Líkan Drudes af málmum

Rafeindagas í jóna-kristalli

Z: gildisrafeindir losna frá hverju atómi

$Z_a - Z$ eru fastar

↑ leiðnirafeindir

Þéttleiki rafeinda

$$n = \frac{N}{V} = N_A \left[mol^{-1}\right] \frac{Z \rho_m \left[g/cm^3\right]}{A \left[g/mol\right]}$$

$$\frac{1}{n} = \frac{4\pi r_s^3}{3} \rightsquigarrow r_s = \left(\frac{3}{4\pi n}\right)^{1/3}$$

$$a_0 = \frac{\hbar^2}{me^2}$$ Bohr geisli

fyrir málma $r_s/a_0 \sim 2-5$

1000 × þéttleiki gass

Samt

① Frjálsar rafeindir, engin víxlverkun!

② Árekstrar við jónir, ekki við rafeindir

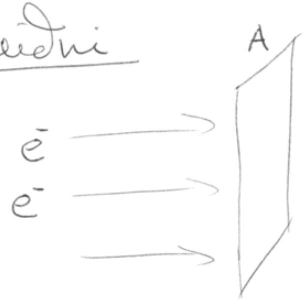
③ Á tímanum dt eru líkur á árekstri dt/τ

τ: slökunartími, meðal tími milli árekstra

④ Staðbundið varmajafnvægi, stefna rafeinda eftir árekstur er slembistærð hraðinn er háð hita

---

DC-leiðni



$$Q = -n(\vec{v}dt)Ae$$

$$\hat{=} \frac{dQ}{dt}\frac{1}{A} = \boxed{\vec{j} = -ne\vec{v}}$$

án ytra sviðs er $\langle \vec{v} \rangle = 0$

með ytra sviði
klukkan t eftir
síðasti árekstur
var við t = 0

$$\langle \vec{v} \rangle = \langle \vec{v}_0 - \frac{e\vec{E}t}{m} \rangle$$

$$= -\frac{e\vec{E}}{m}\langle t \rangle$$

$$= -\frac{e\vec{E}}{m}\tau$$

→ $\vec{j} = \sigma \vec{E}$ með $\sigma = \frac{ne^2\tau}{m}$

Ohms lögmál

σ má mæla ~~til~~ að finna $\tau \sim 10^{-14} - 10^{-15}$ s

meðal fjarlægð á milli árekstra

Herbergis hita

$l = v_0 \tau$: $\frac{1}{2} m v_0^2 = \frac{3}{2} k_B T$ $v_0 \sim 10^7$ cm/s

→ $l \sim 1 - 10$ Å

↑

styður árekstra við jónir

Nými sýni ~~með~~ við $k_B T \sim 0$ $l \sim \mu$, mm, cm

Hreyfijafna rafeinda

meðal skriðþungi

$$\vec{p}(t+dt) = \left(1 - \frac{dt}{\tau}\right)\left(\vec{p}(t)\right) + \vec{f}(t)dt + O(dt)^2 \}$$

↑

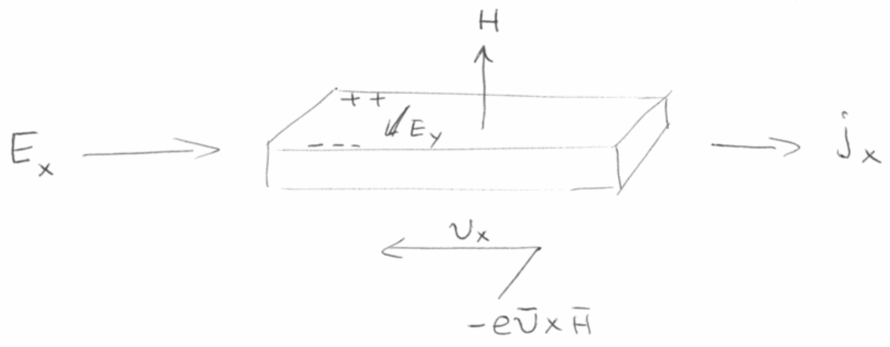
verða ekki fyrir árekstri

$$\rightarrow \frac{d\vec{p}(t)}{dt} = -\frac{\vec{p}(t)}{\tau} + \vec{f}(t)$$

↑

viðnámsliður

Segulviðnám, Hallhrif



Lorentz $\vec{F} = -e(\vec{E} + \bar{v} \times \bar{H}/c)$

Hallsviðið E_y verkar á móti Lorentz kr.

Segulviðnám: $\rho(H) = \frac{E_x}{j_x}$

Hall stuðull $R_H = \frac{E_y}{j_x H}$

gefur formerki bera hleðslu

$$\frac{d\vec{p}}{dt} = -e\left(\vec{E} + \frac{\vec{p}}{mc}\times\vec{H}\right) - \frac{\vec{p}}{\tau}$$

stöðugt ástand $\omega_c \equiv \frac{eH}{mc}$

$$0 = -eE_x - \omega_c p_y - \frac{p_x}{\tau}$$

$$0 = -eE_y + \omega_c p_x - \frac{p_y}{\tau}$$

$$\rightarrow \quad \sigma_0 E_x = \omega_c\tau j_y + j_x$$

$$\sigma_0 E_y = -\omega_c\tau j_x + j_y \qquad \sigma_0 = \frac{ne^2\tau}{m}$$

$$j_y = 0 \rightarrow E_y = -\left(\frac{\omega_c\tau}{\sigma_0}\right) j_x$$

$$= -\left(\frac{H}{nec}\right) j_x \rightarrow R_H = -\frac{1}{nec}$$

einungis háð n -> mæling á R_H
segir til um gæði litans

Háð H almennt
Lágt T eða of sterkt H $\Big\}$ $R_H \rightarrow -\frac{1}{nec}$
hrein sýni

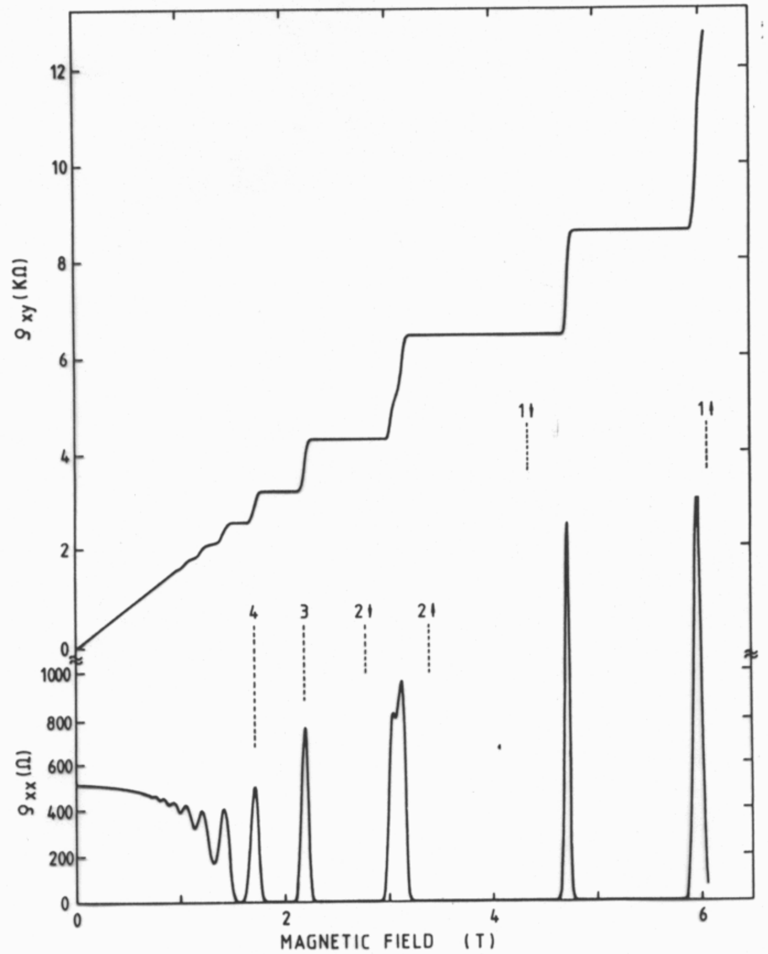


Fig. 14. Experimental curves for the Hall resistance $R_H = \varrho_{xy}$ and the resistivity $\varrho_{xx} \sim R_x$ of a heterostructure as a function of the magnetic field at a fixed carrier density corresponding to a gate voltage $V_g = 0V$. The temperature is about 8mK.

