3	−1	✓
4	0	✓
5	0.618	✗
6	1	✓
7	1.247	✗
8	$\sqrt{2}$	✗
9	1.532	✗
10	1.618	✗

$$\Rightarrow \quad n \in \{1, 2, 3, 4, 6\}$$

Z-1.2

$\Omega^* = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$; $\vec{b}_i = \frac{2\pi}{\Omega} \vec{a}_j \times \vec{a}_k$ $\quad i \to j \to k$

$\Omega^* = \left(\frac{2\pi}{\Omega}\right)^3 (\vec{a}_2 \times \vec{a}_3) \cdot [(\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2)]$

koristimo: $\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B})$

$\Omega^* = \left(\frac{2\pi}{\Omega}\right)^3 (\vec{a}_2 \times \vec{a}_3) \{ \vec{a}_1 [(\vec{a}_3 \times \vec{a}_1) \cdot \vec{a}_2] - \vec{a}_2 [(\vec{a}_3 \times \vec{a}_1) \cdot \vec{a}_1] \}$ (2 → 3 → 1; $\perp \vec{a}_1$, $= 0$)

$= \left(\frac{2\pi}{\Omega}\right)^3 (\vec{a}_2 \times \vec{a}_3) \{ \vec{a}_1 [(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3] - 0 \}$

$= \left(\frac{2\pi}{\Omega}\right)^3 \underbrace{(\vec{a}_2 \times \vec{a}_3) \cdot \vec{a}_1}_{1 \to 2 \to 3 \; = \Omega}$

$= \frac{(2\pi)^3}{\Omega}$

$\Rightarrow \Omega \Omega^* = (2\pi)^3$

Z-1.3

$\vec{a}_i$ – realna rešetka

$\vec{b}_i$ – recipročna rešetka $\Rightarrow \vec{A}_i = \frac{2\pi}{\Omega^*} (\vec{b}_j \times \vec{b}_k)$ $\quad i \to j \to k$

$\vec{A}_1 = \frac{2\pi}{\Omega^*} \left(\frac{2\pi}{\Omega}\right)^2 (\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2)$, $\quad \Omega \Omega^* = (2\pi)^3$

$= \frac{2\pi}{(2\pi)^3/\Omega} \left(\frac{2\pi}{\Omega}\right)^2 \{ \vec{a}_1 \underbrace{[(\vec{a}_3 \times \vec{a}_1) \cdot \vec{a}_2]}_{2 \to 3 \to 1} - \vec{a}_2 [(\vec{a}_3 \times \vec{a}_1) \cdot \vec{a}_1] \} = \vec{a}_1$ ($\perp \vec{a}_1$, $= 0$)

$= \vec{a}_1 [(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3] = \vec{a}_1 \Omega$

$\vec{A}_2 = \frac{2\pi}{\Omega^*} \left(\frac{2\pi}{\Omega}\right)^2 (\vec{a}_1 \times \vec{a}_2) \times (\vec{a}_2 \times \vec{a}_3)$

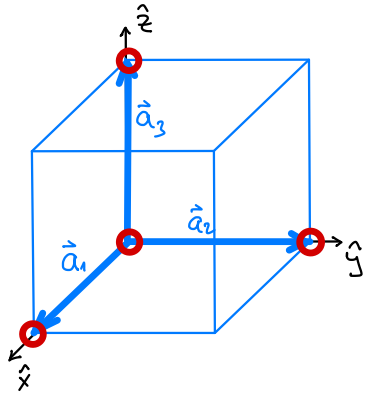
$= \frac{2\pi}{(2\pi)^3/\Omega} \left(\frac{2\pi}{\Omega}\right)^2 \{ \vec{a}_2 \underbrace{[(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3]}_{\Omega} - \vec{a}_3 [(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_2] \} = \vec{a}_2$ ($\perp \vec{a}_2$, $= 0$)

$\vec{A}_3 = \frac{2\pi}{\Omega^*} \left(\frac{2\pi}{\Omega}\right)^2 (\vec{a}_2 \times \vec{a}_3) \times (\vec{a}_3 \times \vec{a}_1)$

$= \frac{2\pi}{(2\pi)^3/\Omega} \left(\frac{2\pi}{\Omega}\right)^2 \{ \vec{a}_3 \underbrace{[(\vec{a}_2 \times \vec{a}_3) \cdot \vec{a}_1]}_{\Omega} - \vec{a}_1 [(\vec{a}_2 \times \vec{a}_3) \cdot \vec{a}_3] \} = \vec{a}_3$ ($\perp \vec{a}_3$, $= 0$)

Z-1.4

a) SC



$$\vec{a}_1 = a\hat{x} = a\begin{pmatrix}1\\0\\0\end{pmatrix}$$

$$\vec{a}_2 = a\hat{y} = a\begin{pmatrix}0\\1\\0\end{pmatrix}$$

$$\vec{a}_3 = a\hat{z} = a\begin{pmatrix}0\\0\\1\end{pmatrix}$$

$$\vec{b}_i = \frac{2\pi}{\Omega}(\vec{a}_j \times \vec{a}_k)$$



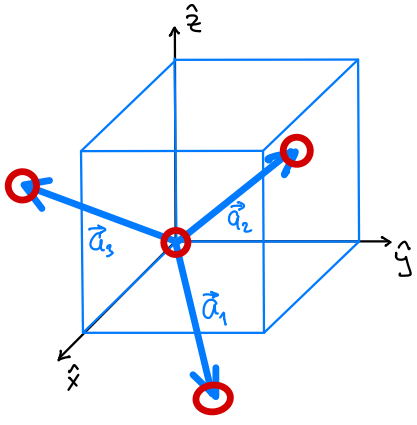
$$\Omega = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = a(1,0,0)\, a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = a^3 \underbrace{(1,0,0)\cdot(1,0,0)}_{1+0+0} = a^3$$

$$\vec{b}_1 = \frac{2\pi}{\Omega}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a^3} a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\0\\0\end{pmatrix}$$

$$\vec{b}_2 = \frac{2\pi}{\Omega}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{a^3} a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}0\\1\\0\end{pmatrix}$$

$$\vec{b}_3 = \frac{2\pi}{\Omega}(\vec{a}_1 \times \vec{a}_2) = \frac{2\pi}{a^3} a^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}0\\0\\1\end{pmatrix}$$

b) BCC



$$\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z}) = \frac{a}{2}\begin{pmatrix}1\\1\\-1\end{pmatrix}$$

$$\vec{a}_2 = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z}) = \frac{a}{2}\begin{pmatrix}-1\\1\\1\end{pmatrix}$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x}-\hat{y}+\hat{z}) = \frac{a}{2}\begin{pmatrix}1\\-1\\1\end{pmatrix}$$

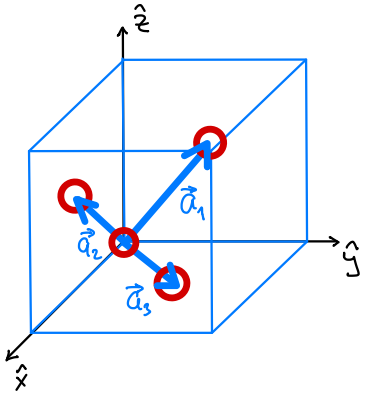
$$\Omega = \vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = \frac{a}{2}(1,1,-1)\frac{a^2}{4}\begin{vmatrix}\hat{x}&\hat{y}&\hat{z}\\-1&1&1\\1&-1&1\end{vmatrix} = \frac{a^3}{8}(1,1,-1)\cdot(2,2,0) = \frac{a^3}{2}$$

$$\vec{b}_1 = \frac{2\pi}{\Omega}(\vec{a}_2\times\vec{a}_3) = \frac{2\pi}{\frac{a^3}{2}}\frac{a^2}{4}\begin{vmatrix}\hat{x}&\hat{y}&\hat{z}\\-1&1&1\\1&-1&1\end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\1\\0\end{pmatrix}$$

$$\vec{b}_2 = \frac{2\pi}{\Omega}(\vec{a}_3\times\vec{a}_1) = \frac{2\pi}{\frac{a^3}{2}}\frac{a^2}{4}\begin{vmatrix}\hat{x}&\hat{y}&\hat{z}\\1&-1&1\\1&1&-1\end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}0\\1\\1\end{pmatrix}$$

$$\vec{b}_3 = \frac{2\pi}{\Omega}(\vec{a}_1\times\vec{a}_2) = \frac{2\pi}{\frac{a^3}{2}}\frac{a^2}{4}\begin{vmatrix}\hat{x}&\hat{y}&\hat{z}\\1&1&-1\\-1&1&1\end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\0\\1\end{pmatrix}$$

c) FCC



$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}) = \frac{a}{2}\begin{pmatrix}0\\1\\1\end{pmatrix}$$

$$\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z}) = \frac{a}{2}\begin{pmatrix}1\\0\\1\end{pmatrix}$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}) = \frac{a}{2}\begin{pmatrix}1\\1\\0\end{pmatrix}$$

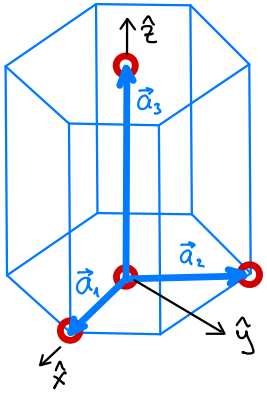
$$\Omega = \vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = \frac{a}{2}(0,1,1)\frac{a^2}{4}\begin{vmatrix}\hat{x}&\hat{y}&\hat{z}\\1&0&1\\1&1&0\end{vmatrix} = \frac{a^3}{8}(0,1,-1)\cdot(-1,1,1) = \frac{a^3}{4}$$

$$\vec{b}_1 = \frac{2\pi}{\Omega}(\vec{a}_2\times\vec{a}_3) = \frac{2\pi}{\frac{a^3}{4}}\frac{a^2}{4}\begin{vmatrix}\hat{x}&\hat{y}&\hat{z}\\1&0&1\\1&1&0\end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}-1\\1\\1\end{pmatrix}$$

$$\vec{b}_2 = \frac{2\pi}{\Omega}(\vec{a}_3\times\vec{a}_1) = \frac{2\pi}{\frac{a^3}{4}}\frac{a^2}{4}\begin{vmatrix}\hat{x}&\hat{y}&\hat{z}\\1&1&0\\0&1&1\end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\-1\\1\end{pmatrix}$$

$$\vec{b}_3 = \frac{2\pi}{\Omega}(\vec{a}_1\times\vec{a}_2) = \frac{2\pi}{\frac{a^3}{4}}\frac{a^2}{4}\begin{vmatrix}\hat{x}&\hat{y}&\hat{z}\\0&1&1\\1&0&1\end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\1\\-1\end{pmatrix}$$

d) 3D heksagonska ćelija



$$\vec{a}_1 = a\begin{pmatrix}1\\0\\0\end{pmatrix}$$

$$\vec{a}_2 = \frac{a}{2}\begin{pmatrix}-1\\\sqrt{3}\\0\end{pmatrix}$$

$$\vec{a}_3 = c\begin{pmatrix}0\\0\\1\end{pmatrix}$$

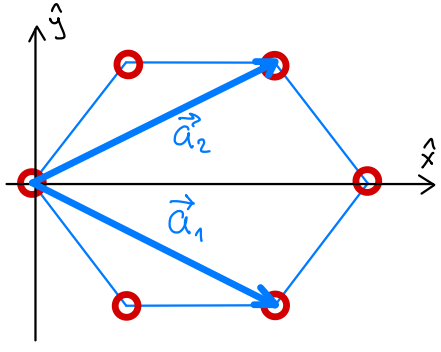
$$\Omega = \vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = a(1,0,0)\frac{ac}{2}\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ -1 & \sqrt{3} & 0\\ 0 & 0 & 1\end{vmatrix} = \frac{a^2c}{2}(1,0,0)\cdot(\sqrt{3},1,0) = \frac{\sqrt{3}a^2c}{2}$$

$$\vec{b}_1 = \frac{2\pi}{\Omega}(\vec{a}_2\times\vec{a}_3) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c}\frac{ac}{2}\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ -1 & \sqrt{3} & 0\\ 0 & 0 & 1\end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\\frac{1}{\sqrt{3}}\\0\end{pmatrix}$$

$$\vec{b}_2 = \frac{2\pi}{\Omega}(\vec{a}_3\times\vec{a}_1) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c}ac\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ 0 & 0 & 1\\ 1 & 0 & 0\end{vmatrix} = \frac{2\pi}{a}\begin{pmatrix}0\\\frac{2}{\sqrt{3}}\\0\end{pmatrix}$$

$$\vec{b}_3 = \frac{2\pi}{\Omega}(\vec{a}_1\times\vec{a}_2) = \frac{2\pi}{\frac{\sqrt{3}}{2}a^2c}\frac{\sqrt{3}a^2}{2}\begin{vmatrix}\hat{x} & \hat{y} & \hat{z}\\ 1 & 0 & 0\\ -1 & \sqrt{3} & 0\end{vmatrix} = \frac{2\pi}{c}\begin{pmatrix}0\\0\\1\end{pmatrix}$$

e) 2D saćasta ("honeycomb") ćelija



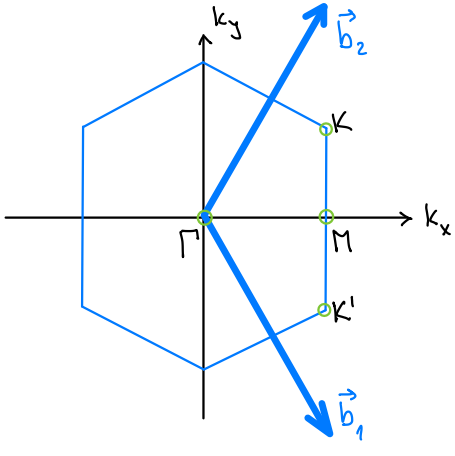
$$\vec{a}_1 = \frac{a}{2}\begin{pmatrix} 3 \\ -\sqrt{3} \end{pmatrix}$$

$$\vec{a}_2 = \frac{a}{2}\begin{pmatrix} 3 \\ \sqrt{3} \end{pmatrix}$$

$$\Omega = |\vec{a}_1 \times \vec{a}_2| = \left(\frac{a}{2}\right)^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 3 & -\sqrt{3} & 0 \\ 3 & \sqrt{3} & 0 \end{vmatrix} = \left(\frac{a}{2}\right)^2 \left|\hat{x}\cdot 0 - \hat{y}\cdot 0 + \hat{z}(3\sqrt{3} + 3\sqrt{3})\right| = \frac{3\sqrt{3}}{2}a^2$$

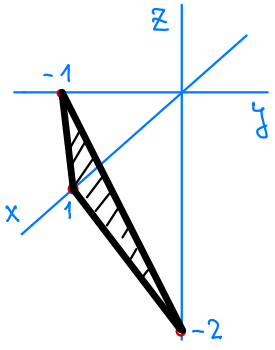
$$\vec{b}_1 = \frac{2\pi}{\Omega}(\vec{a}_2 \times \hat{z}) = \frac{2\pi}{\frac{3\sqrt{3}}{2}a^2}\frac{a}{2}\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 3 & \sqrt{3} & 0 \\ 0 & 0 & 1 \end{vmatrix} = \frac{2\pi}{3a}\begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix}$$

$$\vec{b}_2 = \frac{2\pi}{\Omega}(\hat{z} \times \vec{a}_1) = \frac{2\pi}{\frac{3\sqrt{3}}{2}a^2}\frac{a}{2}\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & 1 \\ 3 & -\sqrt{3} & 0 \end{vmatrix} = \frac{2\pi}{3a}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}$$



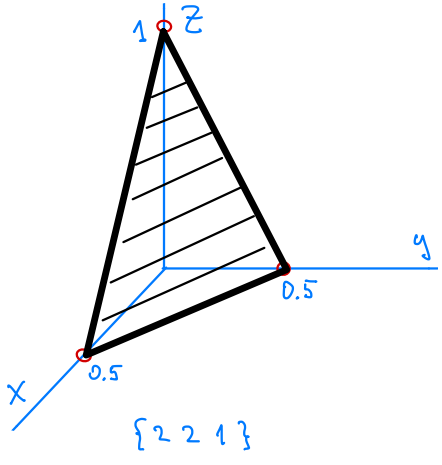
Z-1.5

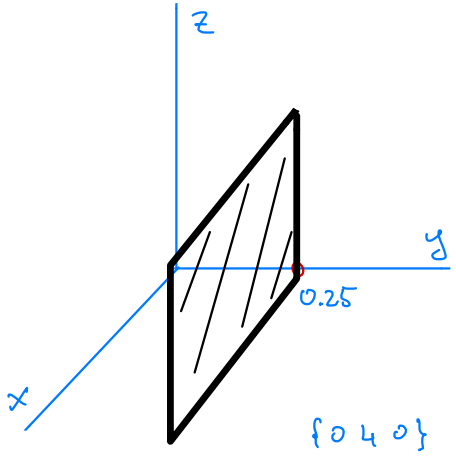
a)



$\frac{1}{1}, \frac{1}{-1}, \frac{1}{-2} \Rightarrow \{2\ \bar{2}\ \bar{1}\}$

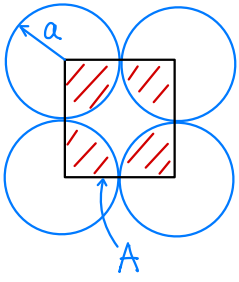
b)





Z-1.6

(1) SC {1 0 0}



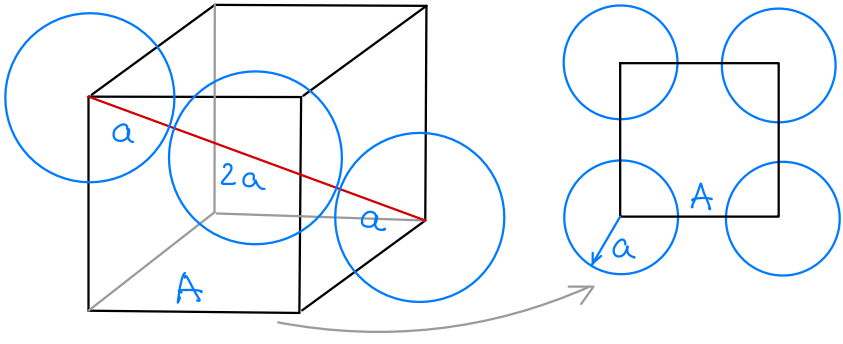
$A = 2a$

$S_o = 4 \cdot \frac{1}{4} a^2 \pi = a^2 \pi$

$S_\square = A^2 = 4a^2$

$\eta = \frac{S_o}{S_\square} = \frac{\pi}{4}$

(2) BCC {1 0 0}



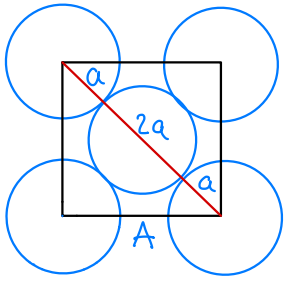
$\sqrt{3} A = 4a$

$S_o = 4 \cdot \frac{1}{4} a^2 \pi = a^2 \pi$

$S_\square = A^2 = \frac{16}{3} a^2$

$\eta = \frac{S_o}{S_\square} = \frac{3\pi}{16} = 0.589$

(3) FCC {1 0 0}



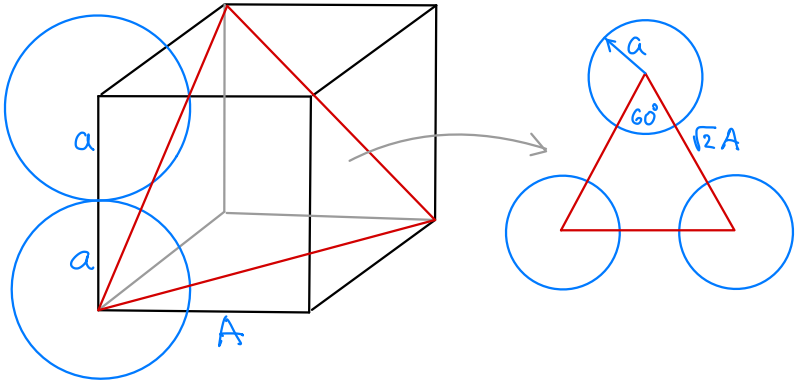
$\sqrt{2} A = 4a$

$S_o = 4 \cdot \frac{1}{4} a^2 \pi + a^2 \pi = 2a^2 \pi$

$S_\square = A^2 = 8a^2$

$\eta = \frac{S_o}{S_\square} = \frac{\pi}{4}$

(4) SC {1 1 1}



$A = 2a$

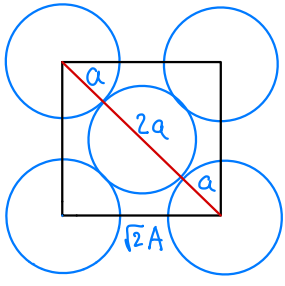
$S_o = 3 \frac{1}{6} a^2\pi = \frac{a^2\pi}{2}$

$S_\Delta = \frac{(A\sqrt{2})^2\sqrt{3}}{4} = 2\sqrt{3}a^2$

$\eta = \frac{S_o}{S_\Delta} = \frac{\pi}{4\sqrt{3}}$

$= 0.454$

(5) BCC {1 1 0}



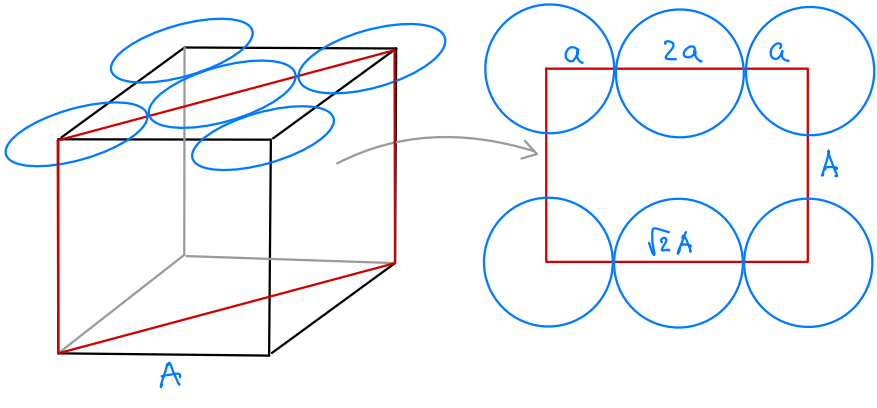
$\sqrt{3}A = 4a$

$S_o = 4 \cdot \frac{1}{4} a^2\pi + a^2\pi = 2a^2\pi$

$S_\square = A \cdot \sqrt{2}A = \frac{16\sqrt{2}}{3} a^2$

$\eta = \frac{S_o}{S_\square} = \frac{3\pi}{8\sqrt{2}} = 0.833$

(6) FCC {1 1 0}



$\sqrt{2}A = 4a$

$S_o = 4 \frac{1}{4} a^2\pi + 2 \frac{1}{2} a^2\pi = 2a^2\pi$

$S_\square = A \cdot \sqrt{2}A = 8\sqrt{2}\, a^2$

$\eta = \frac{S_o}{S_\square} = \frac{\pi}{\sqrt{24}}$

$= 0.555$

Z-1.7

Braggova formula: $n\lambda = 2d \sin\Theta$

$\Rightarrow \sin\Theta = n\frac{\lambda}{2d}$, $n \in \mathbb{N}$

$\frac{\lambda}{2d} = 0.375$

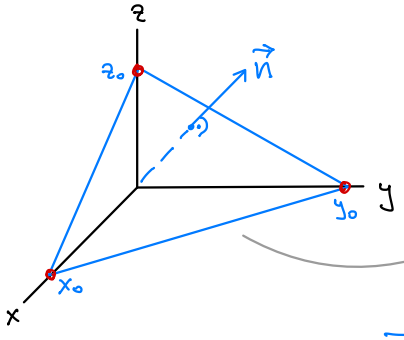
$n = 1$: $\Theta_1 = 22.02°$

$n = 2$: $\Theta_2 = 48.59°$

Z-1.8

jednadžba ravnine: $Ax + By + Cz = D$

udaljenost od ishodišta: $d = \frac{|D|}{\sqrt{A^2+B^2+C^2}}$



Sve koordinate normirane su na konstantu rešetke a (bezdimenzionalne su).

x_0, y_0, z_0 – probodišta koordinatnih osi

$\frac{x}{x_0} + \frac{y}{y_0} + \frac{z}{z_0} = 1$ – ravnina

$\Rightarrow d = \frac{1}{\sqrt{\left(\frac{1}{x_0}\right)^2 + \left(\frac{1}{y_0}\right)^2 + \left(\frac{1}{z_0}\right)^2}}$

Millerovi indeksi: $h = \frac{1}{x_0}$, $k = \frac{1}{y_0}$, $l = \frac{1}{z_0}$

$\Rightarrow d = \frac{1}{\sqrt{h^2+k^2+l^2}}$

def: $\vec{G}_{hkl} = \frac{2\pi}{a}(h,k,l)$

$(|\vec{G}_{hkl}| = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2})$

$\Rightarrow d = \frac{2\pi}{a}\frac{1}{|\vec{G}_{hkl}|}$

udaljenost susjednih ravnina (u jedinicama konstante rešetke tj. $\frac{d}{a}$)

$\Rightarrow d^{(n)}_{hkl} = 2\pi\frac{n}{|\vec{G}_{hkl}|}$ udaljenost n-te ravnine (u jedinicama metra)

Z-1.9

a)

Maksimumi su određeni Laueovom formulom:

$$2k \sin\frac{\theta}{2} = |\vec{G}_{hkl}| \,, \quad \vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