This analysis is based on the equation

$$\frac{1}{C} = \frac{1}{e^2 \cdot D\,(E_F)} + \text{const.} \tag{19}$$

The combination of the different methods for the determination of the DOS leads to a result as shown in Fig. (20). Similar results are obtained from other experiments, too [33, 34] but no theoretical explanation is available.

If one assumes that only the occupation of extended states influences the Hall effect, than the slope $d\varrho_{xy}/dn_s$ in the plateau region should be dominated ground state to the fully spin-polarized ground state at $\nu = \frac{8}{5}$. These exp rimental results lend support to a series of theoretical predictions about tl spin-reversed ground state and excitations [4.23-27] and will be discussed detail in in Sect. 9.4. Finally, following a theoretical prediction about tl possibility of observing the FQHE with *even* denominator fractions in mu tilayer systems [4.28,29], such observations were actually made in a doub layer system [4.30] and will be discussed in Sect. 9.5.

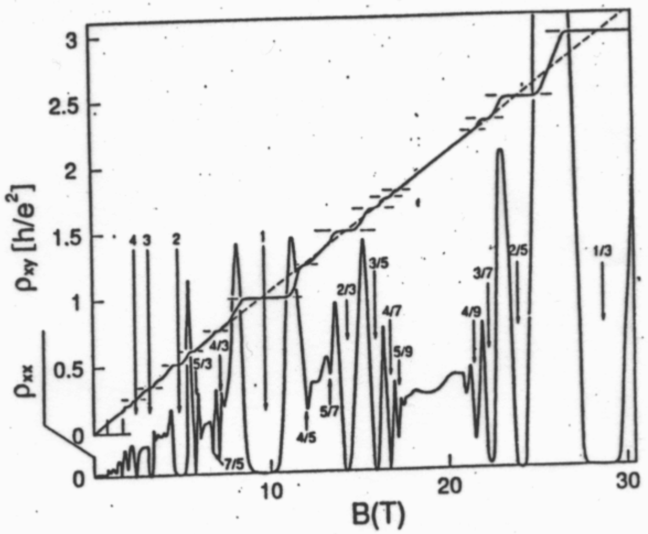


Fig. 4.2. Overview of the observed fractions in the FQHE measurements [4.5]. T Landau level filling factor ν has been defined in the text

In explaining the FQHE, a system of noninteracting electrons is, h wever, inadequate. According to our present understanding of the FQH electron correlations play a major role in this effect, and there have be a variety of theoretical attempts to understand this unique many-electr phenomenon. In the following chapters, we have attempted to survey mc of these theoretical approaches, and have tried to present in detail the cu rent state of our understanding of this fascinating effect.

As the fractional Hall steps are observable only in samples of very hi mobility, impurity potentials are not expected to be very important in coı

---

⑥

AC-leiðni

$$\vec{E}(t) = Re\left(\bar{E}(\omega)e^{-i\omega t}\right)$$

Hreyfijafnan er

$$d_t\vec{p} = -\frac{\vec{p}}{\tau} - e\vec{E}$$

leitað er lausna (stöðugsástands) á forminu

$$\vec{p}(t) = Re(\vec{p}(\omega)e^{-i\omega t})$$

athugum

$$-i\omega\vec{p}(\omega) = -\frac{\vec{p}(\omega)}{\tau} - e\vec{E}(\omega)$$

$$\vec{p}(\omega)\left\{1 - i\omega\tau\right\} = -e\tau\vec{E}(\omega)$$

notum $j = -ne\vec{p}/m$

$$\vec{j}(\omega)\left\{1 - i\omega\tau\right\} = \frac{ne^2\tau}{m}\vec{E}(\omega) = \sigma_0\vec{E}(\omega)$$

$$\vec{j}(\omega) = \sigma(\omega)\vec{E}(\omega), \quad \sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

$\tau\omega >> 1$ $\qquad \sigma_0 = \frac{ne^2\tau}{m}$

$$\epsilon(\omega) = 1 - \frac{4\pi\sigma_0}{\omega^2\tau}$$

$$= 1 - \frac{\left(\frac{4\pi n e^2}{m}\right)}{\omega^2} = 1 - \frac{\omega_p^2}{\omega^2}$$

ef $\omega < \omega_p$ $\to \epsilon \in \mathbb{R}$ $\quad \epsilon < 0$

lausnir (*) dofna

breytist fyrir $\omega = \omega_p$

lausnir sem dofna ekki

málm verður gegnsær

Hverjar eru afleiðingar $\sigma(\omega)$?

Plasma bylgjur (rafgas bylgjur)
gegnsæi málma

Langbylgju nálgun $\boxed{\lambda >> l}$

Maxwells jöfnur

$$\vec\nabla\cdot\vec E = 0, \quad \vec\nabla\cdot\vec H = 0, \quad \vec\nabla\times\vec E = -\frac{1}{c}\partial_t\vec H$$

$$\vec\nabla\times\vec H = \frac{4\pi}{c}\vec j + \frac{1}{c}\partial_t\vec E$$

~~notum~~ leitum lausna með tímaþátt $e^{-i\omega t}$
og notum $\vec j(\omega) = \sigma(\omega)\vec E$

$$\to -\nabla^2\vec E(\omega) = \frac{\omega^2}{c^2}\underbrace{\left(1 + \frac{4\pi i\sigma(\omega)}{\omega}\right)}_{=\epsilon(\omega)}\vec E(\omega) \qquad (*)$$

$$\epsilon(\omega) = 1 + \frac{4\pi i\sigma}{\omega} = 1 + \frac{4\pi i}{\omega}\frac{\sigma_0}{1 - i\omega\tau}$$

athugum mjög háa tíðni $\omega\tau >> 1$

Hitaleiðni

Einangrar -> slæm hitaleiðni

málmar -> góð hitaleiðni

$\downarrow$ Drude

hitaleiðni er vegna leiðni rafeinda

$$\vec{j}^q = -\underset{\substack{\uparrow \\ \text{varmaleiðni}}}{K}\vec{\nabla}T$$

Wiedemann-Franz reglan

$\frac{K}{\sigma T}$ er fasti fyrir marga málma

reynslulögmál

Drude $K = \frac{1}{3}v^2\tau c_v = \frac{1}{3}l v c_v$

með $\left(\frac{dE}{dT}\right)\frac{1}{V} = c_v$ eðlisvarmi rafeinda

---

$$\frac{K}{\sigma} = \frac{\frac{1}{3}c_v m v^2}{ne^2}$$

sígilt gas -> $\frac{K}{\sigma T} = \frac{3}{2}\left(\frac{k_B}{e}\right)^2$

helmingur þess sem mælist

En $(c_v)_{class} = 100\,(c_v)_{ska}$

$(v^2)_{class} = \frac{1}{100}\,(v^2)_{ska}$

við herbergishita

En Ohm reglan, plasma tíðnin benda til þess ~~að~~ víxlverkun rafeindanna sé hverfandi

$\updownarrow$

hvernig getur ~~það~~ verið með þéttleika sem er mjög hár og sterka Coulomb víxlverkun

Sommerfeld líkanið

① Fermi dreifing fyrir leiðni rafeindir.

② Engin víxlverkun milli rafeinda.

③ Jónir → Einsleitur jákvæður bakgr.

④ Skammtafræði, hálfklassískt.

Grunnástand kerfis (T=0)

Hver rafeind hreyfist samkvæmt

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\bar{r}) = \varepsilon\psi(\bar{r})$$

þeim er raðað á orkustig samkvæmt Fermi dreif.

Viljum losna við yfirborðsáhrif, tökum $V \to \infty$. Notum Born-von Karman

$$\psi(\bar{r}+\bar{R}) = \psi(\bar{r})$$

$$\bar{R} = nL\hat{x} + mL\hat{y} + lL\hat{z}$$

Lausn jöfnunnar er

$$\psi_{\bar{k}}(\bar{r}) = \frac{1}{\sqrt{V}}e^{i\bar{k}\cdot\bar{r}}$$

$$\varepsilon(\bar{k}) = \frac{\hbar^2k^2}{2m}$$

$\psi_{\bar{k}}$ er eiginfall skriðþungavirkjans $\vec{p} = -i\hbar\vec{\nabla}$ með eiging. $\vec{p} = \hbar\vec{k}$

$$\vec{v} = \frac{\vec{p}}{m} \quad \text{og} \quad \lambda = \frac{2\pi}{|\vec{k}|}$$

Jaðarskilyrðin gefa

$$\boxed{e^{ik_iL} = 1} \rightarrow \boxed{k_i = \frac{2\pi n_i}{L}}$$

$V \to \infty$ þ.a. bilið á milli k-gilda $\frac{2\pi}{L}$ sé mjög smátt m.v. stærð k-rúmsins sem er setin Ω

(mikill fjöldi rafeinda)

fjöldi k-gilda $= \frac{\Omega}{(2\pi/L)^3}$

þéttni punkta í k-rúminu er $\frac{V}{8\pi^3}$

* * *

Ω : kúlulaga með geisla k_F

$$\to N = \left(\frac{4\pi k_F^3}{3}\right)\left(\frac{V}{8\pi^3}\right) = \frac{k_F^3}{6\pi^2} V$$

↑ fjöldi ástanda

Tvær spuna stefnur →

fjöldi rafeinda $N = \frac{k_F^3}{3\pi^2} V$

→ þéttleiki rafeinda

$$\boxed{n = \frac{k_F^3}{3\pi^2}}$$

Fermi kúla
yfirborð
Skriðþungi $p_F = \hbar k_F$
hraði $v_F = p_F/m$

Athugið vel (2.22) – (2.26)

* * *

Athugum meðalorku

heildar: $E = 2\sum_{k<k_F} \frac{\hbar^2}{2m} k^2$

breytum summu í heildi $V \to \infty$

$$\Delta\vec{k} = \frac{8\pi^3}{V}$$

$$\sum_{\vec{k}} F(\vec{k}) = \frac{V}{8\pi^3}\sum_{\vec{k}} F(\vec{k})\,\Delta\vec{k}$$

$$\to \boxed{\lim_{V\to\infty} \frac{1}{V}\sum_{\vec{k}} F(\vec{k}) = \int \frac{d\vec{k}}{(2\pi)^3} F(\vec{k})}$$

og

$$\frac{E}{V} = \frac{2}{(2\pi)^3}\int_{k<k_F} d\vec{k}\, \frac{\hbar^2 k^2}{2m} = \frac{1}{\pi^2}\frac{\hbar^2 k_F^5}{10m}$$

$$\frac{E/V}{N/V} = \frac{E/V}{n} = \frac{3}{5}\varepsilon_F = \frac{E}{N}$$

↑

mjög stórt m.v. $\left(\frac{E}{N}\right)_{\text{Klass}} = \frac{3}{2}k_BT$

þ. $T \to 0$

Skilgreinum Fermi hita stig

$$T_F k_B = \varepsilon_F$$

$$\to \boxed{T_F = \frac{58.2}{(r_s/a_0)^2}\cdot 10^4\ \text{K}}$$

Rafeindagas málma er Kulgas (degenerate)

Athugum við $T \neq 0$

$$f(\varepsilon_i) = \frac{1}{e^{(\varepsilon_i-\mu)/k_BT}+1}$$

$$2\int \frac{d\vec{k}}{(2\pi)^3} F(\varepsilon(\vec{k})) = 2\cdot 4\pi \int_0^\infty \frac{k^2 dk}{(2\pi)^3} F(\varepsilon(k))$$

$$= \int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon)\, F(\varepsilon)$$

með $g(\varepsilon) = \theta(\varepsilon)\frac{m}{(h\pi)^2}\sqrt{\frac{2m\varepsilon}{\hbar^2}}$

ástanda þéttleikanum

$$g(\varepsilon)d\varepsilon = \frac{\text{fjöldi ástanda milli } \varepsilon \text{ og } \varepsilon + d\varepsilon}{V}$$

$$\boxed{g(\varepsilon_F) = \frac{3}{2}\frac{n}{\varepsilon_F}}$$

Kynna sér vel Sommerfeld nálgunina á bls 45-47 til að reikna

$$\int_{-\infty}^{\infty} H(\varepsilon) f(\varepsilon) d\varepsilon = \int_{-\infty}^{\mu} H(\varepsilon) f(\varepsilon) d\varepsilon + \frac{\pi^2}{6}(k_BT)^2 H'(\mu) + \cdots$$

μ : efnamætti

$$\lim_{T\to 0} \mu = \varepsilon_F$$

$$C_v = \left(\frac{\partial u}{\partial T}\right)_V \quad \text{með} \quad u = \frac{U}{V}$$

þ.s. U er innri orkan

$$U = 2\sum_{\vec{k}} \varepsilon(\vec{k}) f(\varepsilon(\vec{k}))$$

$$\to 2\int \frac{d\vec{k}}{(2\pi)^3} \varepsilon(\vec{k}) f(\varepsilon(\vec{k}))$$

Og efnamættið μ er ákvarðað af

$$n = 2\int \frac{d\vec{k}}{(2\pi)^3} f(\varepsilon(\vec{k}))$$

Heildi þessarar tegundar má leysa með skilgreiningu á ástandaþéttleika

$\varepsilon(\vec{k})$ er fall af $|\vec{k}|$

Með henni finnst

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

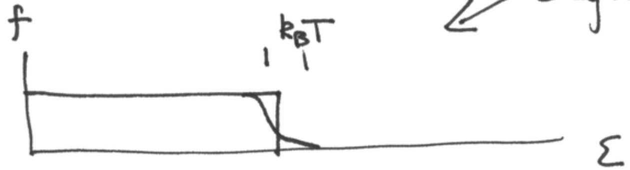
$$U = U_0 + \frac{\pi^2}{6}(k_B T)^2 g(\varepsilon_F)$$

$T=0$

$$\to C_v = \left(\frac{\partial u}{\partial T}\right)_n = \frac{\pi^2}{2}\left(\frac{k_B T}{\varepsilon_F}\right) n k_B$$

Samanborið við $(C_v)_{klass} = 3nk_B/2$

mjög smátt fyrir $T < 300$ K fyrir málma



Skýra hversvegna

Fyrir kristall fast

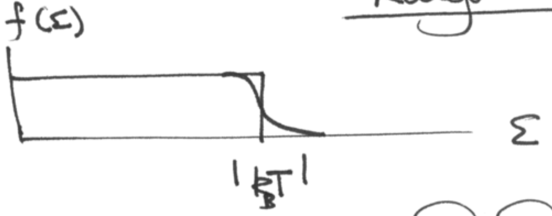
$$C_v = \gamma T + AT^3$$

rafeindir grind

Leiðni þarf flutningslíkan

fyrir hvaða orku geta árekstrar gerst

kulgas



upptaks og laus ástönd verða að vera til

fjöleindafr. með víxlverkun getur (einsleitt)

$$\langle \varepsilon_{kin} \rangle \simeq \frac{2.21}{(r_s/a_0)^2}$$

$$\langle \varepsilon_{pot} \rangle \sim -\frac{0.916}{(r_s/a_0)} + 0.0622\ln\left(\frac{r_s}{a_0}\right) - 0.096 + \mathcal{O}(r_s/a_0)$$

$n \uparrow$

$r_s \downarrow$

$\rightarrow \langle \varepsilon_{kin} \rangle > \langle \varepsilon_{pot} \rangle$ þ. n vex

---

lesa 3 kafla sjálf

Áhrif kristallagrindar

Kristallsgrindur

Hvers vegna? (afltr. rof. grind., nykur.)

Bravais grindur

jónir
atóm
sameind...

① óendanleg grind, þar sem umhverfi allra punkta er eins.

② 3D Bravais grind er mengi allra punkta með stöðuvigur

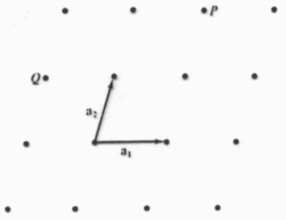
$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

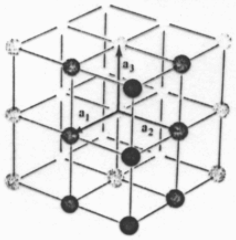
$$n_i \in \mathbb{Z}$$

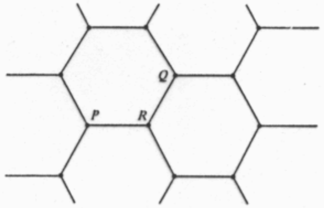
a_i : grunnvigrar grindarinnar

SC [redacted]

ekki B.g.