($k = \frac{2\pi}{\lambda}$)

rešetka je SC (s bazom) s primitivnim vektorima:

$$\vec{a}_1 = a\begin{pmatrix}1\\0\\0\end{pmatrix}, \ \vec{a}_2 = a\begin{pmatrix}0\\1\\0\end{pmatrix}, \ \vec{a}_3 = a\begin{pmatrix}0\\0\\1\end{pmatrix} \rightarrow \vec{b}_1 = \frac{2\pi}{a}\begin{pmatrix}1\\0\\0\end{pmatrix}, \ \vec{b}_2 = \frac{2\pi}{a}\begin{pmatrix}0\\1\\0\end{pmatrix}, \ \vec{b}_3 = \frac{2\pi}{a}\begin{pmatrix}0\\0\\1\end{pmatrix}$$

$$|\vec{G}_{hkl}| = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2}$$

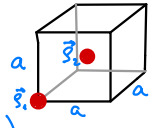
$$\Rightarrow \sin\frac{\theta}{2} = \frac{\lambda}{4\pi}\frac{2\pi}{a}\sqrt{h^2+k^2+l^2}$$

Braggov kut: $\varphi = \frac{\theta}{2}$

$$\Rightarrow \varphi = \arcsin\frac{\lambda}{2a}\sqrt{h^2+k^2+l^2}$$

Vidljivost Braggovog maksimuma određena je strukturnim faktorom baze:

$$F_{hkl} = \sum_i f_i \, e^{i\vec{G}_{hkl}\cdot\vec{s}_i}$$



Za BCC je $f_1 = f_2 \equiv f$; $\vec{s}_1 = \begin{pmatrix}0\\0\\0\end{pmatrix}$, $\vec{s}_2 = a\begin{pmatrix}1/2\\1/2\\1/2\end{pmatrix} = \frac{1}{2}(\vec{a}_1+\vec{a}_2+\vec{a}_3)$

$$F_{hkl} = f\cdot\left(\underbrace{1}_{e^0} + e^{i\vec{G}_{hkl}\cdot\vec{s}_2}\right)$$

$$\vec{G}_{hkl}\cdot\vec{s}_2 = (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)\cdot\frac{1}{2}(\vec{a}_1+\vec{a}_2+\vec{a}_3) \overset{\vec{b}_i\cdot\vec{a}_j = 2\pi\delta_{ij}}{=} \frac{1}{2}2\pi\,(h+k+l)$$

$$= \pi(h+k+l)$$

$$e^{i\vec{G}_{hkl}\cdot\vec{s}_2} = (-1)^{h+k+l} = \begin{cases} 1 \,, & h+k+l \text{ paran} \Rightarrow F_{hkl} = 2f \\ -1 \,, & h+k+l \text{ neparan} \Rightarrow F_{hkl} = 0 \end{cases}$$

Vidljivi maksimumi javljaju se za (h,k,l) kombinacije $(1,1,0)$, $(2,0,0)$, $(2,2,0)$, $(4,0,0)$..., tj. kombinacije za koje je $h^2+k^2+l^2 = 2, 4, 8, 16, \ldots$

Kako je $\varphi \sim h^2+k^2+l^2$, minimalan kut φ dobivamo za $h^2+k^2+l^2 = 2$, a to je za $(h,k,l) = (1,1,0)$, $(1,0,1)$, $(0,1,1)$.

$$\varphi_{min} = \arcsin\frac{\lambda}{2a}\sqrt{2} = \arcsin\frac{\lambda}{\sqrt{2}a} = 17.1^\circ$$

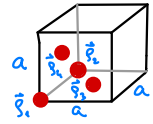
b)

Kao i u (a) zadatku, za primitivnu SC rešetku Braggov kut je:

$$\varphi = \arcsin \frac{\lambda}{2a}\sqrt{h^2+k^2+l^2}$$

Za FCC, baza je $f_1 = f_2 = f_3 = f_4 \equiv f$ i

$$\vec{\rho}_1 = a\begin{pmatrix}0\\0\\0\end{pmatrix},\quad \vec{\rho}_2 = a\begin{pmatrix}1/2\\1/2\\0\end{pmatrix} = \frac{1}{2}(\vec{a}_1+\vec{a}_2),\quad \vec{\rho}_3 = a\begin{pmatrix}1/2\\0\\1/2\end{pmatrix} = \frac{1}{2}(\vec{a}_1+\vec{a}_3),\quad \vec{\rho}_4 = a\begin{pmatrix}0\\1/2\\1/2\end{pmatrix} = \frac{1}{2}(\vec{a}_2+\vec{a}_3)$$



Strukturni faktor baze:

$$F_{hkl} = \sum_i f_i\, e^{i\vec{G}_{hkl}\cdot\vec{\rho}_i} = f\left(1 + e^{i\vec{G}_{hkl}\vec{\rho}_2} + e^{i\vec{G}_{hkl}\vec{\rho}_3} + e^{i\vec{G}_{hkl}\vec{\rho}_4}\right)$$

$$\vec{G}_{hkl} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 \quad , \quad \vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij}$$

$$\vec{G}\cdot\vec{\rho}_1 = 0$$
$$\vec{G}\cdot\vec{\rho}_2 = 2\pi\,\tfrac{1}{2}(h+k) = \pi(h+k)$$
$$\vec{G}\cdot\vec{\rho}_3 = \pi(h+l)$$
$$\vec{G}\cdot\vec{\rho}_4 = \pi(k+l)$$

$$F_{h,k,l} = f\left(1 + e^{i\pi(h+k)} + e^{i\pi(h+l)} + e^{i\pi(k+l)}\right)$$
$$= f\left(\underbrace{1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}}_{\equiv\,\Sigma}\right)$$

(h,k,l)	$(-1)^{h+k}$	$(-1)^{h+l}$	$(-1)^{k+l}$	Σ
1 0 0	-1	-1	-1	0
1 1 0	1	-1	-1	0
1 1 1	1	1	1	4 ✓
2 1 0	-1	1	-1	0
3 2 1	-1	1	-1	0
5 3 1	1	1	1	4 ✓
2 2 4	1	1	1	4 ✓

F_{hkl} je $\neq 0$ samo ako su (h,k,l) ili svi parni, ili svi neparni. Bilo koja parno-neparna kombinacija (h,k,l) vodi na $F_{hkl} = 0$.

Z-1.10

a)

N - broj regularnih mjesta u rešetci

N_s - broj Schottkyevih defekata, $N \gg N_s \gg 1$

B - termodinamička vjerojatnost: broj mikroskopskih konfiguracija koje vode na isto makroskopsko TD stanje - u promatranom slučaju to je broj realizacija razmještanja $N - N_s$ atoma i N_s vakancija na N mjesta u kristalu - kombinacije:

$$B = \binom{N}{N_s} = \frac{N!}{N_s!\,(N-N_s)!}$$

E_s - energija formiranja Sch. defekta

Slobodna energija: $F = U - TS = U_0 + N_s E_s - k_B T \ln B$

Stirlingova formula: $\ln x! \simeq x \ln x - x$, za $x \gg 1$

$$(*)\quad \ln N! = \ln 1 + \ln 2 + \cdots + \ln N = \sum_{x=1}^{N} \ln x \simeq \int_1^N \ln x\, dx = (x \ln x - x)\Big|_1^N = N \ln N - N + \cancel{1}^{N \gg 1}$$

$$\ln \frac{N!}{N_s!\,(N-N_s)!} = \ln N! - \ln N_s! - \ln (N-N_s)!$$

$$\approx N \ln N - \cancel{N} - N_s \ln N_s + \cancel{N_s} - (N-N_s)\ln(N-N_s) + \cancel{(N-N_s)}$$

$$= N \ln N - N_s \ln N_s - (N-N_s)\ln(N-N_s) = \ln B$$

Optimalan broj defekata na temperaturi T: $\frac{\partial F}{\partial T} = 0$

$$\frac{\partial F}{\partial N_s} = E_s - k_B T \left(-\ln N_s - N_s \frac{1}{N_s} + \ln(N-N_s) - (N-N_s)\frac{-1}{N-N_s} \right) = 0$$

$$E_s - k_B T \ln \frac{N-N_s}{N_s} = 0$$

$$\frac{N - \cancel{N_s}^{N_s \ll N}}{N_s} = e^{\frac{E_s}{k_B T}}$$

$$N_s = N e^{-\frac{E_s}{k_B T}}$$

b)

N - broj regularnih mjesta u rešetci
N_F - broj Frenkelovih defekata
N' - broj raspoloživih intersticijskih mjesta, $N, N' >> N_F >> 1$

B - termodinamička vjerojatnost: broj mikroskopskih konfiguracija koje vode na isto makroskopsko TD stanje - u promatranom slučaju to je: B_1 - broj realizacija razmještanja $N - N_F$ atoma i N_F defekata na N mjesta u kristalu (kombinacije) & B_2 - broj realizacija da N_F atoma zauzme N' intersticijskih mjesta

$$B = B_1 \cdot B_2, \quad B_1 = \binom{N}{N_F} = \frac{N!}{N_F!\,(N-N_F)!}, \quad B_2 = \binom{N'}{N_F} = \frac{N'!}{N_F!\,(N'-N_F)!}$$

(E_F: energija formiranja Fr. defekta)

Slobodna energija: $F = U - TS = U_0 + N_F E_F - k_B T \ln B$

Stirlingova formula: $\ln x! \simeq x \ln x - x$, za $x >> 1$

$$\ln \frac{N!\,N'!}{(N_F!)^2 (N-N_F)!\,(N'-N_F)!} = \ln N! + \ln N'! - \ln(N-N_F)! - \ln(N'-N_F)! - 2\ln N_F!$$

$$\approx N \ln N - N + N' \ln N' - N' - (N-N_F)\ln(N-N_F) + (N-N_F) - (N'-N_F)\ln(N'-N_F) + (N'-N_F) - 2N_F \ln N_F + 2N_F$$

$$= N \ln N + N' \ln N' - (N-N_F)\ln(N-N_F) - (N'-N_F)\ln(N'-N_F) - 2N_F \ln N_F = \ln B$$

Optimalan broj defekata na temperaturi T: $\frac{\partial F}{\partial T} = 0$

$$E_F - k_B T \left(-2\ln N_F - 2N_F \frac{1}{N_F} + \ln(N-N_F) - (N-N_F)\frac{-1}{N-N_F} - (N'-N_F)\frac{-1}{N'-N_F} \right) = 0$$

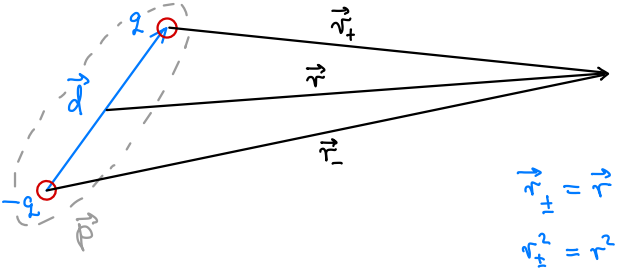
$$E_F - k_B T \ln \frac{(N-N_F)(N'-N_F)}{N_F^2} = 0 \qquad (N_F << N, N')$$

$$N_F = \sqrt{NN'}\, e^{-\frac{E_F}{2k_B T}}$$

II. MEĐUATOMSKE INTERAKCIJE U KRISTALIMA

Z-2.1

a)



$$\vec{r}_\pm = \vec{r} \mp \frac{\vec{d}}{2} = \vec{r}\left(1 \mp \frac{1}{2}\frac{\vec{r}\cdot\vec{d}}{|\vec{r}|^2}\right)$$

$$r_\pm^2 = r^2\left(1 \mp \frac{1}{2}\frac{\vec{r}\cdot\vec{d}}{r^2}\right)^2 = r^2\left(1 \mp \frac{\vec{r}\cdot\vec{d}}{r^2} + \frac{1}{4}\frac{(\vec{r}\cdot\vec{d})^2}{r^4}\right) \approx r^2\left(1 \mp \frac{\vec{r}\cdot\vec{d}}{r^2}\right) \quad (r \gg d)$$

$$\phi(\vec{r}) = \frac{+q}{4\pi\varepsilon_0 r_+} \quad \frac{-q}{4\pi\varepsilon_0 r_-}$$

$$= \frac{q}{4\pi\varepsilon_0}\left(\frac{1}{r_+} - \frac{1}{r_-}\right)$$

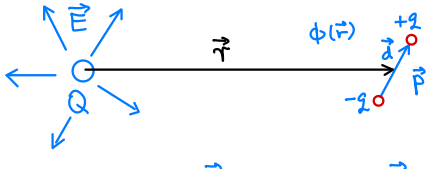
$$= \frac{q}{4\pi\varepsilon_0}\left[\frac{1}{r\sqrt{1-\frac{\vec{r}\cdot\vec{d}}{r^2}}} - \frac{1}{r\sqrt{1+\frac{\vec{r}\cdot\vec{d}}{r^2}}}\right] \quad ; \quad \frac{1}{\sqrt{1\pm x}} \simeq 1 \mp \frac{1}{2}x \;,\; x \ll 1$$

$$\approx \frac{q}{4\pi\varepsilon_0}\frac{1}{r}\left[\cancel{1} + \frac{1}{2}\frac{\vec{r}\cdot\vec{d}}{r^2} - \cancel{1} + \frac{1}{2}\frac{\vec{r}\cdot\vec{d}}{r^2}\right]$$

$$= \frac{q}{4\pi\varepsilon_0}\frac{\vec{r}\cdot\vec{d}}{r^3}$$

$$= \frac{\vec{r}\cdot\vec{p}}{4\pi\varepsilon_0 r^3} \quad (\vec{p} = q\vec{d})$$

b)



$$\phi(\vec{r}) = \frac{Q}{4\pi\varepsilon_0 r}$$

$$U(\vec{r}) = +q\,\phi\left(\vec{r} + \frac{\vec{d}}{2}\right) + (-q)\,\phi\left(\vec{r} - \frac{\vec{d}}{2}\right)$$

$$\approx q\left[\phi(\vec{r}) + \frac{\partial\phi}{\partial\vec{r}}\Big|_{\vec{r}}\cdot\frac{\vec{d}}{2} - \phi(\vec{r}) + \frac{\partial\phi}{\partial\vec{r}}\Big|_{\vec{r}}\cdot\frac{\vec{d}}{2}\right] \;,\; |\vec{d}| \ll |\vec{r}|$$

$$= \underbrace{q\vec{d}}_{=\vec{p}} \cdot \underbrace{\vec{\nabla}\phi(\vec{r})}_{=-\vec{\Pi}}$$

$$= -\vec{p}\cdot\vec{\Pi}$$

c)

$\phi(\vec{r}) = \frac{\vec{p}\cdot\vec{r}}{4\pi\varepsilon_0 r^3}$ - potenciál dipólu $\vec{p}$

$\vec{E}(\vec{r}) = -\vec{\nabla}\phi(\vec{r})$ - elektrické pole dipólu $\vec{p}$

$$\vec{E}(\vec{r}) = -\vec{\nabla}\frac{\vec{p}\cdot\vec{r}}{4\pi\varepsilon_0 r^3}$$

$$= \left[\hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z}\right]\frac{1}{4\pi\varepsilon_0}\frac{p_x x + p_y y + p_z z}{(x^2+y^2+z^2)^{3/2}}$$

$$= -\frac{1}{4\pi\varepsilon_0}\left\{\hat{x}\left[\frac{p_x}{(x^2+y^2+z^2)^{3/2}} - \frac{3}{2}\frac{p_x x + p_y y + p_z z}{(x^2+y^2+z^2)^{5/2}}2x\right] + \right.$$

$$+ \hat{y}\left[\frac{p_y}{(x^2+y^2+z^2)^{3/2}} - \frac{3}{2}\frac{p_x x + p_y y + p_z z}{(x^2+y^2+z^2)^{5/2}}2y\right] +$$

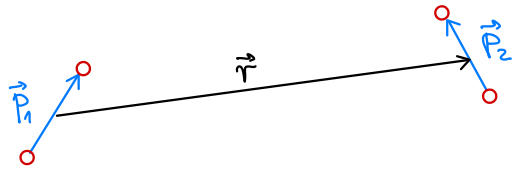
$$\left. + \hat{z}\left[\frac{p_z}{(x^2+y^2+z^2)^{3/2}} - \frac{3}{2}\frac{p_x x + p_y y + p_z z}{(x^2+y^2+z^2)^{5/2}}2z\right]\right\}$$

$$= -\frac{1}{4\pi\varepsilon_0}\left\{\frac{p_x x}{r^3} - 3\frac{\vec{p}\cdot\vec{r}}{r^5}x\hat{x}\quad\frac{p_y y}{r^3} - 3\frac{\vec{p}\cdot\vec{r}}{r^5}y\hat{y}\quad\frac{p_z z}{r^3} - 3\frac{\vec{p}\cdot\vec{r}}{r^5}z\hat{z}\right\}$$

$$= \frac{1}{4\pi\varepsilon_0}\left\{-\frac{\vec{p}}{r^3} + 3\frac{\vec{p}\cdot\vec{r}}{r^5}\vec{r}\right\}$$

$$= \frac{1}{4\pi\varepsilon_0}\frac{3\vec{r}(\vec{p}\cdot\vec{r}) - r^2\vec{p}}{r^5}$$

Z-2.2



$\phi_1(\vec{r}) = \frac{\vec{p}_1 \cdot \vec{r}}{4\pi\varepsilon_0 r^3}$ - potencijal dipola $\vec{p}_1$ na položaju $\vec{r}$

$E_1(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \frac{3\vec{r}(\vec{p}\cdot\vec{r}) - r^2\vec{p}}{r^5}$ - električno polje dipola $\vec{p}_1$ na položaju $\vec{r}$

Za procjenu biramo konfiguraciju $\vec{p}_1 \parallel \vec{r} \parallel \vec{p}_2$ jer je tada pot. en. maksimalna

$\vec{p}_1 \parallel \vec{r} \Rightarrow \vec{p}_1 \cdot \vec{r} = p_1 r$

$\vec{E}_1 = \frac{1}{4\pi\varepsilon_0} \frac{3\vec{r}\, p_1 r - r^2 \vec{p}_1}{r^5} \Rightarrow E_1 = \frac{1}{4\pi\varepsilon_0} \frac{3p_1 r^2 - r^2 p_1}{r^5} = \frac{1}{2\pi\varepsilon_0} \frac{p_1}{r^3}$

Polje $\vec{E}_1$ inducira dipol $\vec{p}_2$ djelovanjem na atom 2:

$\vec{p}_2 = \varepsilon_0 \alpha \vec{E}_1$ ← polarizabilnost atoma

$U = -\vec{p}_2 \cdot \vec{E}_1$ - potencijalna energija dipola $\vec{p}_2$ u polju $\vec{E}_1$

$(\vec{p}_2 \parallel \vec{E}_1)$

$= -\alpha \varepsilon_0 E_1^2$

$= -\frac{\alpha p_1^2}{4\pi^2 \varepsilon_0 r^6} \equiv -\frac{B}{r^6}$

Z-2.3

$$E_p(r) = -\frac{a}{r^n} + \frac{b}{r^{n'}}$$

uvjeti stabilnosti: 1°) $\left.\frac{dE_p}{dr}\right|_{r_0} = 0$ - ekstrem

i 2°) $\left.\frac{d^2E_p}{dr^2}\right|_{r_0} > 0$ - ekstrem je minimum

1°) $\frac{dE_p}{dr} = \frac{na}{r^{n+1}} - \frac{n'b}{r^{n'+1}} = 0$

$\Rightarrow r^{n-n'} = \frac{na}{n'b}$

2°) $\frac{d^2E_p}{dr^2} = -\frac{n(n+1)a}{r^{n+2}} + \frac{n'(n'+1)b}{r^{n'+2}} > 0$

$\Rightarrow r^{n-n'} > \frac{n(n+1)a}{n'(n'+1)b}$

(1°) & (2°):

$$\frac{na}{n'b} > \frac{n(n+1)a}{n'(n'+1)b} \quad \Big| : \frac{na}{n'b}$$

$$1 > \frac{n+1}{n'+1} \Rightarrow n' > n$$

Sustav je stabilan ako na malim udaljenostima dominira odbojni, a na većim privlačni član, što je ostvareno ako je n'>n.

Z-2.4

$$U = -\frac{A}{r^n} + Be^{-\frac{r}{a}}$$

$$\left.\frac{dU}{dr}\right|_{r_0} = 0 \Rightarrow nA\frac{1}{r_0^{n+1}} - \frac{B}{a}e^{-\frac{r_0}{a}} = 0 \rightarrow Be^{-\frac{r_0}{a}} = naA\frac{1}{r_0^{n+1}}$$

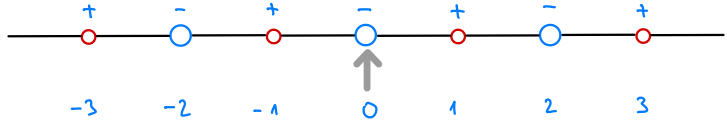
$$\Rightarrow U(r_0) = -\frac{A}{r_0^n} + naA\frac{1}{r_0^{n+1}}$$

$$= -\frac{A}{r_0^n}\left(1 - \frac{na}{r_0}\right)$$

Z-2.5

$\alpha_n = \sum_j \frac{\mp 1}{p_j}$: p_j - diskretna udaljenost ishodišnog iona do j-tog susjeda; „−" za istoimeni, a „+" za raznoimeni naboj

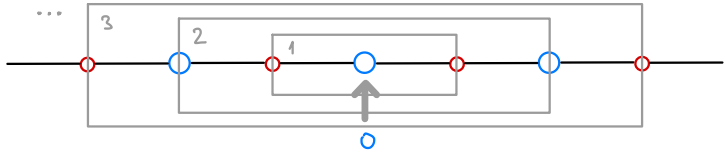
a)



egzaktno:

$$\alpha_n = 2\cdot\left(1 + \frac{-1}{2} + \frac{+1}{3} + \frac{-1}{4} + \cdots\right)$$
$$= 2\left(1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots\right)$$
$$= 2\ln 2 = 1.3863$$

Evjen-Frank: konstruiramo nabojno neutralne ćelije i sumiramo α_n po njima



doprinosi u α_n:

1. E-F ćelija: $2\cdot\frac{1/2}{1} = 1$

2. E-F ćelija: $2\left[\frac{1/2}{1} + \frac{-1/2}{1}\right] = \frac{1}{2} = 0.5$

3. E-F ćelija: $2\left[\frac{-1/2}{2} + \frac{1/2}{3}\right] = -\frac{1}{6} = -0.1667$

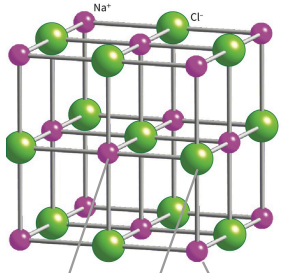
4. E-F ćelija: $2\left[\frac{1/2}{3} + \frac{-1/2}{4}\right] = \frac{1}{12} = 0.0833$

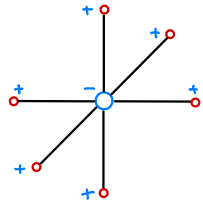
5. E-F ćelija: $2\left[\frac{-1/2}{4} + \frac{1/2}{5}\right] = -\frac{1}{20} = -0.05$

$\sum$: $\alpha_n^{(5)} \simeq 1.3666$

„Obična" sumacija prvih 5 članova alternirajućeg reda, $\alpha_n^{(5)} = 2\left(1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5}\right) \simeq 0.7833$ daje puno lošiji rezultat od E-F metode.

b)





„Hitra sumacija":

		doprinos do
1.	$6\oplus$, $p=1$	$6/1$
2.	$12\ominus$, $p=\sqrt{2}$	$-12/\sqrt{2}$
3.	$8\oplus$, $p=\sqrt{3}$	$8/\sqrt{3}$
4.	$6\ominus$, $p=2$	$-6/2$

Σ: $\alpha_M = \frac{6}{1} - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{2} + \dots$

≈ -0.865

Loše :(

1. E-F ploskev:

$$\alpha_M^{(I)} = \frac{6\cdot\frac{1}{2}}{1} + \frac{12\cdot\left(-\frac{1}{4}\right)}{\sqrt{2}} + \frac{8\cdot\frac{1}{8}}{\sqrt{3}} = 1.46$$

2. E-F ploskev:

$$\alpha_M^{(II)} = 6\frac{1/2}{1} - 12\frac{3/4}{\sqrt{2}} + 8\frac{7/8}{\sqrt{3}} -$$

ostatale 1. ploskve

$$- 4\frac{1/2}{2} + 8\frac{1/2}{\sqrt{5}} - 4\frac{1/4}{\sqrt{8}} +$$

1. ravnina 2. ploskve

$$+2\left\{4\frac{1/2}{\sqrt{5}} - 8\frac{1/2}{\sqrt{6}} + 4\frac{1/4}{\sqrt{9}}\right\} +$$

2. ravnina 2. ploskve × 2

$$+2\left\{-4\frac{1/4}{\sqrt{8}} + 8\frac{1/4}{\sqrt{9}} - 4\frac{1/8}{\sqrt{12}}\right\} + 2\left\{-\frac{1/2}{2} + 4\frac{1/2}{\sqrt{5}} - 4\frac{1/2}{\sqrt{6}}\right\} =$$

3. ravnina 2. ploskve × 2

$$= 3 - \underbrace{\frac{9}{\sqrt{2}} + \frac{7}{\sqrt{3}}}_{0.678} - 1 + \underbrace{\frac{4}{\sqrt{5}} - \frac{1}{\sqrt{8}}}_{0.435} + 2\underbrace{\left\{\frac{2}{\sqrt{5}} - \frac{4}{\sqrt{6}} + \frac{1}{\sqrt{9}}\right\}}_{-0.811} +$$

$$+ 2\underbrace{\left\{-\frac{1}{8} + \frac{2}{\sqrt{9}} - \frac{1}{4\sqrt{3}}\right\}}_{0.338} + 2\underbrace{\left\{-\frac{1}{4} + \frac{2}{\sqrt{8}} - \frac{2}{\sqrt{6}}\right\}}_{-0.344} =$$

$$= 0.30$$

$$\alpha_M^{(I+II)} = 1.76$$

Z-2.6

$$E = N\left[z\frac{A}{R^n} - \frac{q^2}{4\pi\varepsilon_0 R}\alpha_M\right]$$

$$\left.\frac{dE}{dR}\right|_{R_0} = 0$$

$$N\left[-nzA\frac{1}{R_0^{n+1}} + \frac{q^2}{4\pi\varepsilon_0 R^2}\alpha_M\right] = 0$$

$$\Rightarrow \frac{zA}{R_0^n} = \frac{1}{n}\alpha_M\frac{q^2}{4\pi\varepsilon_0 R_0}$$