↑ margir mögulegir grunnvigrar

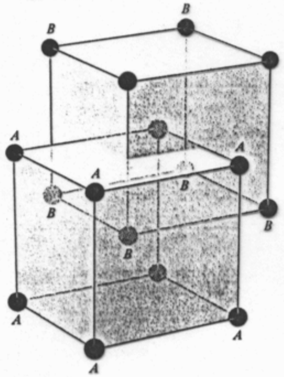
Einkristall, fjölkristall

(endanlegur, óendanlegur)

Dæmi

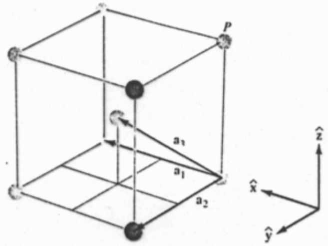
BCC – Body Center Cubic

A ~~eða~~ B í miðju?

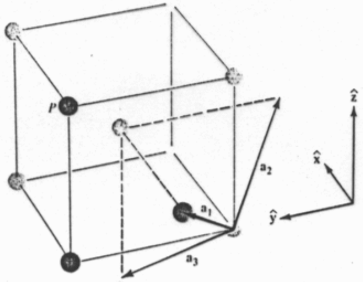


Tvær framsetn.

Ba
Cr
Cs
Fe
K
Li
Mo
Na
⋮

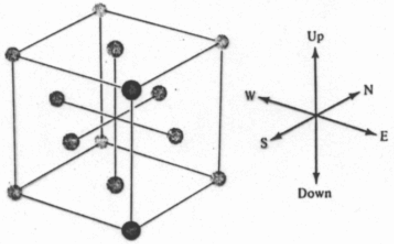


$$\vec{a}_1 = a\hat{x}$$
$$\vec{a}_2 = a\hat{y}$$
$$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$$

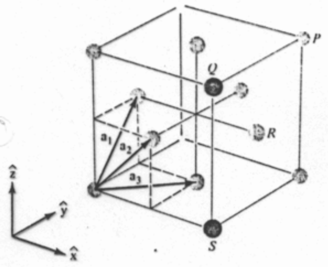


$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}-\hat{x})$$
$$\vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x}-\hat{y})$$
$$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z})$$

FCC - Face Center Cubic



Ar, Ag, Al, Au, Ca, Ce, β-Co, Cu, Ir, Kr, La, Ne, Ni, Pb, Pd, Pr....



$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y})$$

Coordination number

fjöldi næstu granna

SC:	6
BCC:	8
FCC:	12

Frum kristallseiningin (Primitive Unit Cell)

Rúmmál sem hliðrað um alla vigra Bravaisgrindar fyllir allt rúmið án skörunar eða gata er

Frum kristallseiningin

Dæmi

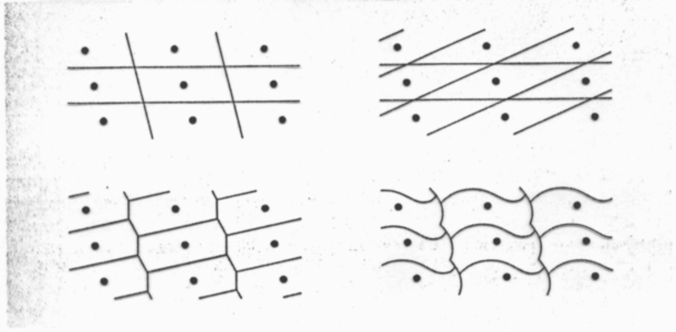
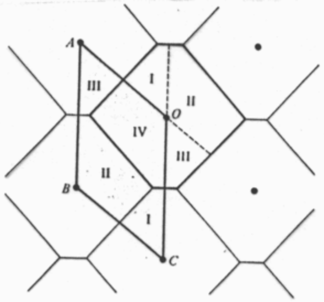


Figure 4.10
Several possible choices of primitive cell for a single two-dimensional Bravais lattice.

Einn grindarpunktur í hverri einingu

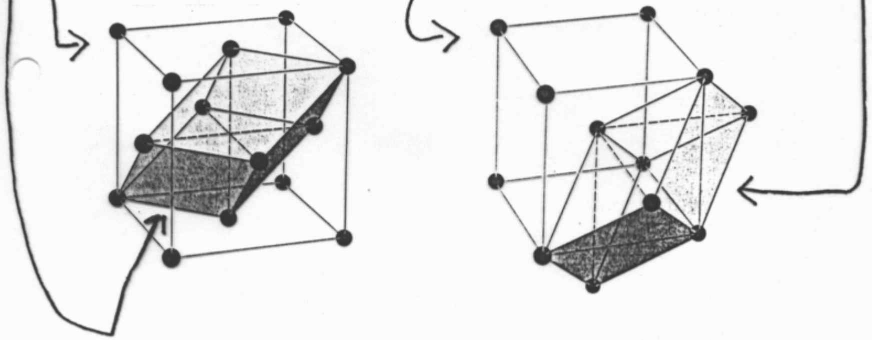


Tvær mögulegar grunneiningar

← búta má hliðra til um grunnvigra

Frum grindareining

Venjuleg grindareining



Frum grindareiningin hefur ekki endilega samhverfu grindareiningar

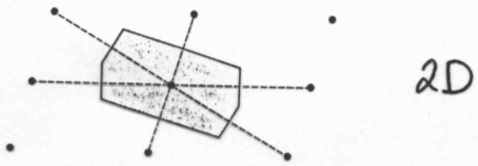
Venjuleg grindareining er stærri

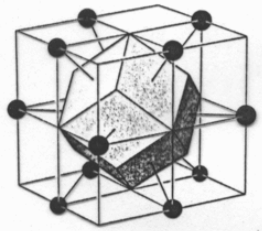
nv = 1

Grindareining með fulla samhverfu grindarinnar

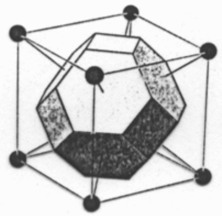
↓

Wigner-Seitz frumeiningin



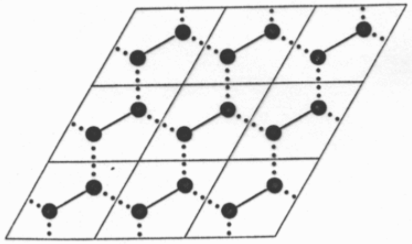


FCC



BCC

Grind með Grunni (basis)

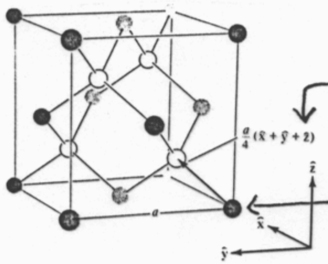


Sameindir: t.d. C_{60}
Einnig til þæginda
t.d. fyrir FCC eða BCC

Dæmi um grindur með grunni

Demantsbygging

Demantur er ekki Bravais grind
En t.d. FCC með grunni
→ tveir punktar $\vec{0}$, $\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$



C
Si
Ge
α-Sn

Zincblende

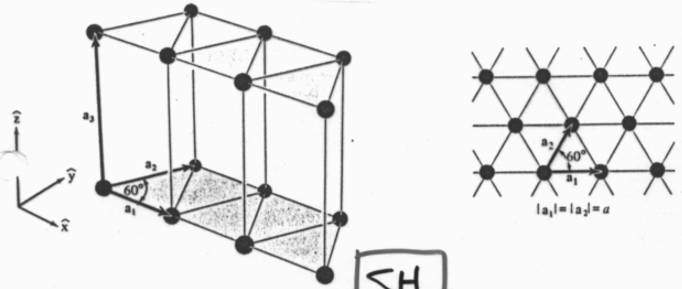
CuF
CuCl
GaAs
InAs
SiC
CdTe
HgTe
AlAs

↑ þá er dekktu punktarnir ein atóm tegund og hinir önnur tegund.

Hexagonal Close-Packed | HCP

Ekki Bravais grind

Be
Mg
Ti
Zn



SH

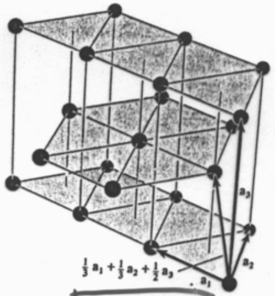
Figure 4.19
The simple hexagonal Bravais lattice. Two-dimensional triangular nets (shown in inset) are stacked directly above one another, a distance *c* apart.

SH

$\vec{a}_1 = a\hat{x}$

$\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}$

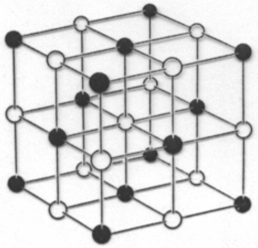
$\vec{a}_3 = c\hat{z}$



HCP

Aðrir þétt pökkunar möguleikar eru til

Natríum-Klór-bygging



FCC með grunni

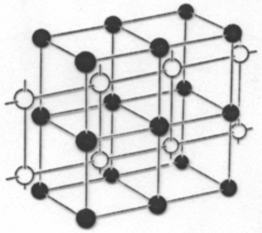
$\vec{0}$: Na

$\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$: Cl

NaCl
LiF
KCl
KF

↑(SC ef einatóma)

Cesín-Klór-bygging



SC með grunni

$\vec{0}$: Ce

$\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$: Cl

↑(BCC ef einatóma)

Nykurgrind

Lotubundin kristallur →

aflfræði kristallsins og rafeindanna er best lýst í „nykurrúminu"

⋮

Skilgreining

Bravaisgrind: mengi punkta með stöðuvigur $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

$n_i \in \mathbb{Z}$ og a_i : eru grunnvigrar....

Vigar~~nir~~ $\vec{K}$ sem uppfylla

$$e^{i\vec{K}\cdot\vec{R}} = 1$$

skilgreina nykurgrind Bravaisgrindarinnar

Nykurgrindin er einnig Bravais grind

②

Önnur skilgr

Bravais grind með frumvigra $\vec{a}_1, \vec{a}_2$ og $\vec{a}_3$ þá er nykurgrindin spönnuð af 3 frumvigrum

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

Sannreynum

Greinilega gildir $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$

$\vec{b}_i$ – geta ekki verið allir í sömu sléttu

því getur hver vigur $\bar{k}$ verið ritaður

$$\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$$

---

③

og $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

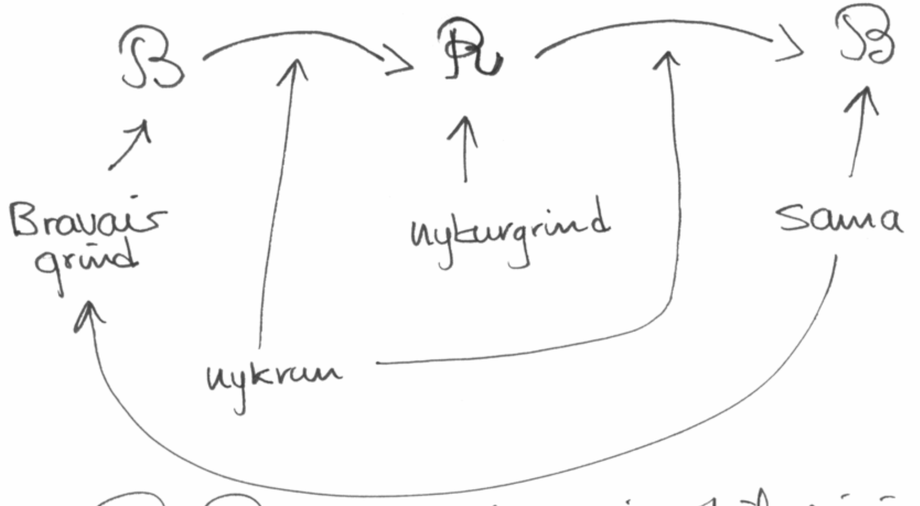
$\rightarrow \vec{k}\cdot\vec{R} = 2\pi(k_1n_1 + k_2n_2 + k_3n_3)$

Ef k_i eru heilar tölur þá gildir

$$e^{i\vec{k}\cdot\vec{R}} = 1$$

$\rightarrow$ $\vec{k}$ er nykurgrindarvigur ef $k_i \in \mathbb{Z}$

$\rightarrow$ $\vec{b}_i$ eru frumvigrar ~~Brava~~ nykurgrindarinnar



Sama með annarri hvorri skilgreiningunni

Dæmi

SC: $\vec{a}_i$ öll hornrétt

↓ önnur skilgreining

$\vec{b}_i$ öll hornrétt

↳ $\mathcal{R}$ er SC

$$\begin{array}{l} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \\ \vec{a}_3 = a\hat{z} \end{array} \longrightarrow \begin{array}{l} \vec{b}_1 = \frac{2\pi}{a}\hat{x} \\ \vec{b}_2 = \frac{2\pi}{a}\hat{y} \\ \vec{b}_3 = \frac{2\pi}{a}\hat{z} \end{array}$$

Venjuleg grindareining

Venjuleg grindarein.

FCC ⟷ BCC

↑

nykrum

Rúmmál

v rúmmál frum Bravais gr.

→ rúmmál frumeiningar

$\mathcal{R}$ er $\frac{(2\pi)^3}{v}$

Fyrsta Brillouin svæðið

Síðar sjáum við hin BS og mikilvægi þeirra.

er Wigner-Seitz frumeining nykurgrindarinnar

Kristalls plön

(innihalda alla punkta $\mathcal{B}$)

Athugum fyrst aðra skilgreiningu á nikurgrindarvigrum

Mengi allra bylgjuvigra $\vec{K}$ sem gefa sléttar bylgjur með lotu $\mathcal{B}$ er ~~kallað~~ nykurgrind $\mathcal{R}$ fyrir $\mathcal{B}$

$$\boxed{e^{i\vec{K}\cdot(\bar{r}+\bar{R})} = e^{i\vec{K}\cdot\bar{r}}}$$

(héðan kemur skilgr. m. $e^{i\vec{K}\cdot\vec{R}} = 1$)

Fyrir
Sérhverja fjölskylda kristallssléttna með bil d eru til nykurvigrar hornréttir á sléttunnar og sá styttsti ~~B~~ er með lengdina $2\pi/d$

eða

Fyrir sérhvern nykurvigur $\vec{K}$ er til fjölsk. kristallssléttna hornrétta á $\vec{K}$ og með bil d þ.a. lengd stysta nykurvigursins samhliða $\vec{K}$ er $2\pi/d$

tengist en lesa sjálf sannanir

Miller vísar fyrir kristallasléttur

Vegna tengingar nykurvigra við kristalls-sléttur er hægt að merkja þær með stysta nikurvigrinum hornréttum á sléttuna. Ef

$$\vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

þá eru Millervísar sléttunnar $\underline{h, k, l}$

: 4 engin sameiginlegur þáttur

Miller vísarnir eru háðir vali á frum(nykur)vigrunum

"Önnur aðferð

Kristalls~~grind~~ slétta með h, k, l er hornrétt á $\vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

→ sléttan liggur í samfelldu sléttunni skilgr. m. $\vec{k}\cdot\vec{r} = A$ = fasti

⑧

sléttan sker ásana $\vec{a}_1, \vec{a}_2, \vec{a}_3$ í
punktunum $x_1\vec{a}_1$, $x_2\vec{a}_2$, $x_3\vec{a}_3$

þ.s. x_i eru ákveðin m. $\vec{k}\cdot(x_i\vec{a}_i) = A$

en $\vec{k}\cdot\vec{a}_1 = 2\pi h$, $\vec{k}\cdot\vec{a}_2 = 2\pi k$, $\vec{k}\cdot\vec{a}_3 = 2\pi l$

$$\rightarrow x_1 = \frac{A}{2\pi h}, \quad x_2 = \frac{A}{2\pi k}, \quad x_3 = \frac{A}{2\pi l}$$