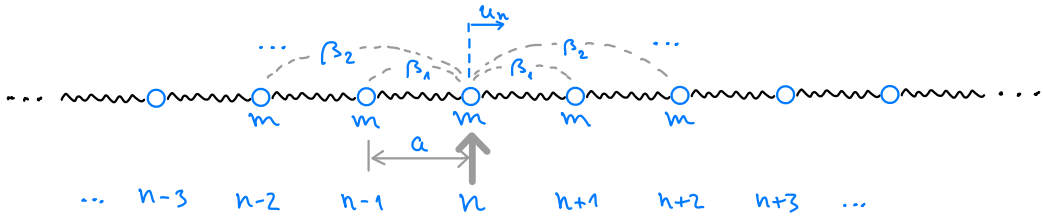
$$E = N\left[\frac{1}{n}\alpha_M\frac{q^2}{4\pi\varepsilon_0 R_0} - \frac{q^2}{4\pi\varepsilon_0 R_0}\alpha_M\right]$$

$$= -N\frac{q^2\alpha_M}{4\pi\varepsilon_0 R_0}\left(1-\frac{1}{n}\right), \quad \text{za 1D kristal je } \alpha_M = 2\ln 2$$

$$= -N\frac{q^2\ln 2}{2\pi\varepsilon_0 R_0}\left(1-\frac{1}{n}\right)$$

III. DINAMIKA KRISTALNE REŠETKE

Z-3.1



$$m\ddot{u}_n = -\left[\beta_1(u_n-u_{n-1}) + \beta_2(u_n-u_{n-2}) + \beta_3(u_n-u_{n-3}) + \cdots + \beta_1(u_n-u_{n+1}) + \beta_2(u_n-u_{n+2}) + \beta_3(u_n-u_{n+3}) + \cdots\right]$$

$$m\ddot{u}_n = -\sum_{\substack{\ell=-N \\ (\ell\neq n)}}^{N} \beta_\ell\,(2u_n - u_{n-\ell} - u_{n+\ell}) \quad , \quad N=5$$

rješenje oblika: $u_n = Ae^{i(kx-\omega t)} = Ae^{i(kna-\omega t)}$

$$-\omega^2 m\, Ae^{i(kna-\omega t)} = -\sum_\ell \beta_\ell \left(2Ae^{i(kna-\omega t)} - Ae^{i(k(n-\ell)a-\omega t)} - Ae^{i(k(n+\ell)a-\omega t)}\right)$$

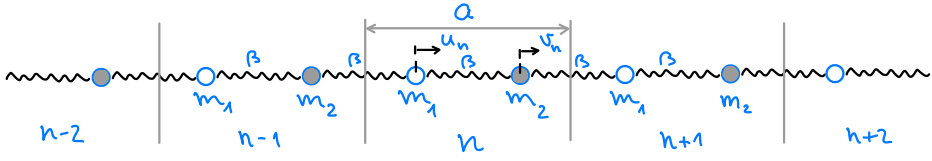
$$\omega^2 m = \sum_\ell \beta_\ell \left(2 - \underbrace{e^{-i\ell ka} - e^{i\ell ka}}_{2\cos(k\ell a)}\right)$$

$1-\cos x = 2\sin^2\frac{x}{2}$

$$\omega_k^2 = \frac{4}{m}\sum_{\ell=-N}^{N} \beta_\ell \sin^2\frac{k\ell a}{2} \quad , \quad N=5$$

{Specijalan slučaj aproksimacije prvih susjeda ($N=1$): $\omega_k^2 = \frac{4}{m}\beta\sin^2\frac{ka}{2}$ }

Z-3.2



$$m_1 \ddot{u}_n = -\beta(2u_n - v_n - v_{n-1}) \quad ; \quad u_n = A\, e^{ikna - i\omega t}$$
$$m_2 \ddot{v}_n = -\beta(2v_n - u_n - u_{n+1}) \quad ; \quad v_n = B\, e^{ikna - i\omega t}$$

$$-m_1\omega^2 A = \beta B(1 + e^{-ikna}) - 2\beta A \quad | : m_1$$
$$-m_2\omega^2 B = \beta A(1 + e^{ikna}) - 2\beta B \quad | : m_2$$

$$\left(\frac{2\beta}{m_1} - \omega^2\right)A - \frac{\beta}{m_1}(1 + e^{-ika})B = 0$$
$$-\frac{\beta}{m_2}(1 + e^{ika})A + \left(\frac{2\beta}{m_2} - \omega^2\right)B = 0 \quad \Rightarrow \quad \begin{vmatrix} \frac{2\beta}{m_1} - \omega^2 & -\frac{\beta}{m_1}(1 + e^{-ika}) \\ -\frac{\beta}{m_2}(1 + e^{ika}) & \frac{2\beta}{m_2} - \omega^2 \end{vmatrix} = 0$$

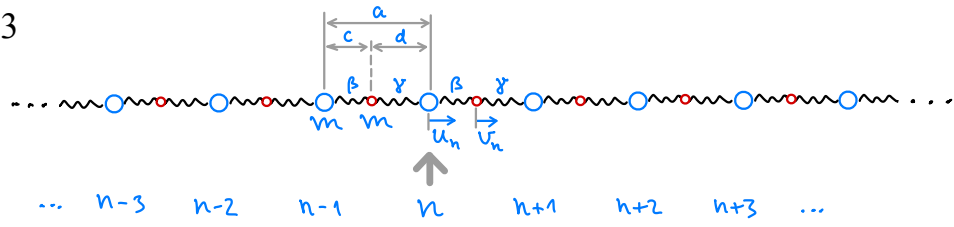
$$\left(\frac{2\beta}{m_1} - \omega^2\right)\left(\frac{2\beta}{m_2} - \omega^2\right) - \frac{\beta^2}{m_1 m_2}\underbrace{(1 + e^{ika})(1 + e^{-ika})}_{= e^{ika/2}(e^{ika/2} + e^{-ika/2})\, e^{-ika/2}(e^{ika/2} + e^{-ika/2}) = 4\cos^2\frac{ka}{2}} = 0$$

$$\omega^4 - 2\beta\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\omega^2 + \underbrace{\frac{4\beta^2}{m_1 m_2} - \frac{\beta^2}{m_1 m_2} 4\cos^2\frac{ka}{2}}_{= \frac{4\beta^2}{m_1 m_2}\sin^2\frac{ka}{2}} = 0$$

$$\omega_\pm^2 = \frac{1}{2}\left[\frac{2\beta}{\mu} \pm \sqrt{\frac{4\beta^2}{\mu^2} - \frac{4\beta^2}{m_1 m_2}\underbrace{\left(4 - 4\cos^2\frac{ka}{2}\right)}_{= 4\sin^2\frac{ka}{2}}}\right] \quad , \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\omega_\pm^2(k) = \frac{\beta}{\mu}\left[1 \pm \sqrt{1 - \frac{4\mu^2}{m_1 m_2}\sin^2\frac{ka}{2}}\right]$$

Z-3.3



$$m\ddot{u}_n = -\beta(u_n - v_n) - \gamma(u_n - v_{n-1}) \quad ; \quad u_n = Ae^{ikna - i\omega t}$$
$$m\ddot{v}_n = -\gamma(v_n - u_{n+1}) - \beta(v_n - u_n) \quad ; \quad v_n = Be^{ikna - i\omega t}, \quad a = c + d$$

$$-m\omega^2 Ae^{ikna} = -\beta(Ae^{ikna} - Be^{ikna}) - \gamma(Ae^{ikna} - Be^{ik(n-1)a})$$
$$-m\omega^2 Be^{ikna} = -\gamma(Be^{ikna} - Ae^{ik(n+1)a}) - \beta(Be^{ikna} - Ae^{ikna}) \quad | : e^{ikna}$$

$$m\omega^2 A = \beta(A - B) + \gamma(A - Be^{-ika})$$
$$m\omega^2 B = \gamma(B - Ae^{ika}) + \beta(B - A)$$

$$[m\omega^2 - (\beta+\gamma)]A + (\beta + \gamma e^{-ika})B = 0 \quad (*)$$
$$(\beta + \gamma e^{ika})A + [m\omega^2 - (\beta+\gamma)]B = 0 \quad \Rightarrow \quad \begin{vmatrix} m\omega^2 - (\beta+\gamma) & \beta + \gamma e^{-ika} \\ \beta + \gamma e^{ika} & m\omega^2 - (\beta+\gamma) \end{vmatrix} = 0$$

$$[m\omega^2 - (\beta+\gamma)]^2 - \underbrace{(\beta + \gamma e^{ika})(\beta + \gamma e^{-ika})}_{= \beta^2 + \gamma^2 + 2\gamma\beta\cos ka} = 0 \quad | \sqrt{\ }$$

$$\omega_\pm^2(k) = \frac{1}{m}\left[\beta + \gamma \pm \sqrt{\beta^2 + \gamma^2 + 2\gamma\beta\cos ka}\right]$$

$ka \ll 1$: $\cos ka \simeq 1 - \frac{1}{2}(ka)^2$

$$\omega_\pm^2 \simeq \frac{1}{m}\left[\beta + \gamma \pm \sqrt{\beta^2 + \gamma^2 + 2\gamma\beta\left(1 - \tfrac{1}{2}(ka)^2\right)}\right]$$
$$= \frac{1}{m}\left[\beta + \gamma \pm (\beta+\gamma)\sqrt{1 - \frac{\beta\gamma}{(\beta+\gamma)^2}(ka)^2}\right]$$
$$\approx \frac{\beta+\gamma}{m}\left[1 \pm \left(1 - \frac{1}{2}\frac{\beta\gamma}{(\beta+\gamma)^2}(ka)^2\right)\right]$$

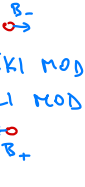
$\omega_-^2(k \ll) = \frac{1}{2m}\frac{\beta\gamma}{\beta+\gamma}(ka)^2$: AKUSTIČKA GRANA

$\omega_+^2(k \ll) = 2\frac{\beta+\gamma}{m}$: OPTIČKA GRANA

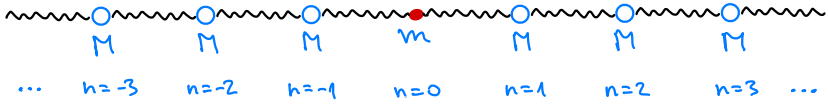
napomena: u jedn. $(*)$ uvrstimo $\omega_\pm(k=0)$ i odredimo $A_\pm$ i $B_\pm$

$\omega_-^2(0) = 0$: $-(\beta+\gamma)A_- + (\beta+\gamma)B_- = 0 \Rightarrow A_- = B_-$ (u fazi) AKUSTIČKI MOD

$\omega_+^2(0) = \frac{2}{m}(\beta+\gamma)$: $(\beta+\gamma)A_+ + (\beta+\gamma)B_+ = 0 \Rightarrow A_+ = -B_-$ (u protufazi) OPTIČKI MOD



Z-3.4



$$m_n \ddot{u}_n = -\beta(2u_n - u_{n+1} - u_{n-1}), \quad m_n = \begin{cases} m, & n=0 \\ M, & n\neq 0 \end{cases}$$

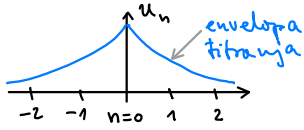
Zbog postojanja defekta problem više nije translacijski invarijantan. Javlja se lokalizirano rješenje za gibanje defekta (primjese) koje eksponencijalno trne kako se udaljavamo od te pozicije na lancu.

modeliranje lokalizacije: $\vec{k} \to \vec{k}_R + i\vec{k}_I$ – kompleksni valni vektor

$$e^{ikx} \Downarrow \to e^{ik_R x} \cdot e^{-k_I |x|}$$ – eksponencijalno trne za $|x| \neq 0$

Tražimo rješenje oblika: $u_n(t) = Ae^{ikx - i\omega t}$

$$= Ae^{ik_R x} e^{-k_I |x|} e^{-i\omega t}$$
$$= Ae^{ik_R na} e^{-\kappa|n|} e^{-i\omega t}, \quad \kappa \equiv k_I a$$



Zbog zrcalne simetrije problema, amplitude titranja za $n<0$ i $n>0$ su iste.

$n=0$:

$$-m\omega^2 A e^{-i\omega t} = -\beta[2Ae^{-i\omega t} - Ae^{ik_R a} e^{-\kappa} e^{-i\omega t} - Ae^{-ik_R a} e^{-\kappa} e^{-i\omega t}]$$
$$m\omega^2 = 2\beta[1 - e^{-\kappa}\cos k_R a]$$

$n\neq 0$:

$$-M\omega^2 A e^{ik_R na} e^{-|n|\kappa} e^{-i\omega t} = -\beta[2Ae^{ik_R na} e^{-|n|\kappa} e^{-i\omega t} - Ae^{ik_R a(n+1)} e^{-|n+1|\kappa} e^{-i\omega t} -$$
$$- Ae^{ik_R a(n-1)} e^{-|n-1|\kappa} e^{-i\omega t}] \quad | : Ae^{-i\omega t} e^{ik_R na} e^{-|n|\kappa}$$
$$M\omega^2 = \beta[2 - e^{ik_R a} e^{(|n|-|n+1|)\kappa} - e^{-ik_R a} e^{(|n|-|n-1|)\kappa}]$$

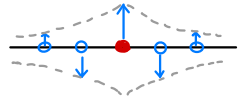
↑ ponište se (analiziraju se posebno slučaj $n>0$ i $n<0$

$$M\omega^2 = \beta[2 - e^{-\kappa + ik_R a} - e^{\kappa - ik_R a}]$$

$\in \mathbb{R} \iff k_R = \pm\frac{\pi}{a}$: Lokalizirano stanje primjese može se realizirati samo na rubu Brillouinove zone.

$$\Downarrow$$

$$u_{n=0}(t) = (-1)^n A e^{-\kappa|n|} e^{-i\omega t}$$



$k_k = \pm \frac{\pi}{a} \Rightarrow m\omega^2 = 2\beta\left[1 - e^{-\kappa}\underbrace{\cos\frac{\pi}{2}}_{=-1}\right]$ & $M\omega^2 = \beta\left[2 - e^{-\kappa}(-1) - e^{-\kappa}(-1)\right] = 2\beta\left[1 + \mathrm{ch}\,\kappa\right]$

$\Rightarrow m\frac{2\beta}{M}(\mathrm{ch}\,\kappa + 1) = 2\beta(e^{-\kappa} + 1) \quad | : 2\beta$

$\left(\frac{m}{2M} - 1\right)e^{-2\kappa} + \left(\frac{m}{M} - 1\right)e^{-\kappa} + \frac{m}{2M} = 0 \quad | \frac{2M}{m-2M}$

$e^{-2\kappa} + 2\frac{m-M}{m-2M}e^{-\kappa} + \frac{m}{m-2M} = 0$

$\hookrightarrow e^{-\kappa_{1,2}} = \frac{1}{2}\left[-2\frac{m-M}{m-2M} \pm \sqrt{4\left(\frac{m-M}{m-2M}\right)^2 - 4\frac{m}{m-2M}}\right] =$

$= -\frac{m - M \mp M}{m - 2M}$

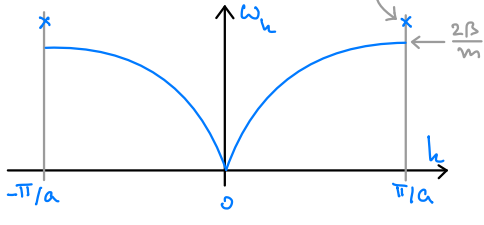
$= \begin{cases} -1 & \text{nemoguće jer } e^{-x} > 0\ ,\ \forall x \\ \frac{m}{2M-m} & \checkmark \end{cases}$

$\Rightarrow \kappa = -\ln\frac{m}{2M-m}$ & $\kappa > 0$ da bi rješenje bilo lokalizirano

$\Rightarrow \frac{m}{2M-m} \leq 1 \iff m < M$ $\checkmark$

frekvencija:

$\omega^2 = \frac{2\beta}{m}(1 + e^{-\kappa}) = \frac{2\beta}{m}\left(1 + \frac{m}{2M-m}\right) \overset{m \ll M}{\approx} \frac{2\beta}{m}\left(1 + \frac{m}{2M}\right)$



Stanje primjese formira se na rubu BZ, izvan vrpce (u procijepu između vrpci ako ih je više).

Z-3.5

$$k_B \Theta_D = \hbar \omega_D \implies \Theta_D = \frac{\hbar}{k_B} v_s k_D$$

$$\omega_D = v_s k_D$$

$k_D = \sqrt[3]{6\pi^2 \frac{N}{L^3}}$; N = broj primitivnih ćelija , L^3 = volumen monokristala

$\Omega = \frac{L^3}{N}$ = volumen jedne primitivne ćelije

FCC ima 4 atoma po jediničnoj ćeliji $\implies \Omega = \frac{a^3}{4}$

$$\Rightarrow k_D = \sqrt[3]{6\pi^2 \frac{4}{a^3}} = \frac{1}{a} \sqrt[3]{24\pi^2}$$

$$\Theta_D = \frac{\hbar v_s}{k_B a} \sqrt[3]{24\pi^2}$$

$$\Theta_D = \begin{cases} 250\ K\ , \ Ca\ \ [a(Ca) = 0.558\,nm\ ,\ v_s = 3 \cdot 10^3\ m/s] \rightarrow \text{eksperiment: } 230\ K \\ 390\ K\ , \ Cu\ \ [a(Cu) = 0.361\,nm\ ,\ v_s = 3 \cdot 10^3\ m/s] \rightarrow \text{eksperiment: } 315\ K \end{cases}$$

Napomena: 2. način:

U Debyevom modelu k_D je radijus kugle u k-prostoru čiji volumen je jednak volumenu 1. BZ, Ω^*:

$$\Omega^* = \frac{4\pi k_D^3}{3}$$

vrijedi: $\Omega \Omega^* = (2\pi)^3$ & $\Omega = \frac{a^3}{n}$, za FCC $n = 4$

$$\frac{4\pi k_D^3}{3} = \frac{(2\pi)^3}{\frac{a^3}{4}} \implies k_D = \frac{1}{a} \sqrt[3]{24\pi^2} \implies \Theta_D = \frac{\hbar v_s}{k_B a} \sqrt[3]{24\pi^2}$$

Z-3.6

Prosječna energija HO na temperaturi T: $\overline{E} = \frac{\hbar\omega}{2} + \hbar\omega\, n(\omega)$

($\frac{\hbar\omega}{2}$ ↑ energija osnovnog stanja; $\hbar\omega\, n(\omega)$ ↑ energija pobuđenih stanja ($n(\omega)$ – Planckova raspodjela))

za 1 mol:

$$W_A = \sum_{\vec{k},\lambda} 1 = \left(\frac{L}{2\pi}\right)^3 \int d^3k = \left(\frac{L}{2\pi}\right)^3 4\pi \int_0^{k_D} k^2\, dk$$

$$= \frac{4\pi}{3}\left(\frac{L}{2\pi}\right)^3 k_D^3 \underset{\uparrow\ \omega_D = v_s k_D}{=} \frac{L^3}{6\pi^2}\frac{\omega_D^3}{v_s^3} \quad \Rightarrow \quad \frac{1}{v_s^3} = \frac{6\pi^2 N_A}{L^3 \omega_D^3} \quad (*)$$

u jednom molu tvari kristala je N_A 3D oscilatora s ukupnom energijom:

$$U = \sum_{\vec{k},\lambda} \frac{\hbar\omega_k}{2} = 3\frac{\hbar}{2}\left(\frac{L}{2\pi}\right)^3 \int \omega_k\, d^3k = 3\frac{\hbar}{2}\left(\frac{L}{2\pi}\right)^3 4\pi \int_0^{k_D} \omega_k k^2\, dk$$

$$\underset{\uparrow\ \omega_D = v_s k_D}{=} \frac{3\hbar L^3}{4\pi^2}\frac{1}{v_s^3}\int_0^{\omega_D} \omega^3 d\omega = \frac{3\hbar L^3}{4\pi^2}\frac{\omega_D^4}{4 v_s^3} \underset{\uparrow\ (*)}{=} \frac{3\hbar L^3}{16\pi^2}\omega_D^4 \frac{6\pi^2 N_A}{L^3\omega_D^3} = \frac{9}{8} N_A \hbar \omega_D$$

$$= \frac{9}{8} N_A k_B \Theta_D = 2.8\ \frac{kJ}{mol}$$

($N_A = 6.02 \cdot 10^{23}\ mol^{-1}$)

Z-3.7

Broj Bose-Einsteinovski pobuđenih fonona (Planckova raspodjela je $n(\omega_k) = \frac{1}{e^{\frac{\hbar\omega(k)}{k_B T}} - 1}$):

$$N = \sum_{\vec{k},\lambda} n(\omega) = 3\left(\frac{L}{2\pi}\right)^3 4\pi \int_0^{k_D} \frac{1}{e^{\frac{\hbar\omega(k)}{k_B T}} - 1} k^2\, dk$$

$$\underset{\uparrow\ \omega_D = v_s k_D}{=} \frac{3L^3}{4\pi^2}\frac{1}{v_s^3}\int_0^{\omega_D} \frac{\omega^2 d\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1} = \left\{ \text{supst. } x \equiv \frac{\hbar\omega}{k_B T} \to \omega = \frac{k_B T}{\hbar}x,\ d\omega = \frac{k_B T}{\hbar}dx;\ x_{max} = \frac{\hbar\omega_D}{k_B T} \left(\equiv k_B\Theta_D\right) = \frac{\Theta_D}{T} \right\}$$

$$= \frac{3L^3}{2\pi^2}\frac{1}{v_s^3}\left(\frac{k_B T}{\hbar}\right)^3 \int_0^{\frac{\Theta_D}{T}} \frac{x^2\, dx}{e^x - 1}$$

$$\frac{1}{v_s^3} = \frac{6\pi^2 N}{L^3 \omega_D^3} \quad \text{(vidi zadatak 3.6)} \quad \& \quad \omega_D^3 = \left(\frac{k_B\Theta_D}{\hbar}\right)^3 \quad (N: \text{broj prim. ćelija})$$

aproksimacija: $\int_0^{\frac{\Theta_D}{T}} \frac{x^2\, dx}{e^x - 1} \underset{T \ll \Theta_D}{\approx} \int_0^{\infty} \frac{x^2\, dx}{e^x - 1} = 2\zeta(3)$; $\zeta(n) \equiv \sum_{j=1}^{\infty} \frac{1}{j^n}$

$\zeta(3) = 1.202\ldots$

$$N \approx 18\, N \left(\frac{T}{\Theta_D}\right)^3 \zeta(3)$$

$$\frac{N}{N} = 18\left(\frac{T}{\Theta_D}\right)^3 \zeta(3) = 0.035$$

Z-3.8

$U = \sum_{k,\lambda} \overline{E}_{k,\lambda} = 3 \sum_{k} \overline{E}_{k}$ za akustične modove (jedini mogući za primitivnu ćeliju s jednim atomom)

$\overline{E}_k = \hbar\omega_k \left(n(\omega_k) + \frac{1}{2}\right), \quad n(\omega_k) = \frac{1}{e^{\frac{\hbar\omega(k)}{k_B T}} - 1}$

$$C_v = \frac{\partial}{\partial T} \sum_{k,\lambda} \overline{E}_k = 3 \sum_{k} \hbar\omega \frac{-1}{\left(e^{\frac{\hbar\omega}{k_B T}} - 1\right)^2} e^{\frac{\hbar\omega}{k_B T}} (-1) \frac{\hbar\omega}{k_B T^2}$$

$$= 3 k_B \left(\frac{L}{2\pi}\right)^3 4\pi \int_0^{k_D} k^2 dk \frac{\left(\frac{\hbar\omega_k}{k_B T}\right)^2 e^{\frac{\hbar\omega_k}{k_B T}}}{\left(e^{\frac{\hbar\omega_k}{k_B T}} - 1\right)^2} = \left\{ \begin{array}{l} \text{supst.} \quad (\omega = v_s k) \\ x = \frac{\hbar\omega}{k_B T}, \quad x_{max} = \frac{\Theta_D}{T} \\ \omega = \frac{k_B T}{\hbar} x, \quad d\omega = \frac{k_B T}{\hbar} dx \end{array} \right\}$$

$$= \frac{3L^3 k_B}{2\pi^2} \underbrace{\frac{1}{v_s^3}} \left(\frac{k_B T}{\hbar}\right)^3 \int_0^{\frac{\Theta_D}{T}} \frac{x^4 e^x dx}{(e^x - 1)^2}$$

$\frac{1}{v_s^3} = \frac{6\pi^2 N}{L^3 \omega_D^3}$ (vidi zadatak 3.6)

$$= 9 N k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{\frac{\Theta_D}{T}} \frac{x^4 e^x dx}{(e^x - 1)^2} \underset{T \ll \Theta_D}{\approx} 9 N k_B \left(\frac{T}{\Theta_D}\right)^3 \underbrace{\int_0^{\infty} \frac{x^4 e^x dx}{(e^x - 1)^2}}_{= \frac{4\pi^4}{15}}$$

$$= \frac{12\pi^4}{5} N k_B \left(\frac{T}{\Theta_D}\right)^3$$

$$\Rightarrow N = \frac{5 C_v}{12\pi^4 k_B} \left(\frac{T}{\Theta_D}\right)^3 = 3 \cdot 10^{23}$$

Z-3.9

$U = \underbrace{1}_{\text{broj polarizacija}} \cdot \int_0^{\omega_D} g(\omega) \hbar\omega\, n(\omega) d\omega \quad ; \quad 1D: g(\omega) = \frac{L}{\pi v_s}$ – gustoća stanja u Debyevoj aproksimaciji po 1 polarizaciji

$$= \int_0^{\omega_D} \frac{L}{\pi v_s} \hbar\omega \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1} d\omega = \left\{ \begin{array}{l} \text{supst.} \\ x = \frac{\hbar\omega}{k_B T}, \quad \omega = \frac{k_B T}{\hbar} x \end{array} \right\}$$

$$= \frac{L}{\pi v_s} \hbar \left(\frac{k_B T}{\hbar}\right)^2 \underbrace{\int_0^{\frac{\Theta_D}{T} \approx \infty, T \ll \Theta_D} \frac{x}{e^x - 1} dx}_{= \frac{\pi^2}{6}} = \frac{\pi}{6} \frac{L k_B^2}{\hbar v_s} T^2$$

$$C_v = \frac{\partial U}{\partial T}$$

$$= \frac{\pi}{3} \frac{L k_B^2}{\hbar v_s} T \sim T^1$$

Z-3.10

Potpuno kruta veza, tj. instantana mogućnost titranja, među razmicima implicira da je problem efektivno 2D.

$$U = 2 \cdot \int_0^{\omega_D} g(\omega)\, \hbar\omega\, n(\omega)\, d\omega \qquad ;\ 2D:\ g(\omega) = \left(\frac{L}{2\pi}\right)^2 \frac{2\pi}{v_s^2}\omega$$

(2 ← broj polarizacija; gustoća stanja u Debyevoj aproksimaciji)

$$= 2\int_0^{\omega_D} \frac{L^2}{2\pi}\frac{\omega}{v_s^2}\frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1}\hbar\omega\, d\omega = \left\{\begin{array}{l} \text{supt.}\\ x = \frac{\hbar\omega}{k_BT} \\ \omega = \frac{k_BT}{\hbar}x \end{array} ;\ x_{max} = \frac{\Theta_D}{T}\right\}$$

$$= \frac{L^2}{\pi v_s^2}\int_0^{\frac{\Theta_D}{T}} \frac{k_BT}{\hbar}x \frac{1}{e^x-1}\hbar\frac{k_BT}{\hbar}x\frac{k_BT}{\hbar}dx$$

$$= \frac{L^2(k_BT)^3}{\pi v_s^2\hbar^2}\underbrace{\int_0^{\frac{\Theta_D}{T}\approx\infty,\ T\ll\Theta_D} \frac{x^2}{e^x-1}dx}_{=2\zeta(3)\ ;\ \zeta(3)=1.202\ldots}$$

$$= \frac{2L^2k_B^3\zeta(3)}{\pi v_s^2\hbar^2}T^3$$

$$C_v = \frac{\partial U}{\partial T} = \frac{6L^2k_B^3\zeta(3)}{\pi v_s^2\hbar^2}T^2 \sim T^2$$

napomena: Faktor $\frac{1}{v_s^2}$ može se naći iz:

$$N = \left(\frac{L}{2\pi}\right)^2 2\pi\int_0^{k_D} k\,dk = \frac{L^2}{2\pi}\frac{1}{v_s^2}\int_0^{\omega_D}\omega\,d\omega = \frac{L^2}{4\pi}\frac{\omega_D^2}{v_s^2}$$

$$\Rightarrow \frac{1}{v_s^2} = \frac{4\pi N}{L^2\omega_D^2}$$

IV. SOMMERFELDOV MODEL METALA

Z-4.1

Fermijeva raspodjela normirana je na broj čestica tj. $\sum_{s,\vec{k}} f(\vec{k}) = N$ pa se prosjek veličine A računa na način:

$$\overline{A} = \frac{\sum_{s,\vec{k}} A_s(\vec{k}) f(\vec{k})}{\sum_{s,\vec{k}} f(\vec{k})} \quad \text{ili} \quad \frac{\int A(\varepsilon) g(\varepsilon) f(\varepsilon) d\varepsilon}{\int g(\varepsilon) f(\varepsilon) d\varepsilon}$$

$$\overline{k} = \frac{\sum_{s,\vec{k}} k f(\vec{k})}{\sum_{s,\vec{k}} f(\vec{k})} = \frac{2\left(\frac{L}{2\pi}\right)^3 \int_0^\infty k f(k) d^3k}{2\left(\frac{L}{2\pi}\right)^3 \int_0^\infty f(k) d^3k} \overset{T=0}{=} \frac{4\pi \int_0^\infty k^3 \Theta(k-k_F) dk}{4\pi \int_0^\infty k^2 \Theta(k-k_F) dk} = \frac{\int_0^{k_F} k^3 dk}{\int_0^{k_F} k^2 dk} = \frac{\frac{1}{4}k_F^4}{\frac{1}{3}k_F^3} = \frac{3}{4}k_F$$

$$\Rightarrow k_F = \frac{4}{3}\overline{k}$$

$$N = \sum_{s,\vec{k}} f(\vec{k}) \overset{T=0}{=} 2\left(\frac{L}{2\pi}\right)^3 4\pi \int_0^\infty k^2 \Theta(k-k_F) dk = \frac{L^3}{\pi^2} \int_0^{k_F} k^2 dk = \frac{L^3}{3\pi^2} k_F^3$$

$$n = \frac{N}{L^3} = \frac{k_F^3}{3\pi^2} = \frac{1}{3\pi^2}\left(\frac{4}{3}\overline{k}\right)^3 = 2.7 \cdot 10^{29}\ m^{-3}$$

Z-4.2

$$P = -\left(\frac{\partial U}{\partial V}\right)_S \quad \& \quad \text{na } T=0 \Rightarrow S = \text{const.}, \text{ pa je } P = -\frac{\partial U_0}{\partial V}$$

$$U_0 = N\langle E_k \rangle_{T=0}$$

$$\langle E_k \rangle_{T=0} = \frac{1}{N} \sum_{s,\vec{k}} E_k f(\vec{k}) \overset{T=0}{=} \frac{2\left(\frac{L}{2\pi}\right)^3 4\pi \int_0^{k_F} k^2 dk \frac{\hbar^2 k^2}{2m}}{2\left(\frac{L}{2\pi}\right)^3 4\pi \int_0^{k_F} k^2 dk} = \frac{3}{5}\frac{\hbar^2}{2m}\frac{k_F^5}{k_F^3} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} = \frac{3}{5}E_F$$

$$U_0 = \frac{3}{5}NE_F$$

$$N = \sum_{s,\vec{k}} f(\vec{k}) = 2\left(\frac{L}{2\pi}\right)^3 4\pi \int_0^{k_F} k^2 dk \overset{L^3=V}{=} \frac{V}{3\pi^2} k_F^3 \Rightarrow k_F = \sqrt[3]{3\pi^2 \frac{N}{V}} \longrightarrow E_F = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{2/3}$$

$$\Rightarrow U_0 = \frac{3}{5} N \frac{\hbar^2}{2m} (3\pi^2 N)^{2/3} V^{-\frac{2}{3}}$$

$$P = -\frac{\partial U_0}{\partial V} = \frac{3}{5} N \frac{\hbar^2}{2m} (3\pi^2 N)^{2/3} \frac{2}{3} V^{-\frac{5}{3}} = \underbrace{\frac{3}{5} N \overbrace{\frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{2/3}}^{E_F} \frac{2}{3} V^{-1}}_{U_0}$$

$$P = \frac{2}{3}\frac{U_0}{V}$$

Z-4.3

Iz zadatka 4.2: $P = \frac{2}{3}\frac{U_0}{V} = \frac{2}{3}\frac{N\langle E\rangle_{T=0}}{V} = \frac{2}{3} n \langle E\rangle_{T=0}$, $n = \frac{N}{V}$ (koncentracija)

$$\langle E\rangle_{T=0} = \frac{\int_0^\infty E\, g(E)\,\Theta(E-\varepsilon_F)\,dE}{\int_0^\infty g(E)\,\Theta(E-\varepsilon_F)\,dE} \quad ; \text{ preko gustoće stanja } g(E) = \frac{m\sqrt{2mE}}{\pi^2\hbar^3}$$

$$= \frac{\int_0^{\varepsilon_F} E\, g(E)\,dE}{\int_0^{\varepsilon_F} g(E)\,dE} = \frac{\int_0^{\varepsilon_F} E^{3/2}\,dE}{\int_0^{\varepsilon_F} E^{1/2}\,dE} = \frac{\frac{2}{5}E_F^{5/2}}{\frac{2}{3}E_F^{3/2}} = \frac{3}{5}E_F = \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

($E_F = \frac{1}{2m}\hbar^2 k_F^2$, $k_F = \sqrt[3]{3\pi^2 n}$)

$$P = \frac{2}{3} n \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2 n)^{2/3} = \frac{\hbar^2(3\pi^2)^{2/3}}{5m} n^{5/3} = 1.9\cdot 10^{10}\ \text{Pa}$$

Z-4.4

$T=0$:

$$N_{T=0} = \sum_{s,\vec{k}} \Theta(k-k_F)$$

$$= 2\left(\frac{L}{2\pi}\right)^2 \int d^2k\,\Theta(k-k_F)$$

$$= 2\left(\frac{L}{2\pi}\right)^2 2\pi \int_0^{k_F} k\,dk = \frac{L^2}{2\pi}k_F^2 = \frac{L^2}{\pi}\frac{mE_F}{\hbar^2} \quad (E_F = \tfrac{\hbar^2k^2}{2m})$$

$T\neq 0$:

$$N_{T\neq 0} = \sum_{s,\vec{k}} f(\vec{k})$$

$$= 2\left(\frac{L}{2\pi}\right)^2 \int d^2k\,\frac{1}{e^{\beta(E_k-\mu)}+1}$$

$$= \frac{L^2}{2\pi^2}2\pi\int_0^\infty \frac{k\,dk}{e^{\beta(E_k-\mu)}+1} = \left\{\begin{array}{l}\text{supst.}\\ x = \beta(E_k-\mu) = \beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)\\ dx = \beta\frac{\hbar^2}{m}k\,dk\end{array}\right\} \quad ; \int_0^\infty dk \to \int_{-\mu\beta}^\infty dx$$

$$= \frac{L^2}{\pi}\frac{m}{\beta\hbar^2}\int_{-\mu\beta}^\infty \frac{dx}{e^x+1} = \frac{L^2}{\pi}\frac{m}{\beta\hbar^2}\int_{-\mu\beta}^\infty \frac{e^{-x}\,dx}{1+e^{-x}}$$

$$= \frac{L^2}{\pi}\frac{m}{\hbar^2\beta}(-1)\ln\left(1+e^{-x}\right)\Big|_{-\mu\beta}^\infty = \frac{L^2}{\pi}\frac{m}{\hbar^2\beta}\ln\left(1+e^{\beta\mu}\right)$$

$N_{T=0} = N_{T\neq 0}$: $\quad E_F = \frac{1}{\beta}\ln\left(1+e^{\beta\mu}\right) \mid \cdot\beta \mid \ln$

$$\Rightarrow e^{\beta E_F} = 1 + e^{\beta\mu} \mid \ln$$

$$\mu = \frac{1}{\beta}\ln\left(e^{\beta E_F}-1\right) \quad ; \quad \text{trik: } \ln\left(e^{\beta E_F}-1\right) = \ln\left[e^{\beta E_F}\left(1-e^{-\beta E_F}\right)\right] = \beta E_F + \ln\left(1-e^{-\beta E_F}\right)$$

$$\mu = E_F + k_B T \ln\left(1-e^{-\frac{E_F}{k_B T}}\right)$$

Uočiti da je korekcija negativna jer je argument ln – funkcije manji od 1.

Z-4.5

Sommerfeldov razvoj: $\int_0^\infty F(\varepsilon) f(\varepsilon)\,d\varepsilon \simeq \int_0^{\mu(T)} F(\varepsilon)\,d\varepsilon + \frac{1}{6}(\pi k_B T)^2 \frac{\partial F}{\partial \varepsilon}\Big|_{\varepsilon=\mu}$

a) $N_{T=0} = \int_0^{\varepsilon_F} g(\varepsilon)\,d\varepsilon = g_0 \int_0^{\varepsilon_F} \sqrt{\varepsilon}\,d\varepsilon = \frac{2}{3} g_0 \varepsilon_F^{3/2}$; $g(\varepsilon) = \frac{m\sqrt{2m}}{\pi^2\hbar^3}\sqrt{\varepsilon} \equiv g_0\sqrt{\varepsilon}$

$N_{T\neq 0} = \int_0^\infty g(\varepsilon) f(\varepsilon)\,d\varepsilon = g_0 \int_0^\infty \sqrt{\varepsilon} f(\varepsilon)\,d\varepsilon \simeq g_0 \left\{ \int_0^\mu \sqrt{\varepsilon}\,d\varepsilon + \frac{1}{6}(\pi k_B T)^2 \frac{1}{2}\mu^{-1/2} \right\} =$

$= g_0 \left(\frac{2}{3}\mu^{2/3} + \frac{\pi^2}{12}(k_B T)^2 \frac{1}{\sqrt{\mu}} \right) = \frac{2}{3} g_0 \mu^{3/2} \left[1 + \frac{3}{2}\frac{\pi^2}{12}(k_B T)^2 \frac{1}{\mu^2} \right]$ ($\frac{1}{\mu^2} \approx 1/\varepsilon_F^2$)

$= \frac{2}{3} g_0 \mu^{3/2} \left[1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\varepsilon_F}\right)^2 \right]$

$N_{T=0} = N_{T\neq 0}$: $\mu^{3/2} = \varepsilon_F^{3/2}\left(1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\varepsilon_F}\right)^2\right)^{-1}$ $\Big|^{2/3}$

$\mu = \varepsilon_F \left(1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\varepsilon_F}\right)^2\right)^{-2/3} \approx \varepsilon_F \left(1 - \frac{2}{3}\frac{\pi^2}{8}\left(\frac{k_B T}{\varepsilon_F}\right)^2\right)$

$\mu(T) = \varepsilon_F \left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\varepsilon_F}\right)^2 \right]$ ⊛

b)

$U = \int_0^\infty \varepsilon g(\varepsilon) f(\varepsilon)\,d\varepsilon = g_0 \int_0^\infty \varepsilon^{3/2} f(\varepsilon)\,d\varepsilon = g_0 \left\{ \int_0^\mu \varepsilon^{3/2} d\varepsilon + \frac{1}{6}(\pi k_B T)^2 \frac{d}{d\varepsilon}\varepsilon^{3/2}\Big|_{\varepsilon=\mu} \right\}$

$= g_0 \left\{ \frac{2}{5}\mu^{5/2} + \frac{1}{6}(\pi k_B T)^2 \frac{3}{2}\mu^{1/2} \right\} \approx \frac{2}{5} g_0 \mu^{5/2} \left[1 + \frac{5\pi^2}{8}\left(\frac{k_B T}{\varepsilon_F}\right)^2 \right]$ ($\mu \simeq \varepsilon_F$)

⊛ $\frac{2}{5} g_0 \varepsilon_F^{5/2} \left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\varepsilon_F}\right)^2 \right]^{5/2} \left[1 + \frac{5\pi^2}{8}\left(\frac{k_B T}{\varepsilon_F}\right)^2 \right]$

$\left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\varepsilon_F}\right)^2 \right]^{5/2} \approx 1 - \frac{5}{2}\frac{\pi^2}{12}\left(\frac{k_B T}{\varepsilon_F}\right)^2$

$\approx \frac{2}{5} g_0 \varepsilon_F^{5/2} \left(1 + \left(\frac{5}{8} - \frac{5}{24}\right)\pi^2 \left(\frac{k_B T}{\varepsilon_F}\right)^2 + \cancel{\mathcal{O}(T^4)} \right) \approx \frac{2}{5} g_0 \varepsilon_F^{5/2} \left(1 + \frac{5\pi^2}{12}\left(\frac{k_B T}{\varepsilon_F}\right)^2 \right)$

$C_V = \frac{\partial U}{\partial T} = \frac{2}{5} g_0 \varepsilon_F^{5/2} \frac{5\pi^2}{12} 2 \left(\frac{k_B}{\varepsilon_F}\right)^2 T = \frac{\pi^2}{3} \underbrace{g_0 \varepsilon_F^{1/2}}_{g_F} k_B^2 T$

$C_V = \frac{\pi^2}{3} g_F k_B^2 T$

napomena: $N = \frac{2}{3} g_F \varepsilon_F \Rightarrow g_F = \frac{3}{2}\frac{N}{\varepsilon_F}$

$\Rightarrow C_V = \frac{\pi^2}{2} N k_B^2 \frac{T}{\varepsilon_F}$

Z-4.6

$$c_V = \frac{\pi^2}{3} g_F k_B^2 T$$

$$g_F = \frac{m}{\pi^2 \hbar^3} \sqrt{2m E_F} \quad \& \quad E_F = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$$

$$\Rightarrow g_F = \frac{m}{\pi^2 \hbar^3} (3\pi^2 n)^{1/3}$$

$$c_V = \frac{k_B^2 m}{\hbar^2} \left(\frac{\pi^2 n}{g}\right)^{1/3} T$$

$$n = \frac{g}{\pi^2} \left(\frac{\hbar^2 c_V}{k_B^2 m T}\right)^2 = 1.5 \cdot 10^{28}\, m^{-3}$$

Z-4.7

$$\frac{c_V^{(el)}}{c_V^{(ph)}} = \frac{\frac{\pi^2}{3} g_F k_B^2 T}{3 N k_B} = \frac{\frac{\pi^2}{3} \frac{3}{2} N k_B \frac{k_B T}{E_F}}{3 N k_B} = \frac{\pi^2}{6} \frac{k_B T}{E_F}$$

$$\frac{c_V^{(el)}}{c_V^{(ph)}} \approx \frac{\pi^2}{6} \frac{3 \cdot 10^2\, K}{10^4\, K} \simeq \frac{\pi^2}{2} \cdot 10^{-2}$$

$\left(c_V^{(ph)} = 3 N k_B \quad @\ T = 300\, K \gg \Theta_D \simeq 200\, K \right)$

Z-4.8

Elektroni energije $E > V_0$ nisu u režimu jake degeneracije pa je:

$$f(E) = \frac{1}{e^{\beta(E-\mu)}+1} \approx e^{-\beta(E-E_F)}$$

Termoelektronska struja iz metala (z-smjer, predznak naboja nije bitan):

$$j_z = \sum_{s,\vec{k}} e v_z(\vec{k}) f(\vec{k}) = \frac{2e}{V} \frac{V}{(2\pi)^3} \int d^3k \, v_z \, e^{-\beta\left(\frac{m|\vec{v}|^2}{2} - E_F\right)}$$

$$= \frac{2e}{(2\pi)^3}\left(\frac{m}{\hbar}\right)^3 \int dv_x dv_y dv_z \, v_z \, e^{-\frac{m}{2k_BT}\left(v_x^2+v_y^2+v_z^2\right)+\frac{E_F}{k_BT}}$$

$$= \frac{2e}{(2\pi)^3}\left(\frac{m}{\hbar}\right)^3 e^{\frac{E_F}{k_BT}} \left[\int_{-\infty}^{\infty} dv_x \, e^{-\frac{mv_x^2}{2k_BT}}\right]\left[\int_{-\infty}^{\infty} dv_y \, e^{-\frac{mv_y^2}{2k_BT}}\right]\left[\int_{v_0}^{\infty} dv_z \, v_z e^{-\frac{mv_z^2}{2k_BT}}\right]$$

$$\int e^{-ax^2} = \frac{1}{2}\sqrt{\frac{\pi}{a}}\,\mathrm{erf}(\sqrt{a}x) \; ; \; \int x e^{-a^2x} dx = -\frac{1}{2a} e^{-ax^2}$$

$$= \frac{2e}{(2\pi)^3}\left(\frac{m}{\hbar}\right)^3 e^{\frac{E_F}{k_BT}} \left[\frac{1}{2}\sqrt{\frac{2\pi k_BT}{m}}\,\underbrace{\mathrm{erf}(x)\Big|_{-\infty}^{\infty}}_{=1-(-1)=2}\right]^2 \left[-\frac{k_BT}{m} e^{-\frac{mv_z^2}{2k_BT}}\Big|_{v_0}^{\infty}\right]$$

$$= \frac{2e}{(2\pi)^3}\left(\frac{m}{\hbar}\right)^3 \frac{1}{4}\frac{2\pi k_BT}{m} 4 \frac{k_BT}{m} e^{-\frac{1}{k_BT}\underbrace{\left(\frac{mv_0^2}{2} - E_F\right)}_{=\Phi}}$$

$$j_z = \frac{4\pi m e}{h^3}(k_BT)^2 e^{-\frac{\Phi}{k_BT}} \equiv A T^2 e^{-\frac{\Phi}{k_BT}}$$

V. ELEKTRON U PERIODIČKOM POTENCIJALU

Z-5.1

$H_0|\phi_n\rangle = E_n^0|\phi_n\rangle$ - egzaktno rješivi problem $\Rightarrow |\phi_n\rangle$ - baza

$(H_0 + V)|\psi_n\rangle = E_n|\psi_n\rangle$ - problem sa smetnjom V; rješenja: ψ_n, E_n

(V: smetnja)

$\rightarrow |\psi_n\rangle = \sum_m c_m|\phi_m\rangle$ - prikaz rješenja u bazi $|\phi_n\rangle$

1. red računa smetnje:

$$E_n = E_n^0 + \langle\phi_n|V|\phi_n\rangle$$

$$|\psi_n\rangle = |\phi_n\rangle + \sum_{\substack{m \\ (n\neq m)}} \frac{\langle\phi_m|V|\phi_n\rangle}{E_n^0 - E_m^0}|\phi_m\rangle$$

slobodni elektron:

$$E_k^0 = \frac{\hbar^2 k^2}{2m}, \quad |\phi_{\vec{k}}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

u periodičkom potencijalu V (smetnja):

$$|\psi_{\vec{k}}\rangle = |\phi_{\vec{k}}\rangle + \sum_{\vec{k}'} \frac{\langle\phi_{\vec{k}'}|V|\phi_{\vec{k}}\rangle}{E_k^0 - E_{k'}^0}|\phi_{\vec{k}'}\rangle$$

$V(\vec{r}) = \sum_n V_{\vec{G}_n} e^{i\vec{G}_n\cdot\vec{r}}$, gdje je $V_{\vec{G}} = \frac{1}{V}\int d^3r\, V(\vec{r})\, e^{-i\vec{G}_n\cdot\vec{r}}$

$$\langle\phi_{\vec{k}'}|V|\phi_{\vec{k}}\rangle = \int_{-L/2}^{L/2} d^3r \frac{1}{\sqrt{V}} e^{-i\vec{k}'\cdot\vec{r}} V(\vec{r}) \frac{1}{\sqrt{V}} e^{+i\vec{k}\cdot\vec{r}}$$

$$= \sum_n V_{\vec{G}_n} \underbrace{\frac{1}{V}\int_{-L/2}^{L/2} e^{i(\vec{k}-\vec{k}'+\vec{G}_n)\cdot\vec{r}} d^3r}_{= \delta_{\vec{k}',\vec{k}+\vec{G}_n}}$$

$$|\psi_{\vec{k}}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} + \sum_n V_{\vec{G}_n} \sum_{\vec{k}'} \frac{2m}{\hbar^2} \frac{\delta(\vec{k}'-\vec{k}-\vec{G}_n)}{k^2 - k'^2} \frac{1}{\sqrt{V}} e^{i\vec{k}'\cdot\vec{r}}$$

$$= \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} + \sum_n V_{\vec{G}_n} \frac{2m}{\hbar^2} \frac{1}{\sqrt{V}} \frac{e^{i(\vec{k}+\vec{G}_n)\cdot\vec{r}}}{k^2 - (\vec{k}+\vec{G}_n)^2}$$

$$= \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \left[1 + \frac{2m}{\hbar^2} \sum_n \frac{V_{\vec{G}_n} e^{i\vec{G}_n\cdot\vec{r}}}{k^2 - (\vec{k}+\vec{G}_n)^2}\right]$$

Z-5.2

nesmetani problem: $E^0_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$, $E^0_{\vec{k}+\vec{G}} = \frac{\hbar^2}{2m}(\vec{k}+\vec{G})^2$

$$\left.\begin{aligned} E^0_{\vec{k}} + E^0_{\vec{k}+\vec{G}} &= \frac{\hbar^2}{2m}\left(k^2 + 2\vec{k}\cdot\vec{G} + G^2\right) \\ E^0_{\vec{k}} - E^0_{\vec{k}+\vec{G}} &= -\frac{\hbar^2}{2m}\left(2\vec{k}\cdot\vec{G} + G^2\right) \end{aligned}\right\}$$

u okolini ruba BZ (Braggova točka $\pm\frac{\vec{G}}{2}$) uzimamo: $\vec{k} = -\frac{\vec{G}}{2} + \Delta\vec{k}$ $(\Delta k \ll G)$

$$\begin{aligned} E^0_{\vec{k}} + E^0_{\vec{k}+\vec{G}} &= \frac{\hbar^2}{2m}\left[2\left(-\frac{\vec{G}}{2} + \Delta\vec{k}\right)^2 + 2\left(-\frac{\vec{G}}{2} + \Delta\vec{k}\right)\cdot\vec{G} + G^2\right] \\ &= \frac{\hbar^2}{2m}\left[\frac{G^2}{2} - \cancel{2\vec{G}\cdot\Delta\vec{k}} + 2\Delta k^2 - \cancel{G^2} + \cancel{2\Delta\vec{k}\cdot\vec{G}} + \cancel{G^2}\right] \\ &= \frac{\hbar^2}{2m}\left[\frac{G^2}{2} + 2\Delta k^2\right] \\ E^0_{\vec{k}} - E^0_{\vec{k}+\vec{G}} &= \frac{\hbar^2}{2m}\left[-2\left(-\frac{\vec{G}}{2} + \Delta\vec{k}\right)\cdot\vec{G} - G^2\right] \\ &= \frac{\hbar^2}{2m}\left[G^2 - 2\vec{G}\cdot\Delta\vec{k} - G^2\right] \\ &= -\frac{\hbar^2}{2m}2\vec{G}\cdot\Delta\vec{k} \end{aligned}$$

$$\begin{aligned} E_\pm(\Delta\vec{k}) &= \frac{1}{2}\left[\frac{\hbar^2}{2m}\left(\frac{G^2}{2} + 2\Delta k^2\right) \pm \sqrt{\left(\frac{\hbar^2}{2m}\right)^2\left(2\vec{G}\cdot\Delta\vec{k}\right)^2 + 4|V_{\vec{G}}|^2}\right] \\ &= \frac{\hbar^2}{2m}\left(\frac{G^2}{4} + \Delta k^2\right) \pm \sqrt{\left(\frac{\hbar^2}{2m}\right)^2\left(2\vec{G}\cdot\Delta\vec{k}\right)^2 + 4|V_{\vec{G}}|^2} \end{aligned}$$