því er hægt að skilgreina vísana

$$\underbrace{h:k:l}_{} = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$$

$\not\equiv$

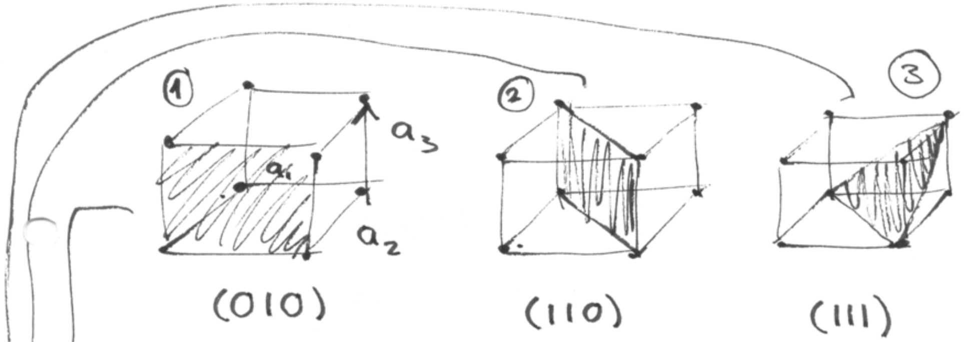
heilar tölur með engan
sameiginlegan þátt.

vísir með $-n \rightarrow \bar{n}$

(100) (010) (001) slétturnar í tenings...
eru jafngildar og merktar með $\{100\}$

⑨

Áttirnar [100] [010] [001] [$\bar{1}$00] [0$\bar{1}$0]
og [00$\bar{1}$] í tenings... eru allar
jafngildar og merktar með <100>



$\vec{a}_1 = (a,0,0)$ $\qquad$ $\vec{b}_1 = \frac{2\pi}{a}(1,0,0)$

$\vec{a}_2 = (0,a,0)$ $\qquad$ $\vec{b}_2 = \frac{2\pi}{a}(0,1,0)$

$\vec{a}_3 = (0,0,a)$ $\qquad$ $\vec{b}_3 = \frac{2\pi}{a}(0,0,1)$

þver nykurvigur $\vec{b}_2 \rightarrow (010)$

$\vec{b}_1 + \vec{b}_2 \rightarrow (110)$

$\vec{b}_1 + \vec{b}_2 + \vec{b}_3 \rightarrow (111)$

Skurðp. xa

① $\frac{1}{\infty} : \frac{1}{1} : \frac{1}{\infty} \rightarrow (010)$

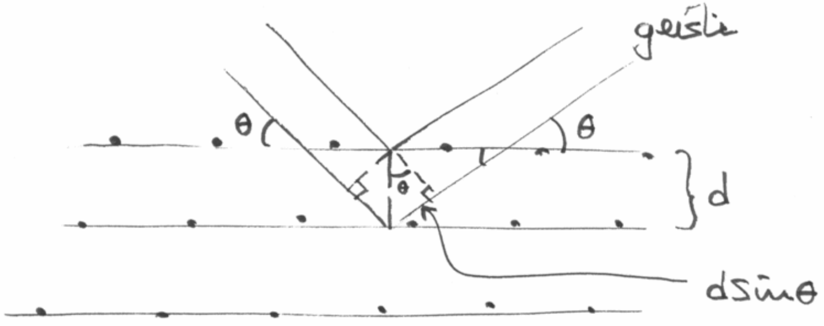
② $\frac{1}{1} : \frac{1}{1} : \frac{1}{\infty} \rightarrow (110)$

③ $\frac{1}{1} : \frac{1}{1} : \frac{1}{1} \rightarrow (111)$

Röngtengreining kristalla

Bragg

toppar í styrkleik spegl~~aðs~~ geisla
af kristalli háðir λ og (θ,φ)



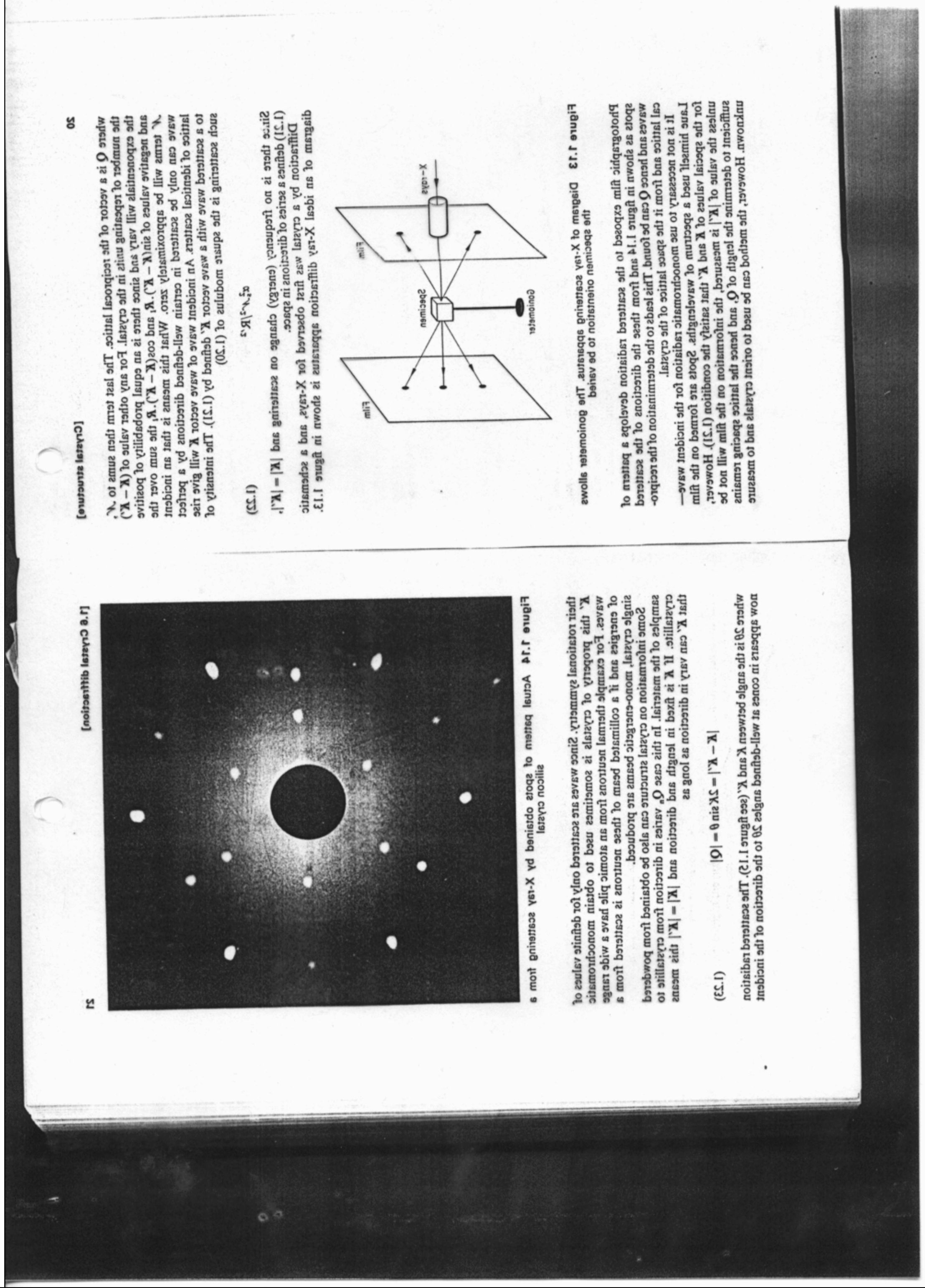
Bylgjueiginleikar röngtengeislans

→ Styrkjandi bylgjuvíxl þegar

$$n\lambda = 2d\sin\theta$$

Stig speglunar

margir toppar ← fjöldi mism.-sléttna

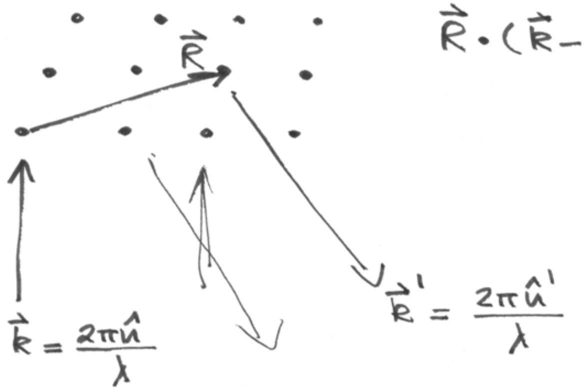


Von Laue

Engin kristallaplön notuð

* Gert ráð fyrir að atóm á Bravais grind geti endurkastað geislum í allar áttir

Styrkjandi víxl möguleg



$$\vec{R}\cdot(\vec{k}-\vec{k}') = 2\pi m$$

fyrir $m \in \mathbb{Z}$
og öll $\vec{R} \in \mathfrak{B}$

þetta er skiljanlegt frá dreifingu bylgna

mjög nærri lagi, en!