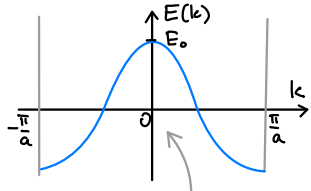
rub BZ: $\Delta k = 0$: $E_\pm = \frac{\hbar^2}{2m}\frac{G^2}{4} \pm |V_{\vec{G}}|$

procijep: $\Delta = E_+ - E_- = 2|V_{\vec{G}}|$

Z-5.3

$$E(k) = E_0 \cos\frac{ka}{2} \quad \Rightarrow \quad \frac{dE_k}{dk} = -\frac{aE_0}{2}\sin\frac{ka}{2}$$

$$\frac{d^2E_k}{dk^2} = -\frac{a^2E_0}{4}\cos\frac{ka}{2}$$



$$m^* = \frac{\hbar^2}{\frac{d^2E_k}{dk^2}} = -\frac{4\hbar^2}{a^2E_0\cos\frac{ka}{2}} \overset{k\approx 0}{\approx} -\frac{4\hbar^2}{a^2E_0} < 0$$

$\cos\frac{ka}{2} \approx 1 - \frac{1}{2}\left(\frac{ka}{2}\right)^2$

- u centru BZ nalaze se šupljine

$$v = \frac{1}{\hbar}\frac{dE_k}{dk} = -\frac{aE_0}{2\hbar}\sin\frac{ka}{2} \overset{k\approx 0}{\approx} -\frac{a^2E_0}{4\hbar}k = \frac{\hbar k}{m^*}$$

$\sin\frac{ka}{2} \approx \frac{ka}{2}$; $-\frac{a^2E_0}{4\hbar} = \frac{\hbar}{m^*}$

Z-5.4

$$\frac{1}{m^*_{\alpha\beta}} = \frac{1}{\hbar^2}\frac{\partial^2 E_k}{\partial k_\alpha \partial k_\beta}, \quad \alpha,\beta \in \{x,y,z\} \quad \& \quad m^*_{\alpha\beta} = m^*_{\beta\alpha}$$

$$\frac{\partial E}{\partial k_x} = -\frac{E_0 a}{2}\left[\sin\frac{k_x a}{2}\cos\frac{k_y b}{2} + \cos\frac{k_z c}{2}\sin\frac{k_x a}{2}\right] = -\frac{E_0 a}{2}\sin\frac{k_x a}{2}\left(\cos\frac{k_y b}{2} + \cos\frac{k_z c}{2}\right)$$

$$\frac{\partial E}{\partial k_y} = -\frac{E_0 b}{2}\sin\frac{k_y b}{2}\left(\cos\frac{k_x a}{2} + \cos\frac{k_z c}{2}\right)$$

$$\frac{\partial E}{\partial k_z} = -\frac{E_0 c}{2}\sin\frac{k_z c}{2}\left(\cos\frac{k_x a}{2} + \cos\frac{k_y b}{2}\right)$$

$$\frac{1}{m^*_{xx}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_x \partial k_x} = -\frac{E_0 a^2}{4\hbar^2}\cos\frac{k_x a}{2}\left(\cos\frac{k_y b}{2} + \cos\frac{k_z c}{2}\right)$$

$$\frac{1}{m^*_{yy}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_y \partial k_y} = -\frac{E_0 b^2}{4\hbar^2}\cos\frac{k_y b}{2}\left(\cos\frac{k_x a}{2} + \cos\frac{k_z c}{2}\right)$$

$$\frac{1}{m^*_{zz}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_z \partial k_z} = -\frac{E_0 c^2}{4\hbar^2}\cos\frac{k_z c}{2}\left(\cos\frac{k_x a}{2} + \cos\frac{k_y b}{2}\right)$$

$$\frac{1}{m^*_{xy}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_x \partial k_y} = \frac{E_0 ab}{4\hbar^2}\sin\frac{k_x a}{2}\sin\frac{k_y b}{2} = \frac{1}{m^*_{yx}}$$

$$\frac{1}{m^*_{xz}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_x \partial k_z} = \frac{E_0 ac}{4\hbar^2}\sin\frac{k_x a}{2}\sin\frac{k_z c}{2} = \frac{1}{m^*_{zx}}$$

$$\frac{1}{m^*_{yz}} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_y \partial k_z} = \frac{E_0 bc}{4\hbar^2}\sin\frac{k_y b}{2}\sin\frac{k_z c}{2} = \frac{1}{m^*_{zy}}$$

Z-5.5

$\sum_{s,\vec{k}} \not\rightarrow 2\left(\frac{L}{2\pi}\right)^3 \int d^3k$ Nije moguće direktno prijeći na sfernosimetrične koordinate zbog anizotropije efektivnih masa

$$m_x^* \neq m_y^* \neq m_z^*$$

def: Uvodimo novi valni vektor s komponentama $q_\alpha \equiv k_\alpha \sqrt{\frac{m}{m_\alpha^*}}$, $\alpha \in \{x, y, z\}$

$$\Rightarrow k_\alpha = \sqrt{\frac{m}{m_\alpha^*}}\, q_\alpha$$

$$E(\vec{k}) = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x^*} + \frac{k_y^2}{m_y^*} + \frac{k_z^2}{m_z^*}\right) \rightarrow E(\vec{q}) = \frac{\hbar^2}{2m}\left(q_x^2 + q_y^2 + q_z^2\right) = \frac{\hbar^2 |\vec{q}|^2}{2m} \quad (*)$$

$$d^3k = dk_x\, dk_y\, dk_z = \frac{\sqrt{m_x^* m_y^* m_z^*}}{m^{3/2}} \underbrace{dq_x\, dq_y\, dq_z}_{= d^3q}$$ (sfernosimetričan!)

$$\sum_{s,\vec{k}} = 2\left(\frac{L}{2\pi}\right)^3 \frac{\sqrt{m_x^* m_y^* m_z^*}}{m^{3/2}} 4\pi \int_0^\infty q^2\, dq = \frac{L^3}{\pi^2} \frac{\sqrt{m_x^* m_y^* m_z^*}}{m^{3/2}} \int_0^\infty q^2\, dq \equiv \int_0^\infty g(E)\, dE$$

$$\Rightarrow g(E) = \frac{L^3}{\pi^2} \frac{\sqrt{m_x^* m_y^* m_z^*}}{m^{3/2}} \frac{q^2}{\frac{dE}{dq}}$$

$\frac{dE}{dq} = \frac{\hbar^2 q}{m}$ (iz $(*)$: $E = \frac{\hbar^2 q^2}{2m}$)

$$= \frac{L^3}{\pi^2} \frac{\sqrt{m_x^* m_y^* m_z^*}}{m^{3/2}} \frac{q\, m}{\hbar^2}$$ (iz $(*)$)

$$= \frac{L^3}{\pi^2} \frac{\sqrt{m_x^* m_y^* m_z^*}}{m^{3/2}} \frac{m\sqrt{2mE}}{\hbar^3}$$

$$= \frac{L^3}{\pi^2} \frac{\sqrt{m_x^* m_y^* m_z^*}}{\hbar^3} \sqrt{2E} \sim \sqrt{E}$$

napomena: može se definirati $m^{**} \equiv \sqrt[3]{m_x^* m_y^* m_z^*}$

$$\Rightarrow g(E) = \frac{L^3}{\pi^2 \hbar^3} m^{**} \sqrt{2 m^{**} E}$$

Z-5.6

$$E(\vec{k}) = E_0 - 2t\cos k_y a - 4t\cos\frac{\sqrt{3}k_x a}{2}\cos\frac{k_y a}{2}$$

$$\approx E_0 - 2t\left(1-\frac{(k_y a)^2}{2}\right) - 4t\left(1-\frac{1}{2}\left(\frac{\sqrt{3}k_x a}{2}\right)^2\right)\left(1-\frac{1}{2}\left(\frac{k_y a}{2}\right)^2\right)$$

$$= E_0 - 2t + t(k_y a)^2 - 4t + 4t\,\frac{1}{2}\,\frac{1}{4}\left(3(k_x a)^2 + (k_y a)^2\right)$$

$$= E_B + t\left((k_y a)^2 + \frac{3}{2}(k_x a)^2 + \frac{1}{2}(k_y a)^2\right)$$

$$= E_B + \frac{3}{2}t\left[(k_x a)^2 + (k_y a)^2\right]$$

$$\frac{1}{m^*_{ij}} = \frac{1}{\hbar^2}\frac{\partial^2 E_{\vec{k}}}{\partial k_i \partial k_j}\bigg|_{E=E_B}, \quad i,j \in \{x,y\}$$

$$\frac{\partial E}{\partial k_x} = 3ta^2 k_x$$

$$\frac{\partial E}{\partial k_y} = 3ta^2 k_y$$

$$\frac{\partial^2 E}{\partial k_x^2} = 3ta^2$$

$$\frac{\partial^2 E}{\partial k_y^2} = 3ta^2$$

$$\frac{\partial^2 E}{\partial k_x \partial k_y} = \frac{\partial^2 E}{\partial k_y \partial k_x} = 0$$

$$\frac{1}{m^*} = \frac{3ta^2}{\hbar^2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

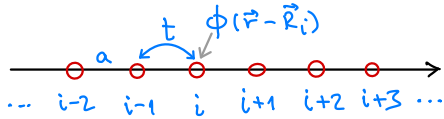
Z-5.7

H_0 - atomski hamiltonijan ; $\phi(\vec{r}-\vec{R}_i) \equiv |\vec{R}_i\rangle$ - atomska valna funkcija na čvoru $\vec{R}_i$

$H = H_0 + V$ - kristalni hamiltonijan s valnim funkcijama $\psi_{\vec{k}}(\vec{r}) \equiv |\vec{k}\rangle$

$H_0|\vec{R}_i\rangle = E^\circ|\vec{R}_i\rangle$

$H|\vec{k}\rangle = E_{\vec{k}}|\vec{k}\rangle$



$|\vec{k}\rangle = \sum_i c_i(\vec{k})|\vec{R}_i\rangle$ - razvoj $\psi_{\vec{k}}(\vec{r})$ u bazi atomskih valnih funkcija $\phi(\vec{r}-\vec{R}_i)$

$H|\vec{k}\rangle = E_{\vec{k}}|\vec{k}\rangle$

$\sum_i c_i(H_0|\vec{R}_i\rangle + V|\vec{R}_i\rangle) = E_{\vec{k}}\sum_i c_i|\vec{R}_i\rangle$

$\sum_i c_i(E^\circ|\vec{R}_i\rangle + V|\vec{R}_i\rangle) = E_{\vec{k}}\sum_i c_i|\vec{R}_i\rangle \;\Big|\; \langle\vec{R}_j|\cdot$

$\sum_i c_i(E^\circ\underbrace{\langle\vec{R}_j|\vec{R}_i\rangle}_{\int\phi^*(\vec{r}-\vec{R}_j)\phi(\vec{r}-\vec{R}_i)d^3r \approx \delta_{ij}} + \underbrace{\langle\vec{R}_j|V|\vec{R}_i\rangle}_{\int\phi^*(\vec{r}-\vec{R}_j)V(\vec{r})\phi(\vec{r}-\vec{R}_i)d^3r \equiv -t(\delta_{i,j-1}+\delta_{i,j+1})}) = E_{\vec{k}}\sum_i c_i\langle\vec{R}_j|\vec{R}_i\rangle$

$(E^\circ - E_{\vec{k}})c_j - t c_{j-1} - t c_{j+1} = 0$

$c_j(\vec{k})$: jer je $\psi(\vec{r}+\vec{R}_j) = e^{i\vec{k}\cdot\vec{R}_j}\psi(\vec{r}) \Rightarrow c_j = e^{i\vec{k}\cdot\vec{R}_j}\underbrace{c_0}_{\equiv c}$ (izbor)

$c_j(\vec{k}) = c\,e^{i\vec{k}\cdot\vec{R}_j} \underset{\vec{k},\vec{R}_j \parallel \hat{x}}{=\!=} c\,e^{ikaj}$; $\vec{R}_j = aj\hat{x}$

$(E^\circ - E_{\vec{k}})e^{ikaj} - t\,e^{ika(j-1)} - t\,e^{ika(j+1)} = 0 \quad |:e^{ikaj}$

$E^\circ - E_{\vec{k}} - t(e^{ika} + e^{-ika}) = 0$

$\underline{E_k = E^\circ - 2t\cos ka}$

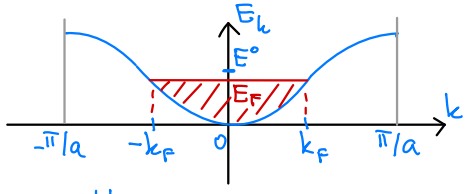
Blochova stanja : $\langle\vec{k}|\vec{k}\rangle = 1$, $|\vec{k}\rangle = \sum_j c\,e^{i\vec{k}\cdot\vec{R}_j}|\vec{R}_j\rangle$

$1 = \sum_{j,j'} c^2 e^{-i\vec{k}\cdot\vec{R}_{j'}} e^{i\vec{k}\cdot\vec{R}_j}\underbrace{\langle\vec{R}_{j'}|\vec{R}_j\rangle}_{\delta_{j,j'}} = \sum_j c^2 \underbrace{e^{-i\vec{k}\cdot\vec{R}_j + i\vec{k}\cdot\vec{R}_j}}_{=1} = c^2\sum_j 1 = c^2 N \Rightarrow c = \frac{1}{\sqrt{N}}$

$\underline{\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_j e^{i\vec{k}\vec{R}_j}\phi(\vec{r}-\vec{R}_j)}$

Z-5.8

$E_{coh} = NE^\circ - \sum_{k_{occ}} E_k$, $E_k = E^\circ - 2t\cos ka$ (E° energija atomskog stanja)



$$E_{coh} = \cancel{NE^\circ} - \cancel{NE^\circ} + 2\frac{L}{2\pi}\int_{-k_F}^{k_F} 2t\cos(ka)\,dk = \frac{2Nat}{\pi}\frac{1}{a}\sin ka\Big|_{-k_F}^{k_F} =$$

($\frac{L}{2\pi} \to \frac{Na}{2\pi}$)

$$= \frac{2Nt}{\pi}\left(\sin k_F a - (-\sin k_F a)\right) = N\frac{1}{\pi}4t\sin k_F a$$

$$E_{coh}^{1at.} = \frac{E_{coh}}{N} = \frac{1}{\pi}4t\sin k_F a$$

Z-5.9

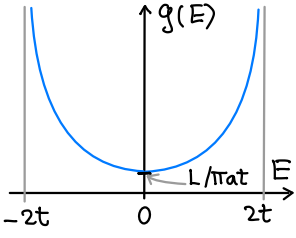
$g(E) = 2\frac{L}{\pi}\frac{1}{\frac{dE}{dk}}$; $E_k = E^\circ - 2t\cos ka \Big|^2 \Rightarrow E^2 = 4t^2\cos^2 ka$ (*)

($E^\circ \equiv 0$ (definiramo ishodište energije))

$$g(E) = \frac{2L}{\pi}\frac{1}{2ta\sin ka} = \frac{2L}{\pi a}\frac{1}{2t\sqrt{1-\cos^2 ka}}$$

$$= \frac{2L}{\pi a}\frac{1}{\sqrt{4t^2 - 4t^2\cos^2 ka}} = \frac{2L}{\pi a}\frac{1}{\sqrt{4t^2 - E^2}}$$

(*) : $= E^2$



$E^\circ \equiv 0$

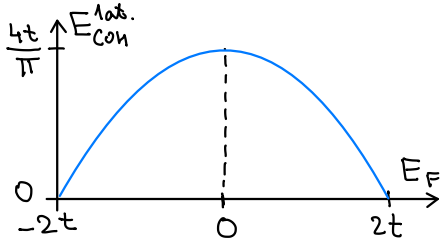
$$E_{coh} = N\cancel{E^\circ} - \int_{E_B}^{E_F} E\,g(E)\,dE \quad , \quad E_B = -2t \text{ (dno vrpce)}$$

($\frac{2L}{\pi a} \to \frac{2Na}{\pi a}$)

$$= -\frac{2N}{\pi}\int_{-2t}^{E_F}\frac{E\,dE}{\sqrt{4t^2 - E^2}} = \frac{2N}{\pi}\sqrt{4t^2 - E^2}\Big|_{-2t}^{E_F} =$$

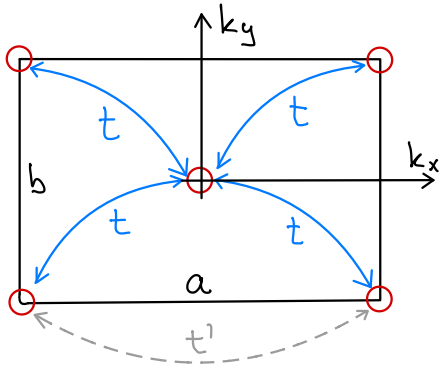
$$= \frac{2N}{\pi}\left(\sqrt{4t^2 - E_F^2} - \sqrt{\cancel{4t^2} - \cancel{4t^2}}\right)$$

$$E_{coh}^{1at.} = \frac{2}{\pi}\sqrt{4t^2 - E_F^2}$$



Z-5.10

a)



t : prvi susjedi

t' : drugi susjedi

$$E_{\vec{k}} = E^0 - \sum_{\vec{\delta}} t(\vec{\delta})\, e^{-i\vec{k}\cdot\vec{\delta}}$$

prvi susjedi:

$$\vec{\delta} = \pm\frac{1}{2}a\hat{x} \pm \frac{1}{2}b\hat{y}$$

$$\Rightarrow \vec{k}\cdot\vec{\delta} = \pm\frac{k_x a}{2} \pm \frac{k_y b}{2}$$

$$E_{\vec{k}} = E^0 - t\left\{e^{-\frac{i}{2}(k_x a + k_y b)} + e^{-\frac{i}{2}(k_x a - k_y b)} + e^{\frac{i}{2}(k_x a + k_y b)} + e^{\frac{i}{2}(k_x a - k_y b)}\right\}$$

$$= E^0 - 2t\left\{\cos\frac{k_x a + k_y b}{2} + \cos\frac{k_x a - k_y b}{2}\right\}$$

$$= E^0 - 2t\left\{\cos\frac{k_x a}{2}\cos\frac{k_y b}{2} - \sin\frac{k_x a}{2}\sin\frac{k_y b}{2} + \cos\frac{k_x a}{2}\cos\frac{k_y b}{2} + \right.$$

$$\left. + \sin\frac{k_x a}{2}\sin\frac{k_y b}{2}\right\}$$

$$= E^0 - 4t\cos\frac{k_x a}{2}\cos\frac{k_y b}{2}$$

centar BZ : $|\vec{k}| = 0$

$$E_{\vec{k}} \approx E^0 - 4t\left(1 - \frac{1}{2}\left(\frac{k_x a}{2}\right)^2\right)\left(1 - \frac{1}{2}\left(\frac{k_y b}{2}\right)^2\right), \quad k_x a,\ k_y b \ll 1$$

$$= E^0 - 4t\left[1 - \frac{1}{8}\left((k_x a)^2 + (k_y b)^2\right) + \frac{1}{64}(k_x a)^2(k_y b)^2\right]$$

$$= E^0 - 4t + \frac{1}{2}t\left[(k_x a)^2 + (k_y b)^2\right]$$

$$= \tilde{E}^0 + \frac{1}{2}t|\vec{K}|^2, \qquad \tilde{E}^0 \equiv E^0 - 4t, \quad \vec{K} \equiv (k_x a, k_y b)$$

b)

$$g(E) = \sum_{\{n\}} \delta(E - E_n) = \sum_{s,\vec{k}} \delta(E - E_{\vec{k}s}) = 2 \sum_{\vec{k}} \delta\left(E - \tilde{E}^0 - \frac{t}{2}|\vec{K}|^2\right)$$

$$g(E) = 2\left(\frac{L}{2\pi}\right)^2 \int dk_x dk_y \, \delta\left(E - \tilde{E}^0 - \frac{t}{2}K^2\right) ; \quad dk_x = \frac{1}{a} dK_x \, , \; dk_y = \frac{1}{b} dK_y$$

$$= \frac{2L^2}{(2\pi)^2 ab} 2\pi \int K dK \, \delta\left(E - \tilde{E}^0 - \frac{t}{2}K^2\right)$$

$$= \frac{L^2}{\pi ab} \int \frac{1}{t} d\underbrace{\left(\frac{t}{2}K^2\right)}_{\equiv x} \delta\left(E - \tilde{E}^0 - \frac{t}{2}K^2\right)$$

$$= \frac{L^2}{\pi ab} \int dx \, \delta(E - \tilde{E}^0 - x)$$

$$= \frac{L^2}{\pi ab} \Theta(E - \tilde{E}^0)$$

$$= \frac{L^2}{\pi ab} \Theta(E - E^0 + 4t)$$

provjera:

$$\frac{1}{t} d\left(\frac{t}{2}K^2\right) = \frac{1}{t} \frac{t}{2} 2K dK = K dK$$

VI. ELEKTRIČNI I TOPLINSKI TRANSPORT

Z-6.1

$m\dot{\vec{v}} = -e\vec{E} - \eta m\vec{v}$: jednadžba gibanja (Newton)

$\dot{\vec{v}} + \eta\vec{v} = -\frac{e}{m}\vec{E}$ ⊛

homogena jednadžba:

$\dot{\vec{v}} + \eta\vec{v} = 0 \xrightarrow[v \sim e^{\lambda t}]{} \lambda\vec{v} + \eta\vec{v} = 0 \Rightarrow \lambda = -\eta$

rješenje: $\vec{v}(t) = \vec{C}e^{-\eta t} + \vec{v}_0$

$\dot{\vec{v}}(t) = -\eta\vec{C}e^{-\eta t}$ - uvrstimo u jedn. ⊛:

$-\eta\vec{C}e^{-\eta t} + \eta\vec{C}e^{-\eta t} + \eta\vec{v}_0 = -\frac{e}{m}\vec{E}$

$\Rightarrow \vec{v}_0 = -\frac{e}{\eta m}\vec{E}$

$\vec{v}(t) = \vec{C}e^{-\eta t} - \frac{e\vec{E}}{\eta m}$

def: $\eta \equiv \frac{1}{\tau}$, τ - relaksacijsko vrijeme : pri $\vec{E} = 0 \rightarrow v \sim e^{-\frac{t}{\tau}}$

tj za $t \gg \tau$: $v \rightarrow 0$

stacionarno rješenje za $t \gg \tau$ ($e^{-t/\tau} \rightarrow 0$):

$\vec{v}(t) = -\frac{e\tau}{m}\vec{E} = \text{const.}$

struja: $\vec{j} = -en\vec{v}$

$= \frac{e^2 n\tau}{m}\vec{E}$ & $\vec{j} \equiv \sigma\vec{E}$ $\Rightarrow \sigma = \frac{e^2 n\tau}{m}$

(Drude)

Z-6.2

$\dot{\vec{v}} + \eta \vec{v} = -\frac{e}{m}\vec{E}_0 e^{-i\omega t}$, $\eta = \frac{1}{\tau}$ - jednadžba gibanja
- τ - relaksacijsko vrijeme

rješenje (odredjeno nehomogenoću jednadžbe):

$\vec{v}(t) = \vec{A} e^{-i\omega t}$ → uvrstimo u jednadžbu

$\Rightarrow -i\omega\vec{A}e^{-i\omega t} + \eta\vec{A}e^{-i\omega t} = -\frac{e}{m}\vec{E}_0 e^{-i\omega t} \Rightarrow \vec{A} = -\frac{e}{m(\eta - i\omega)}\vec{E}_0$

struja:

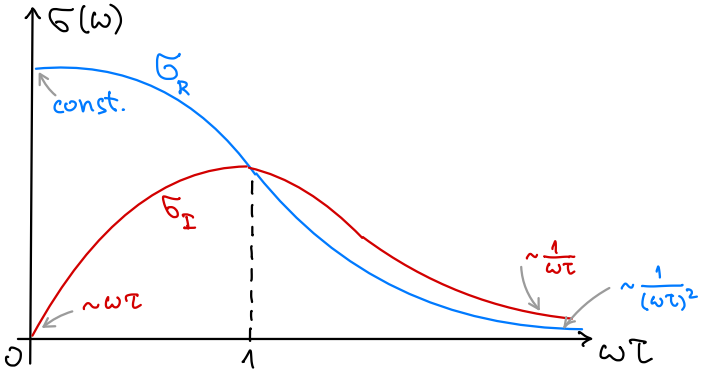
$$\vec{j} = -en\vec{v} = \underbrace{\frac{e^2 n}{m(\eta - i\omega)}}_{=\sigma}\underbrace{\vec{E}_0 e^{-i\omega t}}_{=\vec{E}}$$

$$\sigma(\omega) = \frac{e^2 n}{m(\eta - i\omega)} = \underbrace{\frac{e^2 n \tau}{m}}_{\equiv \sigma_0 \text{ (Drude)}}\frac{1}{1 - i\omega\tau} = \sigma_0 \frac{1 + i\omega\tau}{1 + (\omega\tau)^2}$$

granice:

1.) $\omega\tau \ll 1$: $\sigma(\omega) = \sigma_0 \frac{1 + i\omega\tau}{1 + (\omega\tau)^2} \approx \sigma_0(1 + i\omega\tau)$

2.) $\omega\tau \gg 1$: $\sigma(\omega) = \sigma_0 \frac{1 + i\omega\tau}{1 + (\omega\tau)^2} \approx \sigma_0\left(\frac{1}{(\omega\tau)^2} + \frac{i}{\omega\tau}\right)$



Z-6.3

$\dot{\vec{v}} + \eta \vec{v} = \frac{q}{m}(\vec{E} + \vec{v} \times \vec{B})$: jednadžba gibanja;
τ - relaksacijsko vrijeme ($\eta = \frac{1}{\tau}$)
q - naboj čestice

za $\vec{B} = (0, 0, B) \rightarrow \vec{v} \times \vec{B} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ v_x & v_y & v_z \\ 0 & 0 & B \end{vmatrix} = B(v_y \hat{x} - v_x \hat{y})$

$\Downarrow$

$$\left.\begin{aligned} \left(\frac{d}{dt} + \frac{1}{\tau}\right) v_x &= \frac{q}{m} E_x + \frac{q}{m} v_y B \\ \left(\frac{d}{dt} + \frac{1}{\tau}\right) v_y &= \frac{q}{m} E_y - \frac{q}{m} v_x B \\ \left(\frac{d}{dt} + \frac{1}{\tau}\right) v_z &= \frac{q}{m} E_z \end{aligned}\right\} \xrightarrow[\text{rješenje } \left(\frac{d\vec{v}}{dt} = 0\right)]{\text{stacionarno}} \begin{aligned} v_x - \frac{qB\tau}{m} v_y &= \frac{q\tau}{m} E_x \\ \frac{qB\tau}{m} v_x + v_y &= \frac{q\tau}{m} E_y \\ v_z &= \frac{q\tau}{m} E_z \end{aligned}$$

---

def: $\tilde{\omega}_c \equiv \frac{qB}{m} = \mathrm{sgn}(q) \frac{|q|B}{m}$

$$\begin{aligned} v_x - \tilde{\omega}_c \tau v_y &= \frac{q\tau}{m} E_x \\ \tilde{\omega}_c \tau v_x + v_y &= \frac{q\tau}{m} E_y \quad \Rightarrow v_y = \frac{q\tau}{m} E_y - \tilde{\omega}_c \tau v_x \\ v_z &= \frac{q\tau}{m} E_z \end{aligned}$$

$$v_x - \tilde{\omega}_c \tau \left(\frac{q\tau}{m} E_y - \tilde{\omega}_c \tau v_x\right) = \frac{q\tau}{m} E_x$$

$$v_x \left(1 + (\tilde{\omega}_c \tau)^2\right) = \frac{q\tau}{m} E_x + \tilde{\omega}_c \tau \frac{q\tau}{m} E_y$$

$$v_x = \frac{\frac{q\tau}{m}}{1 + (\tilde{\omega}_c \tau)^2} (E_x + \tilde{\omega}_c \tau E_y)$$

$\Downarrow$

$$\begin{aligned} v_y &= \frac{q\tau}{m} E_y - \frac{\frac{q\tau}{m}}{1 + (\tilde{\omega}_c \tau)^2} (E_x + \tilde{\omega}_c \tau E_y) \\ &= \frac{1}{1 + (\tilde{\omega}_c \tau)^2} \left(\frac{q\tau}{m}(1 + (\tilde{\omega}_c \tau)^2) E_y - \frac{q\tau}{m} \omega_c \tau E_x - \frac{q\tau}{m} (\omega_c \tau)^2 E_y\right) \\ &= \frac{\frac{q\tau}{m}}{1 + (\tilde{\omega}_c \tau)^2} \left(-\tilde{\omega}_c \tau E_x + E_y\right) \end{aligned}$$

$$v_z = \frac{\frac{q\tau}{m}}{1+(\tilde{\omega}_c\tau)^2}\left(1+(\omega_c\tau)^2\right)E_z$$

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

$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \underbrace{\frac{\frac{q^2n\tau}{m}}{1+(\tilde{\omega}_c\tau)^2}}_{\sigma_0} \underbrace{\begin{pmatrix} 1 & \tilde{\omega}_c\tau & 0 \\ -\tilde{\omega}_c\tau & 1 & 0 \\ 0 & 0 & 1+(\tilde{\omega}_c\tau)^2 \end{pmatrix}}_{\equiv \mathbb{M}\text{ - tenzor magnetovodljivosti}} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$$

$\sigma_0 \equiv \frac{q^2n\tau}{m}$ Drudeova vodljivost

$\tilde{\omega}_c = \begin{cases} -\frac{eB}{m}, & \text{za } q=-e \text{ (elektroni)} \\ +\frac{eB}{m}, & \text{za } q=+e \text{ (šupljine)} \end{cases}$

$\frac{eB}{m} \equiv \omega_c$ - ciklotronska frekvencija

Z-6.4

$\vec{j} = \mathbb{M}\vec{E}$; Hallovo polje odredimo iz uvjeta $j_y = 0$:

$$j_y = \frac{\sigma_0}{1+(\tilde{\omega}_c\tau)^2}\left(-\tilde{\omega}_c\tau E_x + E_y\right) = 0 \iff E_y = \tilde{\omega}_c\tau E_x \quad \circledast$$

Hallova konstanta: $R_H = \frac{E_y}{j_x B}$

$$j_x = \frac{\sigma_0}{1+(\tilde{\omega}_c\tau)^2}\left(E_x + \tilde{\omega}_c\tau E_y\right) = \frac{\sigma_0}{1+(\tilde{\omega}_c\tau)^2}\left(E_x + (\tilde{\omega}_c\tau)^2 E_x\right) = \sigma_0 E_x$$

$$R_H = \frac{\tilde{\omega}_c\tau E_x}{\sigma_0 E_x B} = \frac{\frac{q\tau}{m}\tau}{\frac{q^2n\tau}{m}B} = \underline{\frac{1}{qn}}$$

$$\mathbb{M} = \frac{\sigma_0}{1+(\tilde{\omega}_c\tau)^2}\begin{pmatrix} 1 & \tilde{\omega}_c\tau & 0 \\ -\tilde{\omega}_c\tau & 1 & 0 \\ 0 & 0 & 1+(\tilde{\omega}_c\tau)^2 \end{pmatrix}, \qquad \sigma_0 = \frac{q^2 n \tau}{m}, \quad \tilde{\omega}_c = \frac{qB}{m}$$

$\tilde{\omega}_c\tau \ll 1$ (slabo polje B)

$$\omega_c^{e,h} \equiv \mp \frac{eB}{m_{e,h}}$$

$$\vec{j} = \mathbb{M}\vec{E} \Rightarrow j_x = \sigma_0(E_x + \tilde{\omega}_c\tau E_y)$$
$$j_y = \sigma_0(-\tilde{\omega}_c\tau E_x + E_y)$$

$$\mu_{e,h} \equiv \frac{e\tau_{e,h}}{m_{e,h}}$$

$$\sigma_0^{e,h} = \frac{n_{e,h}e^2\tau_{e,h}}{m_{e,h}} = e n_{e,h}\frac{e\tau_{e,h}}{m_{e,h}} = e n_{e,h}\mu_{e,h}$$

Hallova vodljivost: $\sigma_{xy} = \sigma_{xy}^e + \sigma_{xy}^h$, $\sigma_{xy}^{e,h} = \sigma_0^{e,h}\tilde{\omega}_c^{e,h}\tau_{e,h}$

$$\sigma_{xy} = e n_e \mu_e \frac{-eB}{m_e}\tau_e + e n_e \mu_e \frac{+eB}{m_e}\tau_e$$
$$= e(n_h\mu_h^2 - n_e\mu_e^2)B$$

$$j_y = j_y^e + j_y^h = e n_e \mu_e\left(\underbrace{\frac{eB\tau_e}{m_e}}_{\mu_e B}E_x + E_y\right) + e n_h\mu_h\left(-\underbrace{\frac{eB\tau_h}{m_h}}_{\mu_h B}E_x + E_y\right)$$
$$= e\{(n_e\mu_e^2 - n_h\mu_h^2)BE_x \; (n_e\mu_e + n_h\mu_h)E_y\}$$

Hall: $j_y = 0 \Rightarrow E_y = -\frac{n_e\mu_e^2 - n_h\mu_h^2}{n_e\mu_e + n_h\mu_h}BE_x \sim B$

$$j_x = j_x^e + j_x^h = e n_e\mu_e\left(E_x - \underbrace{\frac{eB\tau_e}{m_e}E_y}_{\sim B^2}\right) + e n_h\mu_h\left(E_x - \frac{eB\tau_h}{m_h}E_y\right) \sim B$$
$$\approx e(n_e\mu_e + n_h\mu_h)E_x$$

$$R_H = \frac{-\frac{n_e\mu_e^2 - n_h\mu_h^2}{n_e\mu_e + n_h\mu_h}BE_x}{e(n_e\mu_e + n_h\mu_h)E_x B} = \frac{n_h\mu_h^2 - n_e\mu_e^2}{e(n_e\mu_e + n_h\mu_h)^2}$$

Z-6.6

$$\mathbb{M} = \frac{\sigma_0}{1+(\tilde{\omega}_c\tau)^2}\begin{pmatrix} 1 & \tilde{\omega}_c\tau & 0 \\ -\tilde{\omega}_c\tau & 1 & 0 \\ 0 & 0 & 1+(\tilde{\omega}_c\tau)^2 \end{pmatrix} \approx \sigma_0 \begin{pmatrix} (\tilde{\omega}_c\tau)^{-2} & (\tilde{\omega}_c\tau)^{-1} & 0 \\ -(\tilde{\omega}_c\tau)^{-1} & (\tilde{\omega}_c\tau)^{-2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$\tilde{\omega}_c\tau \gg 1$ (jako pole B)

Hallova vodljivost:

$$\sigma_{xy} = \sigma^e_{xy} + \sigma^h_{xy} = \frac{\sigma^e_0}{\omega^e_c\tau_e} + \frac{\sigma^h_0}{\omega^h_c\tau_h} = \frac{\frac{e^2 n_e \tau_e}{m_e}}{-\frac{eB}{m_e}\tau_e} + \frac{\frac{e^2 n_h \tau_h}{m_h}}{\frac{eB}{m_h}\tau_h}$$

$$= \frac{e}{B}(n_h - n_e)$$

Hallova konstanta: $R_H = \frac{E_y}{j_x B}$, za $j_y = 0$

$$j_y = j^e_y + j^h_y = \left(-\frac{\sigma^e_0}{\omega^e_c\tau_e}E_x + \frac{\sigma^e_0}{(\omega^e_c\tau_e)^2}E_y\right) + \left(-\frac{\sigma^h_0}{\omega^h_c\tau_h}E_x + \frac{\sigma^h_0}{(\omega^h_c\tau_h)^2}E_y\right)$$

$$= \left[-\frac{\frac{n_e e^2\tau_e}{m_e}}{-\frac{eB}{m_e}\tau_e} - \frac{\frac{n_h e^2\tau_h}{m_h}}{\frac{eB}{m_h}\tau_h}\right]E_x + \left[\frac{\frac{n_e e^2\tau_e}{m_e}}{\left(-\frac{eB}{m_e}\tau_e\right)^2} + \frac{\frac{n_h e^2\tau_h}{m_h}}{\left(\frac{eB}{m_h}\tau_h\right)^2}\right]E_y$$

$$= \frac{e}{B}(n_h - n_e)E_x + \frac{1}{B^2}\left(\frac{n_e \cdot m_e}{\tau_e} + \frac{n_h \cdot m_h}{\tau_h}\right)E_y = 0$$

$$\Rightarrow E_y = eB\,\frac{n_h - n_e}{\frac{n_e \cdot m_e}{\tau_e} + \frac{n_h \cdot m_h}{\tau_h}}E_x \sim B \quad \text{(Hallovo polje)}$$

⊛

$$j_x = j_x^e + j_x^h = \left(\frac{\sigma_0^e}{(\omega_c^e \tau_e)^2} E_x + \frac{\sigma_0^e}{\omega_c^e \tau_e} E_y\right) + \left(\frac{\sigma_0^h}{(\omega_c^h \tau_h)^2} E_x + \frac{\sigma_0^h}{\omega_c^h \tau_h} E_y\right)$$

$$= \left[\frac{\frac{n_e e^2 \tau_e}{m_e}}{\left(-\frac{eB}{m_e}\tau_e\right)^2} + \frac{\frac{n_h e^2 \tau_h}{m_h}}{\left(\frac{eB}{m_h}\tau_h\right)^2}\right] E_x + \left[\frac{\frac{n_e e^2 \tau_e}{m_e}}{-\frac{eB}{m_e}\tau_e} + \frac{\frac{n_h e^2 \tau_h}{m_h}}{\frac{eB}{m_h}\tau_h}\right] E_y$$

$$= \left[\frac{n_e \cdot m_e}{B \cdot \tau_e} + \frac{n_h \cdot m_h}{B \cdot \tau_h}\right] E_x + \left[-\frac{n_e e}{B} + \frac{n_h e}{B}\right] E_y$$

$$= \frac{1}{B^2}\left(\frac{n_e \cdot m_e}{\tau_e} + \frac{n_h \cdot m_h}{\tau_h}\right) E_x + \frac{e}{B}(n_h - n_e) E_y$$

$$\overset{\text{(*)}}{=} \underbrace{\frac{1}{B^2}\left(\frac{n_e \cdot m_e}{\tau_e} + \frac{n_h \cdot m_h}{\tau_h}\right) E_x}_{\sim 1/B^2} + \underbrace{\frac{e}{B} eB}_{\sim 1} \frac{(n_h - n_e)^2}{\frac{n_e \cdot m_e}{\tau_e} + \frac{n_h \cdot m_h}{\tau_h}} E_x$$

$$\approx \frac{e^2 (n_h - n_e)^2}{\frac{n_e \cdot m_e}{\tau_e} + \frac{n_h \cdot m_h}{\tau_h}} E_x$$

$$R_H = \frac{eB \dfrac{n_h - n_e}{\frac{n_e \cdot m_e}{\tau_e} + \frac{n_h \cdot m_h}{\tau_h}} E_x}{\dfrac{e^2 (n_h - n_e)^2}{\frac{n_e \cdot m_e}{\tau_e} + \frac{n_h \cdot m_h}{\tau_h}} E_x B}$$

$$= \frac{1}{e(n_h - n_e)}$$

Z-6.7

$$E(\vec{k}) = \hbar^2\left(\frac{k_x^2+k_t^2}{2m_t} + \frac{k_z^2}{2m_l}\right) ,$$

$$(1)\quad \hbar\frac{d\vec{k}}{dt} = -e\vec{v}\times\vec{B} \underset{\vec{B}=(0,0,B)}{=} -eB(v_z\hat{y} - v_y\hat{z})$$

$$(2)\quad \vec{v} = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}E(\vec{k})$$

$$(2):\quad v_x = \frac{1}{\hbar}\frac{\hbar^2}{2m_t}2k_x = \frac{\hbar k_x}{m_t}$$

$$v_y = \frac{\hbar k_y}{m_t}$$

$$v_y = \frac{\hbar k_z}{m_l}$$

$$(1):\quad \frac{dk_x}{dt} = 0$$

$$\frac{dk_y}{dt} = -\frac{eB}{\hbar}v_z = -\frac{eB}{m_l}k_z = -\omega_c^{(l)}k_z \;\Big|\frac{d}{dt}\;;\quad \omega_c^{(l)} \equiv \frac{eB}{m_l}$$

$$\frac{dk_z}{dt} = \frac{eB}{\hbar}v_y = \frac{eB}{m_t}k_y = \omega_c^{(t)}k_y \qquad ;\quad \omega_c^{(t)} \equiv \frac{eB}{m_l}$$

$$\frac{d^2k_y}{dt^2} = -\omega_c^{(l)}\frac{dk_z}{dt}$$

$$= -\omega_c^{(l)}\omega_c^{(t)}k_y$$

$$\ddot{k}_y + \omega_c^{(l)}\omega_c^{(t)}k_y = 0 \xrightarrow{H.O.} \omega_c \equiv \sqrt{\omega_c^{(l)}\cdot\omega_c^{(t)}} = \frac{eB}{\sqrt{m_l m_t}}$$

Z-6.8

Wiedemann–Franz: $\frac{k_e}{\sigma T} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$

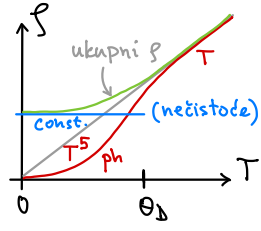
$\sigma = \frac{1}{\rho} \Rightarrow \underbrace{\frac{k_e \rho}{T}}$

$k_e = \frac{1}{3} v l_0 c_v^{el.}$

$\bar{n}_{ph} \sim \begin{cases} T^3, & T \ll \Theta_D \\ T, & T \gg \Theta_D \end{cases}$ – prosječan broj fonona

$l_0 \sim \bar{n}_{ph}^{-1} \sim \begin{cases} \text{const.}, & T \ll\ll \Theta_D \\ T^{-3}, & T \ll \Theta_D \\ T^{-1}, & T \gg \Theta_D \end{cases}$

$\rho \sim \begin{cases} \text{const.}, & T \ll\ll \Theta_D \\ T^5, & T \ll \Theta_D \text{ – čist uzorak} \\ \text{const.}, & T \ll \Theta_D \text{ – uzorak s nečistoćama} \\ T^1, & T \gg \Theta_D \end{cases}$



$c_v^{el.} \sim T$

$\frac{k_e \rho}{T} \sim \frac{l_0 c_v^{el.} \rho}{T} \sim \begin{cases} \frac{\text{const} \cdot T \cdot \text{const}}{T} \sim \text{const} \checkmark, & T \ll\ll \Theta_D \text{ – da} \\ \frac{T^{-3} \cdot T \cdot T^5}{T} \sim T^2 \times \\ \frac{T^{-3} \cdot T \cdot \text{const}}{T} \sim T^{-3} \times \end{cases}, T \ll \Theta_D \text{ – ne!}$

$\frac{T^{-1} \cdot T \cdot T}{T} \sim \text{const} \checkmark, \quad T \gg \Theta_D$ – da

VII. POLUVODIČI

Z-7.1

$$E_g(T) = E_g(0) - \alpha \frac{T^2}{T + T_0}$$

$$\Rightarrow T_0 = T\left(\frac{\alpha T}{E_g(0) - E_g(T)} - 1\right) = 60\,K$$

$E_g(0) - E_g(T) = 0.08\,eV$

Z-7.2

$$N_e = \frac{2}{h^3}\left(2\pi m_e^* k_B T\right)^{3/2} e^{-\frac{E_c - E_F}{k_B T}}$$

$$N_h = \frac{2}{h^3}\left(2\pi m_h^* k_B T\right)^{3/2} e^{-\frac{E_F - E_v}{k_B T}}$$

intrinsični polprevodič: $N_e = N_h \Rightarrow$

$$\left(\frac{m_e^*}{m_h^*}\right)^{3/2} = e^{\frac{E_c + E_v - 2E_F}{k_B T}} \quad \Big| \ln$$

$$E_F = \frac{E_c + E_v}{2} - \frac{3}{4} k_B T \cdot \ln \frac{m_e^*}{m_h^*}$$

Z-7.3

elektroni: $E^e(k) = E_c + \frac{\hbar^2 k^2}{2m_e^*}$, $g^e(E) = \frac{m_e^*}{\pi^2 \hbar^3}\sqrt{2m_e^*(E-E_c)}$

šupljine: $E^h(k) = E_v - \frac{\hbar^2 k^2}{2m_e^*}$, $g^h(E) = \frac{m_h^*}{\pi^2 \hbar^3}\sqrt{2m_h^*(E_v-E)}$

za male koncentracije nosilaca: $f_e(E) \simeq e^{-\frac{E-E_F}{k_B T}}$

$f_h(E) \simeq e^{-\frac{E_F-E}{k_B T}}$

$$N_e = \int_{E_c}^{\infty} g_e(E) f_e(E)\,dE = \frac{m_e^*\sqrt{2m_e^*}}{\pi^2\hbar^3} e^{\frac{E_F}{k_B T}} \int_{E_c}^{\infty} \sqrt{E-E_c}\, e^{-\frac{E}{k_B T}}\,dE =$$

$$\left\{ \text{supst: } x^2 = \frac{E-E_c}{k_B T},\ dE = 2k_B T \times dx,\ \int_{E_c}^{\infty} dE \to \int_0^{\infty} dx \right\}$$

$$= \frac{m_e^*\sqrt{2m_e^*}}{\pi^2\hbar^3} e^{\frac{E_F}{k_B T}} \int_0^{\infty} e^{-\frac{E_c}{k_B T}} \sqrt{k_B T} \times e^{-x^2} \cdot 2k_B T \times dx$$

$$= 2\frac{m_e^*\sqrt{2m_e^*}}{\pi^2\hbar^3} e^{\frac{E_F - E_c}{k_B T}} (k_B T)^{3/2} \underbrace{\int_0^{\infty} x^2 e^{-x^2} dx}_{=\sqrt{\pi}/4}$$

$$= \frac{2}{\hbar^3}(2\pi m_e^* k_B T)^{3/2} e^{-\frac{E_c - E_F}{k_B T}}$$

$$N_e = \int_{-\infty}^{E_v} g_h(E) f_h(E)\,dE = \frac{m_h^*\sqrt{2m_h^*}}{\pi^2\hbar^3} e^{-\frac{E_F}{k_B T}} \int_{-\infty}^{E_v} \sqrt{E_v - E}\, e^{\frac{E}{k_B T}}\,dE =$$

$$\left\{ \text{supst: } x^2 = \frac{E_v - E}{k_B T},\ dE = -2k_B T \times dx,\ \int_{-\infty}^{E_v} dE \to \int_{\infty}^{0} dx \right\}$$

$$= 2\frac{m_h^*\sqrt{2m_h^*}}{\pi^2\hbar^3} e^{\frac{E_v - E_F}{k_B T}} (k_B T)^{3/2} \underbrace{\int_0^{\infty} x^2 e^{-x^2} dx}_{=\sqrt{\pi}/4}$$

$$= \frac{2}{\hbar^3}(2\pi m_h^* k_B T)^{3/2} e^{-\frac{E_F - E_v}{k_B T}}$$

ZAM: $n_i = \sqrt{N_e N_h} = \frac{2}{\hbar^3}(2\pi k_B T)^{3/2} (m_e^* m_h^*)^{3/2} e^{-\frac{E_g}{2k_B T}}$

Z-7.4

intrinsični polvodič: $n_i^2 = C T^3 e^{-\frac{E_g}{k_B T}} \Rightarrow C = \frac{n_i^2}{T^3} e^{\frac{E_g}{k_B T}}$

$T = T_1$: $C = \frac{n_i^2}{T_1^3} e^{\frac{E_g}{k_B T_1}}$

$T = T_2$: $n_i^2(T_2) = C T_2^3 e^{-\frac{E_g}{k_B T}}$

$$\Rightarrow \frac{n_i^2(T_2)}{n_i^2(T_1)} = \left(\frac{T_2}{T_1}\right)^3 e^{-\frac{E_g}{k_B}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)} = 1.16335$$

$T_1 = 300\,K$, $T_2 = 301\,K$

$$\frac{n_i(T_2)}{n_i(T_1)} = 1.0786$$

$$\xi = \frac{n_i(T_2) - n_i(T_1)}{n_i(T_1)} = 7.86\,\%$$

Z-7.5

$N_D = 5 \cdot 10^{14}\,cm^{-3} > N_A = 3 \cdot 10^{14}\,cm^{-3} \Rightarrow$ n-tip

koncentracija večinskih nosilaca:

$$n + N_A = p + N_D$$

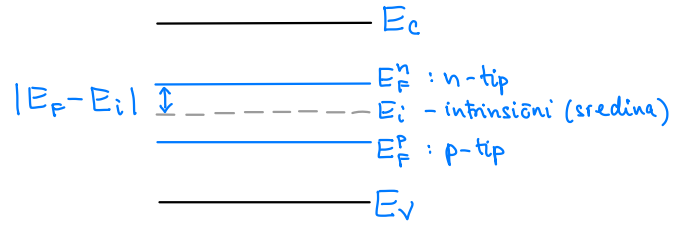
$$n = \frac{1}{2}\left[\underbrace{N_D - N_A}_{2 \cdot 10^{14}} + \sqrt{\underbrace{(N_D - N_A)^2}_{(2 \cdot 10^{14})^2} + \cancel{4n_i^2}}\right] \approx 2 \cdot 10^{14}\,cm^{-3}$$

$(2 \cdot 10^{14})^2 \gg (1.45 \cdot 10^{10})^2$

koncentracija manjinskih nosilaca:

$$p = \frac{n_i^2}{n} = \frac{(1.45 \cdot 10^{10})^2}{2 \cdot 10^{14}} = 1.05 \cdot 10^6\,cm^{-3}$$

Z-7.6



$|E_F - E_i| = ?$

$|E_F - E_i| = k_B T \ln \frac{N}{n_i}$

večinski nosilci: $N_A > N_D \Rightarrow$ p-tip

$$p = \frac{1}{2}\left[N_A - N_D + \sqrt{(N_A - N_D)^2 + 4n_i^2}\right] \approx 3 \cdot 10^{16}\ cm^{-3}$$

($N_A - N_D \sim 3\cdot 10^{16}$, $(N_A - N_D)^2 \sim (10^{16})^2$, $4n_i^2 \sim (10^{13})^2$)

$$|E_F - E_i| = k_B T \ln \frac{p}{n_i} = 0.185\ eV$$

($T = 300K$, $n_i = 2.4 \cdot 10^{13}\ cm^{-3}$)

Z-7.7

$|E_F - E_i| = k_B T \ln \frac{n(T)}{n_i(T)}$ → iščemo na $T_2 = 400K$ v odnosu na $T_1 = 300K$

$n_i^2(T_1) = C T_1^3 e^{-\frac{E_g}{k_B T_1}} \Rightarrow C = \frac{n_i^2(T_1)}{T_1^3} e^{\frac{E_g}{k_B T_1}} = 2.17 \cdot 10^{31}\ cm^{-6} K^{-3}$

($E_g = 1.1\ eV$, $T_1 = 300K$, $n_i = 1.45 \cdot 10^{10}\ cm^{-3}$)

$n_i^2(T_2) = C T_2^3 e^{-\frac{E_g}{k_B T_2}} = 1.975 \cdot 10^{25}\ cm^{-6}$

($T_2 = 400K$)

$n_i(T_2) = 4.44 \cdot 10^{12}\ cm^{-3}$

koncentracija večinskeih nosilcev:

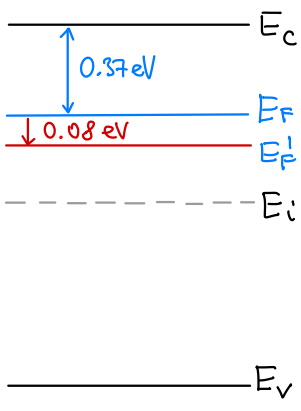
$$n = \frac{1}{2}\left[N_D + \sqrt{N_D^2 + 4n_i^2}\right] \approx N_D = 10^{14}\ cm^{-3}$$