Sama bylgjulengd ⇔ fjaðrandi!

jafngildir $\exp\left\{i(\vec{k}-\vec{k}')\cdot\vec{R}\right\} = 1$

Bera saman við skilgreiningu á $\mathfrak{R}$

→ von Laue skilyrðin fyrir styrkjandi víxlun

$$\boxed{\begin{array}{l}\text{breyting bylgjuvigursins}\\ \qquad \vec{K} \equiv \vec{k}' - \vec{k}\\ \text{er vigur} \in \mathfrak{R}\end{array}}$$

lesa sjálf um túlkun röntgentilrauna á kristöllum bls. 101 – 104

Dreifing bylgna vegna einatóma grindar með grunni

; rúmfr. byggingarstuðullinn

Innan grindareiningar eru dreifimiðjur með stöðuvigra $\vec{d}_1 \ldots \vec{d}_n$ sem gefa mism. víxlun

Geislinn sem dreifist frá frumgrindar einingunni fær líkindavísi með þáttinn

$$S_{\vec{K}} = \sum_{j=1}^{n} e^{i\vec{K}\cdot\vec{d}_j}$$

↗

byggingarstuðull ∠ rúmfræðilegur

Segir hve mikið víxl frá grunni deyfa Bragg toppinn tengdum $\vec{K}$

dæmi   BCC sem SC með grunni

Bragg toppur þegar $\vec{K}$ er vigur. í fcc nyturgrindinni

Ef notum SC með $a\hat{x}$, $a\hat{y}$ og $a\hat{z}$

með grunni $\vec{d}_1 = 0$ $\vec{d}_2 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z}$

$\mathcal{R}$ grindin er SC með $\frac{2\pi}{a}$ -hlið

Ef hver toppur deyfist með

$$S_{\vec{K}} = 1 + \exp\left\{i\vec{K}\cdot\tfrac{1}{2}a(\hat{x}+\hat{y}+\hat{z})\right\}$$

í SC gildir $\vec{K} = \frac{2\pi}{a}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z})$

$$\rightarrow S_{\vec{K}} = 1 + \exp\left\{i\pi(n_1+n_2+n_3)\right\}$$

$$= 1 + (-1)^{n_1+n_2+n_3}$$

$$= \begin{cases} 2 & \text{ef } n_1+n_2+n_3 = \text{jöfn} \\ 0 & \text{ef } \cdots\cdots \text{ ójöfn} \end{cases}$$

Sama ef við hefðum beint reiknað fyrir BCC $\in \mathcal{B}$ $\curvearrowright$ fcc $\in \mathcal{R}$

(6)

Fjölatóma kristallar

Atóm(byggingar) stuðull

Ef jónirnar eru ekki allar eins

$$\longrightarrow \; S_{\vec{K}} = \sum_{j=1}^{n} f_j(\vec{K})\, e^{i\vec{K}\cdot\vec{d}_j}$$

með f_j : atómstuðullinn

Fyrsta stigs truflunar reikningur fyrir f_j gefur (Born nálgun)

$$f_j(\vec{K}) = -\frac{1}{e}\int dr\, e^{i\vec{K}\cdot r}\, \rho_j(r)$$

Sem er Fourier umformun hleðsluþéttleika jónar j.

(7)

Við munum ekki fara í 7 kafla sem fjallar um kristallssamhverfur

7 Kristallskerfi

14 Bravais grindur

230 punktgrúpur

⋮

Við höldum beint í 8 kafla og könnum aflfræði í lotubundnu mætti

Lotubundið mætti

Algerlega lotubundið, heim lota

↑ athugum síðar frávik

Lotubundið mætti jóna
+ víxlverkun rafeinda innbyrðis

Nálgun H, HF, LDA ......

↓

óháðar rafeindir í
lotubundnu virku mætti

Athugum fyrst áhrif lotu án þess að tiltaka nákvæmlega mættið innan hverrar lotu

$$U(\bar{r}+\bar{R}) = U(\bar{r})$$

Því nægir að skoða einnar-eindar hreyfijöfnu:

$$H\psi = \left\{-\frac{\hbar^2}{2m}\bar{\nabla}^2 + U(\bar{r})\right\}\psi = \varepsilon\psi$$

Bloch rafeindir <-> frjálsar rafeindir

Setning Blochs

Eiginföll H hér að ofan eru

$$\psi_{n\bar{k}}(\bar{r}) = e^{i\bar{k}\cdot\bar{r}}\, u_{n\bar{k}}(\bar{r})$$

með $u_{n\bar{k}}(\bar{r}+\bar{R}) = u_{n\bar{k}}(\bar{r})$

fyrir alla $\bar{R} \in \mathcal{B}$

sem jafngildir

$$\psi_{n\bar{k}}(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot(\bar{r}+\bar{R})}\, u_{n\bar{k}}(\bar{r}+\bar{R})$$
$$= e^{i\bar{k}\cdot\bar{R}} \cdot e^{i\bar{k}\cdot\bar{r}}\, u_{n\bar{k}}(\bar{r})$$
$$= e^{i\bar{k}\cdot\bar{R}}\, \psi_{n\bar{k}}(\bar{r})$$

Sönnun

Skilgreinum hliðrunarvirkjann

$$T_{\bar R} f(\bar r) = f(\bar r + \bar R), \quad \bar R \in \mathcal{B}$$

$$T_{\bar R} H\psi = H(\bar r + \bar R)\psi(\bar r + \bar R)$$

$$= H(\bar r)\psi(\bar r + \bar R) = H T_{\bar R}\psi$$

fyrir öll ψ -> $[H, T_{\bar R}] = 0$

og greinilega

$$[T_{\bar R}, T_{\bar R'}] = 0, \quad T_{\bar R} T_{\bar R'} = T_{\bar R + \bar R'}$$

$\boxed{\text{H og } T_{\bar R} \text{ hafa sameiginleg ástönd}}$

$$H\psi = \varepsilon\psi$$
$$T_{\bar R}\psi = c(\bar R)\psi$$

finnum eigingildin $c(\bar R)$

$$T_{\bar R'} T_{\bar R}\psi = c(\bar R') T_{\bar R}\psi = c(\bar R') c(\bar R)\psi$$

$$\hookrightarrow = T_{\bar R' + \bar R}\psi = c(\bar R + \bar R')\psi$$

því $\quad c(\bar R + \bar R') = c(\bar R) c(\bar R')$

Veljum $\vec a_i$ grunnvigrana í $\mathcal{B}$.

það er alltaf hægt að skrifa

$$c(\vec a_i) = e^{2\pi i x_i}$$

ef x_i er valið rétt.

$$\bar R = n_1 \bar a_1 + n_2 \bar a_2 + n_3 \bar a_3 \in \mathcal{B}$$

$$\to c(\bar R) = c(\bar a_1)^{n_1} c(\bar a_2)^{n_2} c(\bar a_3)^{n_3}$$

en athugum

$$e^{i\bar k \cdot \bar R}$$ með $\bar k = x_1 \bar b_1 + x_2 \bar b_2 + x_3 \bar b_3$

og $\quad \bar b_i \cdot \bar a_j = 2\pi\delta_{ij}$

$$\hookrightarrow \exp\{i2\pi(n_1 x_1 + n_2 x_2 + n_3 x_3)\}$$

$$= \left(e^{2\pi i x_1}\right)^{n_1} \left(e^{2\pi i x_2}\right)^{n_2} \left(e^{2\pi i x_3}\right)^{n_3}$$

$$\to c(\bar R) = e^{i\bar k \cdot \bar R} \qquad \bar R \in \mathcal{B},$$

⑤

því fæst

$$T_R\psi = C(\bar{R})\psi = e^{i\bar{k}\cdot\bar{R}}\psi(\bar{r})$$

$$\hookrightarrow = \psi(\bar{r}+\bar{R})$$

Bloch setningin

Bloch bylgjuvigurinn hefur enn ekki verið ákveðinn. Það gerist með hreyfijöfnunni og jaðarskilyrðunum. ($\bar{k}$ þarf ekki að vera vigur í $\mathfrak{R}$!)