($N_D \sim (10^{14})^2 \gg 4n_i^2 \sim (10^{12})^2$)

$|E_F - E_i| = 0.11\ eV$

($n = 10^{14}\ cm^{-3}$, $n_i = 4.44 \cdot 10^{12}\ cm^{-3}$, $T = 400K$)

Z-7.8



$$E_F - E_i = k_B T \ln \frac{n}{n_i}$$

$$E_c - E_i = E_c + E_F - E_F - E_i$$

$$= (E_c - E_F) + (E_F - E_i)$$

$(E_c - E_F) = \frac{E_g}{2}$; $(E_F - E_i)$ = ?

$$\Rightarrow E_F - E_i = \frac{E_g}{2} - (E_c - E_i)$$

$\frac{E_g}{2} = 0.55\,eV$; $(E_c - E_i)$ zadano: 0.37eV

$$n_i^2(T) = C T^3 e^{-\frac{E_g}{k_B T}} = 1.24 \cdot 10^{24}\,cm^{-6} \Rightarrow n_i(T) = 1.12 \cdot 10^{12}\,cm^{-3}$$

$T = 370\,K$

većinski nosioci:

$$n = n_i e^{\frac{E_F - E_i}{k_B T}} = 3.16 \cdot 10^{14}\,cm^{-3}$$

$E_F - E_i = 0.18\,eV$

$$n' = n_i e^{\frac{E_F' - E_i}{k_B T}} = 2.57 \cdot 10^{13}\,cm^{-3}$$

$E_F - E_i = 0.10\,eV$

manjinski nosioci: $p \cdot n = n_i^2$

$$p = \frac{n_i^2}{n} = 3.97 \cdot 10^{9}\,cm^{-3}$$

$$p' = \frac{n_i^2}{n'} = 4.88 \cdot 10^{10}\,cm^{-3}$$

$\Delta p = p' - p = 4.48 \cdot 10^{10}\,cm^{-3}$: koncentracija akceptora koju treba dodati da se E_F pomakne za 0.08 eV prema E_i

VIII. DIELEKTRIČNI ODZIV

Z-8.1

$$\vec{\nabla} \times \vec{H} = \vec{j}_f + \varepsilon_r' \varepsilon_0 \frac{\partial \vec{E}}{\partial t}$$

$\varepsilon_r' = 1$ (intrinsična od rešetke; $\varepsilon_r^{latt.} = 1$)

$$\& \Updownarrow$$

$$\vec{\nabla} \times \vec{H} = \varepsilon_r \varepsilon_0 \frac{\partial \vec{E}}{\partial t}$$

ε_r: totalna permitivnost (intrinsična + inducirana)

Ohmov zakon: $\vec{j} = \sigma \vec{E}$

za $\vec{E} = \vec{E}_0 e^{-i\omega t}$; $\frac{\partial \vec{E}}{\partial t} = -i\omega \underbrace{\vec{E}_0 e^{-i\omega t}}_{\vec{E}}$

$$\begin{cases} \vec{\nabla} \times \vec{H} = \sigma \vec{E} + 1 \cdot \varepsilon_0 (-i\omega) \vec{E} = (\sigma - i\omega\varepsilon_0) \vec{E} \\ \vec{\nabla} \times \vec{H} = \varepsilon_r \varepsilon_0 (-i\omega) \vec{E} \end{cases}$$

$$(\sigma - i\omega\varepsilon_0) \vec{E} = -i\omega \varepsilon_0 \varepsilon_r \vec{E}$$

$$\Rightarrow \varepsilon_r(\omega) = 1 + i \frac{\sigma(\omega)}{\varepsilon_0 \omega}$$

$\varepsilon_{pl}(\omega) = \varepsilon_r(\omega)$:

$$1 - \frac{\omega_p^2}{\omega^2 + i\omega\tau^{-1}} = 1 + i \frac{\sigma(\omega)}{\varepsilon_0 \omega}$$

$$\Rightarrow \sigma(\omega) = i\varepsilon_0 \frac{\omega_p^2}{\omega + i\tau^{-1}} = \varepsilon_0 \frac{e^2 n \tau}{\varepsilon_0 m} \frac{1}{1 - i\omega\tau}$$

$\omega_p^2 = \frac{e^2 n}{\varepsilon_0 m}$; $\frac{e^2 n \tau}{\varepsilon_0 m} = \sigma_0$

$$= \frac{\sigma_0}{1 - i\omega\tau}$$

Z-8.2

$$\varepsilon_r(\vec{q},\omega) = 1 - \frac{e^2}{\varepsilon_0 q^2} \sum_{s,\vec{k}} \frac{f(E_{\vec{k}}) - f(E_{\vec{k}+\vec{q}})}{\hbar\omega + E_{\vec{k}} - E_{\vec{k}+\vec{q}}}$$

$k \to 0$ granica:

$$E_{\vec{k}} = \frac{\hbar^2 k^2}{2m} \; ; \; q \to 0 \Rightarrow f(E_{\vec{k}+\vec{q}}) \simeq f(E_{\vec{k}}) + (E_{\vec{k}+\vec{q}} - E_{\vec{k}}) \left.\frac{df}{dE}\right|_{E=E_{\vec{k}}} + \ldots$$

$T=0$: $f(E) = \Theta(E_F - E)$: $\lim_{T\to 0} \frac{df}{dE} = -\delta(E - E_F)$

$$\left.\frac{df}{dE}\right|_{E=E_{\vec{k}}} = -\delta(E_{\vec{k}} - E_F)$$

a) Thomas-Fermi ($\omega = 0$):

$$\varepsilon_r(q) = 1 - \frac{e^2}{\varepsilon_0 q^2} \sum_{s,\vec{k}} \frac{f(E_{\vec{k}}) - f(E_{\vec{k}}) - (E_{\vec{k}+\vec{q}} - E_{\vec{k}})(-\delta(E_{\vec{k}} - E_F))}{E_{\vec{k}} - E_{\vec{k}+\vec{q}}} \quad (-1)$$

$$= 1 + \frac{e^2}{\varepsilon_0 q^2} \underbrace{\sum_{s,\vec{k}} \delta(E_{\vec{k}} - E_F)}_{= g_F}$$

(jer je $g(E) = \sum_\eta \delta(E - E_\eta)$ & $\delta(x) = \delta(-x)$)

$$= 1 + \frac{e^2 g_F}{\varepsilon_0 q^2}$$

$$= 1 + \frac{k_{TF}^2}{q^2} \; , \; k_{TF}^2 \equiv \frac{e^2 g_F}{\varepsilon_0}$$

b) granica plazme ($\omega \neq 0$)

$$E_{\vec{k}+\vec{q}} - E_{\vec{k}} = \frac{\hbar^2}{2m}\left((\vec{k}+\vec{q})^2 - k^2\right) = \frac{\hbar^2}{2m}\left(k^2 + 2\vec{k}\cdot\vec{q} + \cancel{q^2} - k^2\right) \quad (q^2 \ll)$$

$$\approx \frac{\hbar^2}{m}\vec{k}\cdot\vec{q} = \frac{\hbar^2}{m} kq\cos\vartheta$$

$$\varepsilon_r(\omega) = 1 - \frac{e^2}{\varepsilon_0 q^2}\sum_{s,\vec{k}} \frac{\delta(E_{\vec{k}} - E_F)(E_{\vec{k}+\vec{q}} - E_{\vec{k}})}{\hbar\omega + E_{\vec{k}} - E_{\vec{k}+\vec{q}}}$$

$$= 1 - \frac{e^2}{\varepsilon_0 q^2}\frac{2}{(2\pi)^3}\frac{\hbar^2}{m}\int d^3k \frac{\delta(E_{\vec{k}} - E_F)\, kq\cos\vartheta}{\hbar\omega - \frac{\hbar^2}{m}kq\cos\vartheta}$$

$$= 1 - \frac{e^2}{\varepsilon_0 q^2}\frac{2\hbar^2}{(2\pi)^3 m}\int_0^\infty \int_0^\pi \int_0^{2\pi} k^2 dk \sin\vartheta\, d\vartheta\, d\varphi \frac{\delta(E_k - E_F) kq\cos\vartheta}{\hbar\omega - \frac{\hbar^2}{m}kq\cos\vartheta}$$

$$\left\{ k = \frac{\sqrt{2mE}}{\hbar},\ dk = \frac{\sqrt{2m}}{2\hbar}\frac{dE}{\sqrt{E}}\ ;\ \sin\vartheta\, d\vartheta = -d(\underbrace{\cos\vartheta}_{\equiv x}) \right\}$$

$$= 1 - \frac{e^2}{\varepsilon_0 q^2}\frac{4m}{(2\pi)^2\hbar^2} q \int_0^\infty dE \int_{-1}^{1} dx \frac{E\,\delta(E - E_F)\, x}{\hbar\omega - \hbar\sqrt{\frac{2}{m}}q\sqrt{E}\,x}$$

$$= 1 - \frac{e^2}{\varepsilon_0 q^2}\frac{4m\,E_F}{(2\pi)^2\hbar^3}\sqrt{\frac{m}{2E_F}}\int_{-1}^{1} \frac{x\,dx}{\sqrt{\frac{m}{2E_F}}\frac{\omega}{q} - x}$$

$$\left\{ \int \frac{x\,dx}{ax+b} = \frac{x}{a} - \frac{b}{a^2}\ln(ax-b)\ ;\ a = -1,\ b = \sqrt{\frac{m}{2E_F}}\frac{\omega}{q} \right\}$$

$$= 1 - \frac{e^2}{\varepsilon_0 q^2}\frac{4m^{3/2}\sqrt{E_F}}{\sqrt{2}\hbar^3(2\pi)^2}\left[-x - \sqrt{\frac{m}{2E_F}}\frac{\omega}{q}\ln\left(-x + \sqrt{\frac{m}{2E_F}}\frac{\omega}{q}\right)\right]\Bigg|_{-1}^{1}$$

$$\left\{ -b\left[\ln(-1+b) - \ln(1+b)\right] = b\ln\frac{b+1}{b-1} \approx 2b\left(\frac{1}{b} + \underbrace{\frac{1}{3b^3}} + \cancel{\frac{1}{5b^5} + \ldots}\right) \right\}$$

$$= 1 - \frac{e^2}{\varepsilon_0 q^2} \frac{4m^{3/2}\sqrt{E_F}}{\sqrt{2}\hbar^3(2\pi)^2}\left[-2 + 2\sqrt{\frac{m}{2E_F}}\frac{\omega}{q}\frac{1}{\sqrt{\frac{m}{2E_F}}\frac{\omega}{q}} + \sqrt{\frac{m}{2E_F}}\frac{\omega}{q}\frac{2}{3}\frac{1}{\left(\frac{m}{2E_F}\right)^{3/2}\left(\frac{\omega}{q}\right)^3}\right]$$

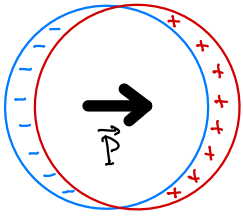
$$= 1 - \frac{e^2}{\varepsilon_0 \omega^2}\frac{2}{3}\underbrace{\frac{m\sqrt{2mE_F}}{\pi^2\hbar^3}}_{=g_F}\frac{E_F}{m} \quad ; \quad g_F = \frac{m\sqrt{2mE_F}}{\pi^2\hbar^3}$$

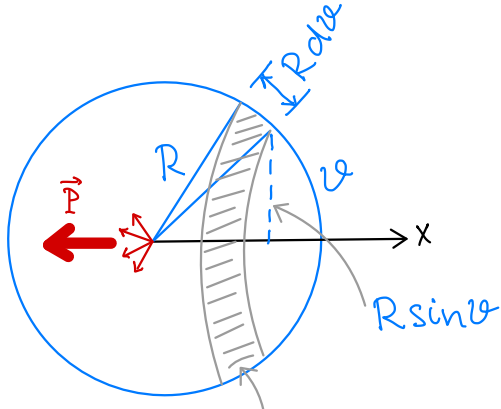
$$\& \quad g_F = \frac{3}{2}\frac{n}{E_F} \Rightarrow n = \frac{2}{3}g_F E_F$$

$$= 1 - \underbrace{\frac{e^2 n}{\varepsilon_0 m}}_{=\omega_p^2}\frac{1}{\omega^2}$$

$$= 1 - \frac{\omega_p^2}{\omega^2}$$

Z-8.3





površina prstena: $2\pi R\sin\vartheta \cdot R d\vartheta = 2\pi R^2 \sin\vartheta d\vartheta$

$$\varrho \sim \vec{\nabla}\cdot\vec{P} \longrightarrow \int_V \vec{\nabla}\cdot\vec{P}\,dV = \oint_S \vec{P}\cdot d\vec{S} \Rightarrow \sigma \sim P$$

polje:

$$E_x = \int_0^\pi \frac{P\cos\vartheta\, dS \cdot \cos\vartheta}{4\pi\varepsilon_0 R^2}$$

samo E_x projekcija je konačna, ostale E_y i E_z iščezavaju zbog simetrije

$$= \frac{P}{2\varepsilon_0}\underbrace{\int_0^\pi \cos^2\vartheta \sin\vartheta\, d\vartheta}_{-\frac{1}{3}\cos^3\vartheta\,|_0^\pi = \frac{2}{3}} = \frac{P}{3\varepsilon_0}, \quad E_y = E_z = 0$$

Z-8.4

a)

$$\alpha(\omega)\Big|_{\tilde{\omega}} = \frac{Q^2}{M_r}\frac{1}{\tilde{\omega}^2-\omega^2}$$

$$\vec{P} = n\alpha(\omega)\vec{E}\Big|_{\omega_T}$$

$$\vec{P}^* = \frac{n\alpha(\omega)}{1-\frac{n\alpha(\omega)}{3\varepsilon_0}}\vec{E}\Big|_{\omega_0}$$

$$\vec{P}\Big|_{\omega_T} = \vec{P}^*\Big|_{\omega_0}$$

$$n\frac{Q^2}{M_r}\frac{1}{\omega_T^2-\omega^2}\vec{E} = \frac{n\frac{Q^2}{M_r}\frac{1}{\omega_0^2-\omega^2}}{1-\frac{n}{3\varepsilon_0}\frac{Q^2}{M_r}\frac{1}{\omega_0^2-\omega^2}}\vec{E}$$

$$\frac{1}{\omega_T^2-\omega^2} = \frac{\frac{1}{\omega_0^2-\omega^2}}{\frac{\omega_0^2-\omega^2-\frac{nQ^2}{3\varepsilon_0 M_r}}{\omega_0^2-\omega^2}} \quad \Rightarrow \omega_T^2 = \omega_0^2 - \frac{nQ^2}{3\varepsilon_0 M_r}$$

b)

$$\varepsilon_r(\omega) = \varepsilon^{(\infty)} + \frac{\varepsilon^{(0)}-\varepsilon^{(\infty)}}{1-\frac{\omega^2}{\omega_T^2}} \quad ; \quad \varepsilon^{(0)} = \varepsilon^{(\infty)}\frac{\omega_L^2}{\omega_T^2} \quad \text{(LST)}$$

$$= \varepsilon^{(\infty)}\left[1+\frac{\omega_L^2-\omega_T^2}{\omega_T^2-\omega^2}\right]$$

$$= \varepsilon^{(\infty)}\frac{\omega_L^2-\omega^2}{\omega_T^2-\omega^2}$$

Z-8.5

$$\omega(k) = \frac{c}{\sqrt{\varepsilon_r(\omega)}}k \Big|^2 \quad , \quad \varepsilon_r(\omega) = \varepsilon^{(\infty)} + \frac{\varepsilon^{(0)} - \varepsilon^{(\infty)}}{1 - \frac{\omega^2}{\omega_T^2}}$$

$$\omega^2\left(\varepsilon^\infty + \omega_T^2 \frac{\varepsilon^0 - \varepsilon^\infty}{\omega_T^2 - \omega^2}\right) = c^2k^2$$

$$(\omega_T^2 - \omega^2)\omega^2\varepsilon^\infty + \omega^2\omega_T^2(\varepsilon^0 - \varepsilon^\infty) - c^2k^2(\omega_T^2 - \omega^2) = 0$$

$$\varepsilon^\infty\omega^4 - (\omega_T^2\varepsilon^0 + c^2k^2)\omega^2 + \omega_T^2c^2k^2 = 0$$

$$\omega_\pm^2(k) = \frac{1}{2\varepsilon^\infty}\left[\omega_T^2\varepsilon^0 + c^2k^2 \pm \sqrt{(\omega_T^2\varepsilon^0 + c^2k^2)^2 - 4\varepsilon^\infty\omega_T^2c^2k^2}\right]$$

(1) granica $k \to 0$

$$\omega_\pm^2(k\to 0) \simeq \frac{1}{2\varepsilon^\infty}\left[\omega_T^2\varepsilon^0 + c^2k^2 \pm \sqrt{\omega_T^4\varepsilon^{0^2} + 2\omega_T^2\varepsilon^0c^2k^2 + \cancel{c^4k^4} - 4\varepsilon^\infty\omega_T^2c^2k^2}\right]$$

$$= \frac{1}{2\varepsilon^\infty}\left[\omega_T^2\varepsilon^0 + c^2k^2 \pm \omega_T^2\varepsilon^0\sqrt{1 + 2\frac{\varepsilon^0 - 2\varepsilon^\infty}{2\varepsilon^0}\frac{c^2k^2}{\varepsilon^0\omega_T^2}}\right]$$

$$\hookrightarrow \sqrt{1+x^2} \approx 1 + \tfrac{1}{2}x^2$$

$$= \frac{1}{2\varepsilon^\infty}\left[\omega_T^2\varepsilon^0 \pm \omega_T^2\varepsilon^0 + c^2k^2\left(1 \pm \frac{\varepsilon^0 - 2\varepsilon^\infty}{\varepsilon^0}\right)\right]$$

LST

$$= \frac{1}{2}\left[\omega_L^2 \pm \omega_L^2 + \frac{c^2k^2}{\varepsilon^\infty}\left(1 \pm 1 \mp 2\frac{\omega_T^2}{\omega_L^2}\right)\right]$$

$$1 - 2\frac{\varepsilon^\infty}{\varepsilon^0} = 1 - 2\frac{\omega_T^2}{\omega_L^2} \quad \text{(LST)}$$

$$\frac{\varepsilon^0}{\varepsilon^\infty} = \frac{\omega_L^2}{\omega_T^2}$$

$$\omega_+^2(k\to 0) = \omega_L^2 + \frac{c^2k^2}{2\varepsilon^\infty}\left(2 - 2\frac{\omega_T^2}{\omega_L^2}\right) = \omega_L^2 + \left(1 - \frac{\omega_T^2}{\omega_L^2}\right)\frac{c^2}{\varepsilon^\infty}k^2$$

$$\omega_+(k\to 0) = \sqrt{\omega_L^2 + \left(1 - \frac{\omega_T^2}{\omega_L^2}\right)\frac{c^2}{\varepsilon^\infty}k^2} \quad ; \quad \omega_+(k=0) = \omega_L$$

$$\omega_-^2(k\to 0) = \frac{1}{2}\frac{c^2k^2}{\varepsilon^\infty}2\frac{\omega_T^2}{\omega_L^2} \underset{\text{LST}}{=\!=} \frac{c^2k^2}{\varepsilon^0}$$

$$\omega_-(k\to 0) = \frac{c}{\sqrt{\varepsilon^0}}k \quad ; \quad \omega_-(k=0) = 0$$

(2) granica $k \to \infty$

$$\omega_{\pm}^2(k\to 0) \approx \frac{1}{2\varepsilon^\infty}\left[\omega_T^2\varepsilon^0 + c^2k^2 \pm \sqrt{\omega_T^4\varepsilon^{0^2} + 2\omega_T^2\varepsilon^0 c^2k^2 + c^4k^4 - 4\varepsilon^\infty\omega_T^2c^2k^2}\right]$$

$$= \frac{1}{2\varepsilon^\infty}\left[\omega_T^2\varepsilon^0 + c^2k^2 \pm c^2k^2\sqrt{1 + 2(\varepsilon^0 - 2\varepsilon^\infty)\frac{\omega_T^2}{c^2k^2}}\right]$$

$$\hookrightarrow \sqrt{1+x^2} \approx 1 + \tfrac{1}{2}x^2$$

$$\approx \frac{1}{2\varepsilon^\infty}\left[\omega_T^2\varepsilon^0 + c^2k^2 \pm \left(c^2k^2 + (\varepsilon^0 - 2\varepsilon^\infty)\omega_T^2\right)\right]$$

(LST)

$$\frac{\varepsilon^0}{\varepsilon^\infty} = \frac{\omega_L^2}{\omega_T^2}$$

LST ↓

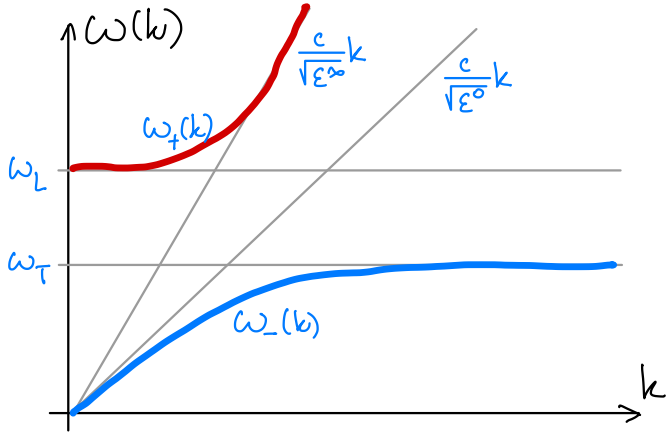
$$= \frac{1}{2}\left[\omega_L^2 \mp \left(2 - \frac{\varepsilon^0}{\varepsilon^\infty}\right)\omega_T^2 + \frac{1}{\varepsilon^\infty}\left(c^2k^2 \pm c^2k^2\right)\right]$$

$$\omega_+^2(k\to\infty) \approx \frac{c^2}{\varepsilon^\infty}k^2$$

$$\omega_+(k\to\infty) \approx \frac{c}{\sqrt{\varepsilon^\infty}}k$$

$$\omega_-^2(k\to\infty) = \frac{1}{2}\left[\omega_L^2 + 2\omega_T^2 - \underbrace{\frac{\varepsilon^0}{\varepsilon^\infty}\omega_T^2}_{=\omega_L^2}\right] = \omega_T^2$$

$$\omega_-(k\to\infty) = \omega_T$$



Z-8.6

$$\ddot{x} + \gamma\dot{x} + \omega_0^2 x = -\frac{e}{m}E_0 e^{-i\omega t}$$

↳ tjerani oscilator → rješenje: $x(t) = Ae^{-i\omega t}$

uvrstimo $x(t)$ u jednadžbu gibanja:

$$A\left[-\omega^2 - i\omega\gamma + \omega_0^2\right] = -\frac{e}{m}E_0 \Rightarrow A = -\frac{eE_0}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

Pomak elektrona stvara dipolni moment: $p = -ex$

$$p = \frac{e^2 E_0}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}e^{-i\omega t} = \frac{e^2}{m}\frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega}E$$

polarizacija: $P = np$

$$P = \frac{ne^2}{m(\omega_0^2 - \omega^2 - i\gamma\omega)}E$$

dielektrični pomak: $\vec{D} = \varepsilon\vec{E}$ $(\varepsilon = \varepsilon_0\varepsilon_r)$

$$\left.\begin{aligned}(1)\quad \vec{D} &= \varepsilon_0\vec{E} + \vec{P}\\ (2)\quad \vec{D} &= \varepsilon_0\varepsilon_r\vec{E}\end{aligned}\right\} \Rightarrow \vec{D} = \varepsilon_0\vec{E} + \frac{ne^2}{m(\omega_0^2 - \omega^2 - i\gamma\omega)}\vec{E}$$

$$= \varepsilon_0\underbrace{\left[1 + \frac{ne^2}{\varepsilon_0 m(\omega_0^2 - \omega^2 - i\gamma\omega)}\right]}_{=\varepsilon_r(\omega)}\vec{E}$$

$$\underline{\varepsilon_r(\omega) = 1 + \frac{ne^2}{\varepsilon_0 m(\omega_0^2 - \omega^2 - i\gamma\omega)}}$$

Z-8.7

$$n(\omega) = \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2 - \omega^2}}\,, \qquad \omega_p^2 = \frac{n e^2}{\varepsilon_0 m}$$

$\omega_{at} \sim 10^{16}\,\mathrm{Hz}$, $\omega_p \sim \omega_{at}$; $\omega_{at}, \omega_p \gg \omega$

$$n(\omega) = \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2\left(1 - \frac{\omega^2}{\omega_{at}^2}\right)}} \approx \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2}\left(1 + \frac{\omega^2}{\omega_{at}^2}\right)}$$

$(1-x)^{-1} \simeq 1 + x\,,\ x \ll 1$

$$= \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2}} \cdot \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^4\left(1 + \frac{\omega_p^2}{\omega_{at}^2}\right)}\omega^2} \approx$$

$\sqrt{1+x} \simeq 1 + \frac{1}{2}x\,,\ x \ll 1$

$$\approx \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2}}\left[1 + \frac{1}{2}\,\frac{1}{1 + \frac{\omega_p^2}{\omega_{at}^2}}\,\frac{\omega_p^2}{\omega_{at}^4}\omega^2\right]$$

$\omega = 2\pi\frac{c}{\lambda}$

$\Downarrow$

$$n(\lambda) = \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2}} + \frac{1}{2}\,\frac{1}{\sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2}}}\,\frac{\omega_p^2}{\omega_{at}^4}\,\frac{4\pi^2 c^2}{\lambda^2}$$

def:

$$n_0 \equiv \sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2}}$$

$$\lambda_0 \equiv 2\pi^2 c^2 \frac{\omega_p^2}{\omega_{at}^4}\,\frac{1}{\sqrt{1 + \frac{\omega_p^2}{\omega_{at}^2}}}$$

$$n(\lambda) = n_0 + \left(\frac{\lambda_0}{\lambda}\right)^2$$ Cauchyeva formula

IX. MAGNETSKA SVOJSTVA TVARI

Z-9.1

$$\chi_d = -\frac{N_A e^2 \mu_0}{6m} \sum_i \overline{r_i^2}$$, i - suma po atomskim ljuskama:

vodikov atom → 1 elektron

u s-ljusci: $\sum_i \overline{r_i^2} \to \langle r^2 \rangle_s \equiv \overline{r^2}$;

$$\chi_d = -\frac{N_A e^2 \mu_0}{6m} \overline{r^2}$$

$$\overline{r^2} = \int \psi_s^*(\vec{r})\, r^2\, \psi_s(\vec{r})\, \underbrace{d^3r}_{\uparrow\, r^2 dr \sin\vartheta d\vartheta d\varphi}$$, $\psi_s(\vec{r}) = \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}$

s-ljuska $\psi_s(\vec{r})$ je sferno simetrična

pa je $\int \sin\vartheta\, d\vartheta d\varphi = 4\pi$

$$= 4\pi \int_0^\infty \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} r^2 \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} r^2 dr$$

$$= \frac{4}{a_0^3} \int_0^\infty r^4 e^{-\frac{2r}{a_0}} dr = \left\{ \begin{array}{l} \text{supst.} \\ x = \frac{2r}{a_0} \to r = \frac{a_0}{2} x,\ dr = \frac{a_0}{2} dx \end{array} \right\}$$

$$= \frac{4}{a_0^3} \frac{a_0^5}{32} \underbrace{\int_0^\infty x^4 e^{-x} dx}_{=4!} = 3a_0^2$$

$$\chi_d = -\frac{N_A e^2 \mu_0}{6m} 3a_0^2$$

$$= -\frac{N_A e^2 \mu_0}{6m} \frac{\varepsilon_0^2 h^4}{\pi^2 m^2 e^4}$$

$$= -\frac{N_A \mu_0 \varepsilon_0^2 h^4}{2\pi^2 m^3 e^2} = -2.99 \cdot 10^{-11}\ \mathrm{m^3/mol}$$

Z-9.2

pretp. $\vec{B} \parallel \hat{z}$

particijska funkcija: $Z = \sum_i e^{-\beta E_i}$, $E_i = -\mu_i B$, $\beta \equiv \frac{1}{k_B T}$

$$Z = \sum_i e^{\beta \mu_i B}$$

magnetizacija: $M = n \bar{\mu}_z$

$$\bar{\mu}_z = \frac{\sum_i \mu_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} \; ; \quad \sum_i e^{-\beta E_i} = Z$$

$$(*) \quad \sum_i \mu_i e^{-\beta E_i} = \sum_i \mu_i e^{\beta \mu_i B} = \frac{1}{\beta} \frac{\partial}{\partial B} \overbrace{\sum_i e^{\beta \mu_i B}}^{=Z}$$

$$\bar{\mu}_z = \frac{1}{Z} \frac{1}{\beta} \frac{\partial}{\partial B} Z \; ; \quad [*] \; \frac{1}{y(x)} \frac{\partial y(x)}{\partial x} = \frac{\partial}{\partial x} \ln y(x)$$

$$= \frac{1}{\beta} \frac{\partial}{\partial B} \ln Z$$

s druge strane: $F = -n k_B T \ln Z$

$$\Rightarrow \ln Z = -\frac{F}{n k_B T}$$

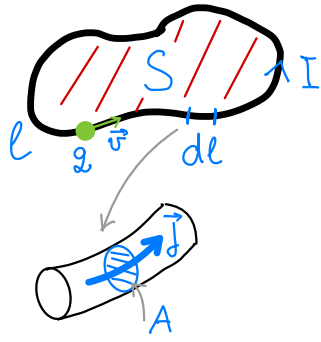
$$M = n \bar{\mu}_z$$

$$= n \frac{1}{\beta} \frac{\partial}{\partial B} (-1) \frac{F}{n k_B T}$$

$$= -\frac{\partial F}{\partial B}$$

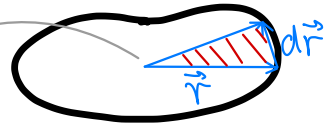
Z-9.3

$\mu = I \cdot S$, I - struja kroz petlju
S - površina petlje
ℓ - duljina petlje



def: $\lambda = \frac{q}{\ell}$ - linearna gustoća struje

$I = qv = \lambda \ell v$ (↳ $= jA$) $\Big\} \lambda \ell v = jA$



$d\vec{\mu} = \lambda \ell v \, d\vec{S}$; $d\vec{S} = \frac{1}{2}\vec{r} \times d\vec{r}$

$= \frac{1}{2} \underbrace{\lambda \ell v}_{jA} \vec{r} \times d\vec{r}$

$= \frac{1}{2}\vec{r} \times \vec{j}\, dV$

$d\vec{r} \parallel \vec{v} \parallel \vec{j}$

$j A \, d\vec{r} = j \hat{r} \underbrace{A\, dr}_{dV} = \vec{j}\, dV$

$\vec{\mu} = \frac{1}{2} \int \vec{r} \times \vec{j}\, dV$

Za točkasti naboj q, koji se giba po petlji ℓ, možemo pisati:

$\vec{j}(\vec{r},t) = q\vec{v}(t)\,\delta(\vec{r} - \vec{r}(t))$; $\int \vec{j}(\vec{r},t)\, d^3r = q\vec{v}(t)$

$\vec{\mu} = \frac{1}{2}\int \vec{r} \times \vec{j}\, d^3r \overset{\downarrow}{=}$

$= \frac{q}{2}\int \vec{r} \times \vec{v}(t)\,\delta(\vec{r} - \vec{r}(t))\, d^3r$

$= \frac{q}{2}\vec{r}(t) \times \vec{v}(t) \cdot \frac{m}{m}$

$= \frac{q}{2m}\vec{r} \times (\underbrace{m\vec{v}}_{\vec{p}})$

$= \frac{q}{2m}\vec{L}$

Z-9.4

$$Z = \sum_i e^{-\beta E_i} \overset{E_i = -\mu_i B,\ \mu_i \in \{-\mu, 0, \mu\}}{=} e^{-\beta\mu B} + 1 + e^{\beta\mu B}, \quad \beta = \frac{1}{k_B T}$$

$$F = -nk_BT \ln Z = -\frac{n}{\beta} \ln\left(e^{-\beta\mu B} + 1 + e^{\beta\mu B}\right)$$

$$M = -\frac{\partial F}{\partial B} = \frac{n}{\beta} \frac{-\beta\mu e^{-\beta\mu B} + \beta\mu e^{\beta\mu B}}{e^{-\beta\mu B} + 1 + e^{\beta\mu B}}$$

$$= n\mu \frac{e^{-\beta\mu B} - e^{\beta\mu B}}{1 + e^{-\beta\mu B} + e^{\beta\mu B}}$$

Za $\mu B \ll k_B T \rightarrow \beta\mu B \ll 1$: $e^{\pm\beta\mu B} \simeq 1 \pm \beta\mu B$

$$M = n\mu \frac{1 + \beta\mu B - 1 + \beta\mu B}{1 + 1 - \beta\mu B + 1 + \beta\mu B} = \frac{2}{3} n\mu^2 \beta B = \frac{2}{3} \frac{n\mu^2}{k_B T} B$$

$$\chi = \frac{M}{H} \underset{B = \mu_0 H}{=} \frac{2}{3} \frac{n\mu_0\mu^2}{k_B T}$$

napomena:

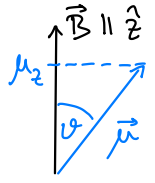
Uočiti da se radi o slučaju „kvantnog paramagnetizma s:

$2j+1 = 3$ tj. $j = 1$ ($l = j = 1$, $s = 0$)

kada je: $g = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} = 1$, $p \equiv g\sqrt{j(j+1)} = \sqrt{2}$

$$\Rightarrow \chi_p \overset{\mu = \mu_B}{=} \frac{n\mu_0 p^2 \mu_B}{3k_B T} = \frac{2}{3} \frac{n\mu_0\mu_B^2}{k_B T}$$ ✓

Z-9.5



$$M = n\overline{\mu_z} = n\mu\langle\cos\vartheta\rangle$$

$$\overline{\mu_z} = \frac{\int \mu\cos\vartheta\, e^{-\beta E_i}\, d^3r}{\int e^{-\beta E_i}\, d^3r}$$

$$E_i = -\vec{\mu}\cdot\vec{B} = -\mu B\cos\vartheta$$

$\{$ supst. $x = \cos\vartheta \}$ ↓

$$\overline{\mu_z} = \mu\, \frac{\int_0^{\bar{r}} r^2 dr \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\vartheta d\vartheta\, \cos\vartheta\, e^{\beta\mu B\cos\vartheta}}{\int_0^{\bar{r}} r^2 dr \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\vartheta d\vartheta\, e^{\beta\mu B\cos\vartheta}} =$$

$$= \mu\, \frac{\int_{-1}^{1} x\, e^{\beta\mu B x}\, dx}{\int_{-1}^{1} e^{\beta\mu B x}\, dx} = \mu\, \frac{\int_{-1}^{1} x\, e^{ax}\, dx}{\int_{-1}^{1} e^{ax}\, dx}$$

$a \equiv \beta\mu B$

$$= \begin{cases} \text{parcijalno int.} \\ u = x\ ;\ du = dx \\ dv = e^{ax}dx\ ; \\ v = \frac{1}{a}e^{ax} \end{cases}$$

$$= \mu\, \frac{\frac{1}{a}x\, e^{ax}\Big|_{-1}^{1} - \frac{1}{a}\int_{-1}^{1} e^{ax}dx}{\int_{-1}^{1} e^{ax}dx} = \mu\left[\frac{\frac{1}{a}(e^{a}+e^{-a})}{\frac{1}{a}(e^{a}+e^{-a})} - \frac{1}{a}\right] =$$

$$= \mu\left(\operatorname{cth} a - \frac{1}{a}\right)$$

⇓

$$M = n\mu L(a)\ ;\ L(a) \equiv \operatorname{cth} a - \frac{1}{a},\ a \equiv \frac{\mu B}{k_B T}$$

$2a\, k_B T \gg \mu B$ $(a \ll 1)$: $\operatorname{cth} a \simeq \frac{1}{a} + \frac{a}{3} - \frac{a^3}{45} + \dots$

$$M \approx n\mu\left(\frac{1}{a} + \frac{a}{3} - \frac{1}{a}\right) = \frac{1}{3}n\mu a$$

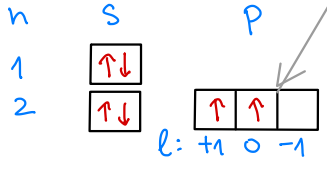
prvi neiščezavajući član

$$\chi = \frac{M}{H} = \frac{n\mu_0\mu^2}{3k_B T}$$

Z-9.6

Koristimo Hundova pravila: (1) s - poprima max. vrijednost u skladu s P.P.; (2) l - poprima max. vrijednost konzistentnu s (1); (3) za ljusku manje od polupopunjenu je j=|l-s|, a za ljusku više od polupopunjene je j=|l+s|.

a) C^6 : $[He]\,2s^2\,2p^2$ — djelomično popunjena!



$S = \frac{1}{2} + \frac{1}{2} = 1$

$l = 1\cdot(+1) + 1\cdot 0 + 0\cdot(-1) = 1$

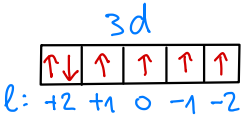
$n = 2$ – popunjenje

$N_p = 6$ – max. popunjenje p

$n = 2 < \frac{N_p}{2} = 3 \Rightarrow j = |l - s|$

$j = |1 - 1| = 0$

b) Fe^{26} : $[Ar]\,3d^6\,4s^2$



$S = 5\cdot\frac{1}{2} + 1\cdot\left(-\frac{1}{2}\right) = 2$

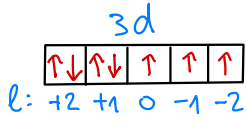
$l = 2\cdot(+2) + 1\cdot(+1) + 1\cdot 0 + 1\cdot(-1) + 1(-2) = 2$

$n = 6$, $N_d = 10$

$n = 6 > \frac{N_d}{2} = 5 \Rightarrow j = |l + s|$

$j = |2 + 2| = 4$

c) Co^{27} : $[Ar]\,3d^7\,4s^2$



$S = 5\cdot\frac{1}{2} + 2\cdot\left(-\frac{1}{2}\right) = \frac{3}{2}$

$l = 2\cdot(+2) + 2\cdot(+1) + 1\cdot 0 + 1\cdot(-1) + 1(-2) = 3$

$n = 7$, $N_d = 10$

$n = 7 > \frac{N_d}{2} = 5 \Rightarrow j = |l + s|$

$j = |3 + \frac{3}{2}| = \frac{9}{2}$

Z-9.7

$$H \simeq \frac{e}{2m}\left(\vec{L}+2\vec{S}\right) + \alpha \vec{L}\cdot\vec{S}$$

napomena:

$$H_1 = -\vec{\mu}\cdot\vec{B} = -\frac{-e}{2m}\left(g_L\vec{L}+g_S\vec{S}\right) = \frac{e}{m}\left(\vec{L}+2\vec{S}\right)$$

$$H_2 = -\vec{\mu}\cdot\vec{B}_{eff} = \frac{e}{m}\vec{S}\cdot\vec{B}_{eff} \equiv \alpha\vec{L}\cdot\vec{S}$$

a) Za B<<, L-S član dominira fizikom angularnog momenta - uzrokuje precesiju L i S vektora oko vektora J. Problem možemo aproksimativno riješiti tako da prvo projiciramo vektore L i S na J, a potom na os kvantizacije određenu poljem B.

$$\left(\vec{L}+2\vec{S}\right)_{\substack{L\text{-}S\\ \text{precesija}}} = L_{\parallel\vec{J}}\hat{J} + 2S_{\parallel\vec{J}}\hat{J} = \frac{\vec{L}\cdot\vec{J}}{J^2}\vec{J} + 2\frac{\vec{S}\cdot\vec{J}}{J^2}\vec{J};$$

$\vec{L}\cdot\vec{J} = ?$ & $\vec{S}\cdot\vec{J} = ?$

$\vec{J} = \vec{L}+\vec{S}$

1) $\vec{S} = \vec{J}-\vec{L}\ \big|^2$

$S^2 = J^2 + L^2 - 2\vec{J}\cdot\vec{L}$

$\Rightarrow \vec{J}\cdot\vec{L} = \frac{1}{2}\left(J^2+L^2-S^2\right)$

2) $\vec{L} = \vec{J}-\vec{S}\ \big|^2$

$L^2 = J^2+S^2-2\vec{J}\cdot\vec{S}$

$\Rightarrow \vec{J}\cdot\vec{S} = \frac{1}{2}\left(J^2+S^2-L^2\right)$

$$H \simeq \frac{e}{2m}\left(\frac{J^2+L^2-S^2}{2J^2}\vec{J} + 2\frac{J^2+S^2-L^2}{2J^2}\vec{J}\right)\cdot\vec{B}$$

$$= \frac{e}{2m}\frac{1}{2J^2}\underbrace{\left(J^2+L^2-S^2+2J^2+2S^2-2L^2\right)}_{3J^2-L^2+S^2}\underbrace{\vec{J}\cdot\vec{B}}_{J_z B}\cdot\frac{\hbar}{\hbar}$$

$$= \frac{e\hbar}{2m}\left(1 + \frac{J^2+L^2-S^2}{2J^2}\right)\frac{J_z}{\hbar}B$$

$$= \mu_B\left(1 + \frac{J^2+L^2-S^2}{2J^2}\right)j_z B$$

stanja: J^2 je dobar kvantni broj; $|J| = \hbar\sqrt{j(j+1)}$ itd.

$$J^2|J, J_z\rangle = \hbar^2 j(j+1)|J, J_z\rangle$$

energija: ZEEMANOV EFEKT

$$E = \langle J, J_z|H|J, J_z\rangle = \mu_B\left(1 + \underbrace{\frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)}}_{= g_j \text{ LANDEOV FAKTOR}}\right)j_z B$$

b) Za B>>, L-S član je praktično zanemariv. L i S vektori evoluiraju svaki zasebno i direktno se projiciraju na os kvantizacije određenu poljem B.

$$H \simeq \frac{e}{2m}(\vec{L} + 2\vec{S})\cdot\vec{B} = \frac{e}{2m}(L_z + 2S_z)B \cdot \frac{\hbar}{\hbar} = \mu_B(l_z + 2s_z)B$$

L, L_z, S, S_z su dobri kvantni brojevi: $L_z|\vec{L}, L_z\rangle = \hbar l_z|\vec{L}, L_z\rangle$

$S_z|\vec{S}, S_z\rangle = \hbar S_z|\vec{S}, S_z\rangle$

energija: PASCHEN-BACHOV EFEKT

$$E = \langle H\rangle = \mu_B(l_z + 2s_z)B$$

Z-9.8

$$M = n\mu_B \operatorname{th}\frac{\mu_B(B+\mu_0\lambda M)}{k_BT}$$

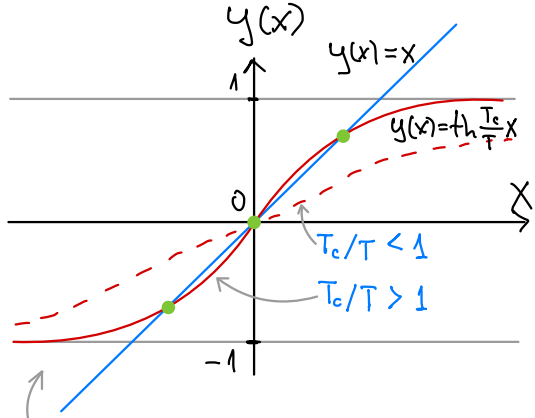
a) spontana magnetizacija : $B=0$

$$M = n\mu_B \operatorname{th}\frac{\mu_B\mu_0\lambda M}{k_BT}$$

$$\underbrace{\frac{M}{n\mu_B}}_{\equiv X} = \operatorname{th}\left[\underbrace{\frac{\mu_B^2\mu_0\lambda}{k_BT}}_{\equiv T_c/T}\underbrace{\frac{M}{n\mu_B}}_{\equiv X}\right]$$

$$X = \operatorname{th}\left[\frac{T_c}{T}X\right] \quad (*)$$

↑ Transcedentna jednadžba (rješava se numerički ili grafički).



Rješenja s $X \neq 0 \Rightarrow M \neq 0$ (spontana magnetizacija) nalazimo za $T_c/T > 1$ tj. $T < T_c \equiv \frac{\mu_B^2\mu_0\lambda}{k_B}$.

b) u granici $T \to T_c$ razvijamo $\operatorname{th}(x) \simeq x - \frac{1}{3}x^3$

$$(*) \Rightarrow X = \frac{T_c}{T}X - \frac{1}{3}\left(\frac{T_c}{T}X\right)^3 \;\Big|\; :X\neq 0 \;(T<T_c)\;;\; \text{za } T>T_c : X=0 \;(M=0)$$

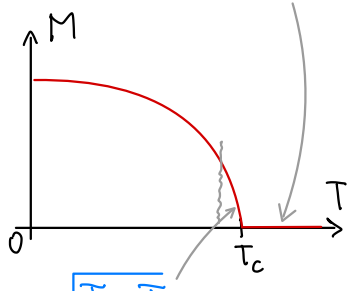
$$\frac{1}{3}\frac{T_c^3}{T^3}X^2 = \left(\frac{T_c}{T}-1\right)\Big|\cdot T$$

$$X^2 = 3\frac{T^2}{T_c^3}(T_c-T) \underset{T\to T_c}{\approx} 3\frac{1}{T_c}(T_c-T)$$

$$X = \frac{\sqrt{3}}{\sqrt{T_c}}\sqrt{T_c-T} \quad ;\; (M = n\mu_B X)$$

$$M = n\mu_B\frac{\sqrt{3}}{\sqrt{T_c}}\sqrt{T_c-T} = \frac{\sqrt{3}\,n\sqrt{k_B}}{\sqrt{\lambda}}\sqrt{T_c-T} \sim \sqrt{T_c-T}$$

$$T_c = \frac{\mu_B^2\mu_0\lambda}{k_B}$$



c) u granici $k_B T \gg \mu_B (B + \mu_0 \lambda M) \Rightarrow \text{th}\, x \simeq x$

$$M = n\mu_B \frac{\mu_B (B + \mu_0 \lambda M)}{k_B T} = \frac{n\mu_B^2 B}{k_B T} + \frac{n\mu_0 \mu_B^2 \lambda}{k_B T} M \qquad T_c$$

$$\left(1 - \frac{T_c}{T}\right) M = \frac{n\mu_B^2 B}{k_B T} \Rightarrow M \simeq \frac{n\mu_B^2 B}{k_B (T - T_c)}$$

$$\chi_p \simeq \frac{M}{H} \simeq \frac{n\mu_B^2 \mu_0}{k_B (T - T_c)} \equiv \frac{C}{T - T_c} \quad \text{(Curie-Weiss)}$$

Z-9.9

$$E_\uparrow(k) = E(k) - \mu_B B \qquad \vec{B} \uparrow \uparrow$$
$$E_\downarrow(k) = E(k) + \mu_B B \qquad \vec{B} \uparrow \downarrow$$
$$, \quad E(k) = \frac{\hbar^2 k^2}{2m}$$

$$M = \mu_B (n_\uparrow - n_\downarrow)$$
$$= \mu_B \int_0^\infty \underbrace{\frac{1}{2} g(E)}_{\text{po polu gustoće stanja za spin} \uparrow \text{ i} \downarrow;\ g(E) = \frac{m\sqrt{2mE}}{\pi^2 \hbar^3}} \left[f(E - \mu_B B) - f(E + \mu_B B) \right] dE$$

za $\mu_B B \ll E_F$: $f(E \pm \mu_B B) \approx f(E) \pm \mu_B B \left.\frac{df}{dE}\right|_{E \text{ u blizini } E_F}$

$$M = \mu_B \int_0^\infty \frac{1}{2} g(E) \left[\cancel{f(E)} - \mu_B B \frac{df}{dE} - \cancel{f(E)} - \mu_B B \frac{df}{dE} \right] dE$$
$$= -\mu_B^2 B \int_0^\infty g(E) \frac{df}{dE} dE$$

$T = 0$: $f(E) = \Theta(E_F - E) \Rightarrow \frac{df}{dE} = -\delta(E - E_F)$

$$M_{T=0} = \mu_B^2 B \int_0^\infty g(E) \delta(E - E_F) = \mu_B^2 g_F B$$

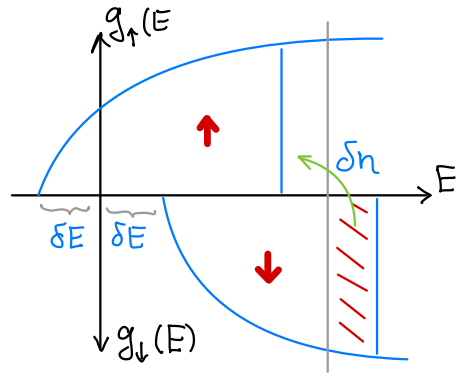
$$\chi_p = \frac{M}{H} = \mu_0 \mu_B^2 g_F$$

Z-9.10

$$H = \frac{p^2}{2m} - g_s \mu_B \vec{S}\cdot\vec{B} + U n_\uparrow n_\downarrow$$

$$M_{T=0} = -\frac{\partial(\Delta E)}{\partial B}$$

$$\Delta E = \Delta E_{KIN} + \Delta E_{MAG} + \Delta E_{INT}$$



δn – broj elektrona koji zbog mag. polja + interakcije promijene spin („spin-flip")

δE – promjena energije zbog redistribucije elektrona mag. poljem i interakcijom („spin-flip") koju treba odrediti optimizacijom totalne energije

gustoća stanja: $g_s(E \approx E_F) \approx \frac{g_F}{2}$

$$\delta n = \frac{g_F}{2}\delta E$$

$$\Delta E_{KIN} = \delta E \cdot \delta n = \frac{g_F}{2}(\delta E)^2$$

$$\Delta E_{MAG} = -\mu_B B \cdot 2\delta n = -\mu_B B g_F \delta E$$

$$\Delta E_{INT} = E_{INT} - E_{INT}^{(0)} = U\left[\left(\frac{N}{2}+\delta n\right)\left(\frac{N}{2}-\delta n\right) - \frac{N}{2}\cdot\frac{N}{2}\right]$$

$$= -U(\delta n)^2 = -\frac{1}{4}U g_F^2 (\delta E)^2$$

$$\Delta E = \frac{g_F}{2}(\delta E)^2 - \mu_B B g_F \delta E - \frac{1}{4}U g_F^2 (\delta E)^2$$

$$\frac{\partial(\Delta E)}{\partial(\delta E)} = 0 \quad \Rightarrow g_F \delta E - \mu_B g_F B - \frac{1}{2}U g_F^2 \delta E = 0$$

$$\Rightarrow \delta E = \frac{\mu_B B}{1 - \frac{U g_F}{2}}$$: uvrstimo u izraz za ΔE

$$\Delta E = \frac{g_F}{2}\frac{\mu_B B}{\left(1-\frac{U g_F}{2}\right)^2} - \mu_B g_F B \frac{\mu_B B}{1-\frac{U g_F}{2}} - \frac{1}{4}\frac{U g_F^2 \mu_B^2 B^2}{\left(1-\frac{U g_F}{2}\right)^2}$$

$$= \frac{1}{4}\frac{g_F \mu_B^2 B^2}{\left(1-\frac{U g_F}{2}\right)^2}\left[2 - 4\left(1-\frac{U g_F}{2}\right) - U g_F\right]$$

$$= -\frac{1}{2}\frac{g_F \mu_B^2}{1-\frac{U g_F}{2}} B^2$$

$$M_{T=0} = -\frac{\partial(\Delta E)}{\partial B} = \frac{g_F \mu_B^2}{1-\frac{U g_F}{2}} B$$

$$\chi = \frac{M}{H} = \frac{g_F \mu_0 \mu_B^2}{1-\frac{U g_F}{2}} \Rightarrow \text{uvjet spontane magnetizacije:}$$

$$1 - \frac{U g_F}{2} = 0 \quad \text{(Stonerov kriterij)}$$