Jaðarskilyrði

Endurbætum Born-von Karman

$$\psi(\bar{r}+N_i\bar{a}_i) = \psi(\bar{r}) \qquad i=1,2,3$$

$N_1N_2N_3 = N$ fjöldi punkta í grind

⑥

$$\psi_{n\bar{k}}(\bar{r}+N_i\bar{a}_i) = e^{iN_i\bar{k}\cdot\bar{a}_i}\psi_{\text{[redacted]}}(\bar{r})$$

↑ Bloch skilyrði

til þess að uppfylla B-vK þarf því

$$e^{iN_i\bar{k}\cdot\bar{a}_i} = 1$$

$$\to e^{2\pi i N_i x_i} = 1 \quad \text{ef } \bar{k} = x_1\bar{b}_1 + x_2\bar{b}_2 + x_3\bar{b}_3$$

og því $x_i = \frac{m_i}{N_i}$ með $m_i \in \mathbb{Z}$

Bloch bylgjuvigrarnir eru því

$$\vec{k} = \frac{m_1}{N_1}\bar{b}_1 + \frac{m_2}{N_2}\bar{b}_2 + \frac{m_3}{N_3}\bar{b}_3$$

Rúmmál $\Delta\vec{k}$ í k-rúminu um hvert $\bar{k}$ er

$$\boxed{\begin{aligned}\Delta\bar{k} &= \frac{\bar{b}_1}{N_1}\cdot\left(\frac{\bar{b}_2}{N_2}\times\frac{\bar{b}_3}{N_3}\right)\\ &= \frac{1}{N}\bar{b}_1\cdot(\bar{b}_2\times\bar{b}_3)\\ &= \frac{(2\pi)^3}{V}\end{aligned}}$$

sama og fyrir frjálsu ástöndin

fjöldi leifðra bylgjuvigra í frumeiningu nykurrúmsins er jafn heildarfjölda punkta í kristallinum

N ↙

Lesa sjálf um hina sönnun Bloch setningarinnar bls 137-139

Við munum athuga bráðlega líkan með gefnu lotubundnu mætti: Kronig-Penney-líkanið.

En athugum nú almennar staðreyndir um lotubundin mætti

Um H fyrir lotubundið mætti gildir

$$[\bar{p}, H] = [\bar{p}, U(\bar{r})] \neq 0 \quad , \quad \vec{p} = -i\hbar\vec{\nabla}$$

H er ekki með hliðrunarsamhverfu nema um $\bar{R} \in \mathfrak{B}$

→ H og $\vec{p}$ hafa ekki sameiginleg ástönd

$\hbar\vec{k}$ er ekki skriðþungi rafeindar

$$\vec{p}\,\psi_{n\bar{k}} = -i\hbar\vec{\nabla}\left(e^{i\bar{k}\cdot\bar{r}}u_{n\bar{k}}(\bar{r})\right)$$

$$= \hbar\bar{k}\psi_{n\bar{k}} + e^{i\bar{k}\cdot\bar{r}}\frac{\hbar}{i}\vec{\nabla}u_{n\bar{k}}(\bar{r})$$

$\{\psi_{nk}$ er ekki eiginástand $\bar{p}$!$\}$

$\boxed{\hbar\vec{k} \text{ er kristallsskriðþungi rafeindar}}$

útvíkkun á $\vec{p}$ yfir í lotubundið mætti

$\vec{k}$ er alltaf á fyrsta Brillouinsvæðinu

því ef visst $\bar{k}'$ er það ekki þá gildir

$$\bar{k}' = \bar{k} + \vec{K}$$

í fyrsta Brillouin sv.

og
$$e^{i\bar{k}'\cdot\bar{R}} = e^{i(\bar{k}+\bar{K})\cdot\bar{R}} = e^{i\bar{k}\cdot\bar{R}}$$

skammtatalan n merkir lausn Schrödinger-jöfnunnar fetar, því ef

$$\psi(\bar r) = e^{i\bar k\cdot\bar r}\,u(\bar r)$$

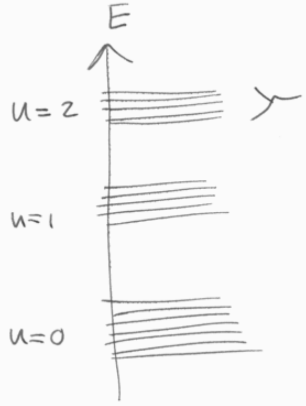
þá fæst

$$H\psi = e^{i\bar k\cdot\bar r}\left\{\frac{\hbar^2}{2m}\left(-i\bar\nabla+\bar k\right)^2 + U(\bar r)\right\}u_k(\bar r)$$

$$= e^{i\bar k\cdot\bar r}\,\varepsilon_{\bar k}\,u_k(\bar r)\,, \quad u_{\bar k}(\bar r) = u_{\bar k}(\bar r+\bar R)$$

gefur Schrödinger jöfnu fyrir frumeiningu kristallsins

líklega flokkast eigingildin saman í borða merktum með n



> leyfileg k-gildi innan borða

$\bar k$ er hægt að takmarka við fyrsta Brillouin svæðið

því

$$\left(\psi_{n,\bar k+\bar K}(\bar r) = \psi_{n,\bar k}\right)$$

$$\varepsilon_{n,\bar k+\bar K} = \varepsilon_{n\bar k}$$

$\varepsilon_n(\bar k)$: gefur borðabygginguna storta

Meðalhraði rafeindar með $\vec k$ er

$$v_n(\bar k) = \frac{1}{\hbar}\vec\nabla_{\bar k}\,\varepsilon_n(\bar k)$$

Hraðinn breytist ekki vegna árekstra við jónir, hann er stöðugur fyrir ástand $|n\bar k\rangle$

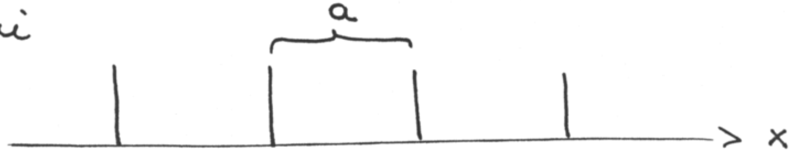
sjá viðbót E

Lotubundin mætti

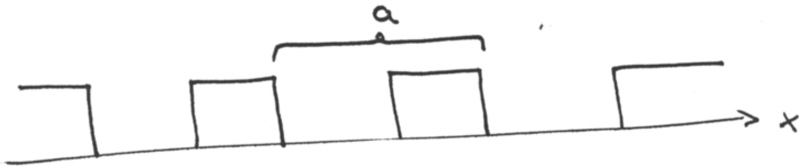
Hér verður farið lauslega í lotubundin mætti þ.a. aðaláherslan verður á frásögu af lausn og niðurstöðum

$$V(x+an) = V(x) \quad \text{ef } n \in \mathbb{Z}$$

dæmi

①


②


③


a: lotulengd mættis

Allir punktar sem eru hliðraðir um na eru jafngildir í x-rúmi

→ við verðum að krefjast

$$|\psi(x+a)|^2 = |\psi(x)|^2$$

því getur almennt gilt um ψ að

$$\boxed{\psi(x+a) = e^{ika}\,\psi(x)} \quad (*)$$

{ þannig má tákna alla mögulega fasastuðla }

þ.s. $e^{2\pi i n} = 1$ þá nægir að takmarka k þ.a.

$$\boxed{-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}}$$

(✱) er aðeins hægt að uppfylla ef

$$\boxed{\begin{array}{l}\psi(x) = e^{ikx}\,u_k(x) \\ \text{með} \quad u_k(x) = u_k(x+a)\end{array}}$$

Setning Blochs

$$\rightarrow \underline{\psi(x+a)} = e^{ik(x+a)}\,u_k(x+a)$$

$$= e^{ika}\left\{e^{ikx}u_k(x)\right\} = \underline{e^{ika}\psi(x)}$$

Athugum nú lotuna $0 \le x \le a$

Gerum ráð fyrir að hér sé almenn lausn

$$\psi(x) = Au(x) + Bv(x)$$

Þá gildir á bilinu $a \le x \le 2a$ (vegna (✱))

$$\psi(x) = e^{ika}\left\{Au(x-a) + Bv(x-a)\right\}$$

Nú verða $\psi(x)$ og $\psi'(x)$ að vera samfeld í $x = a$

$$\rightarrow \begin{cases} \overbrace{Au(a)+Bv(a)}^{0\le x\le a} = \overbrace{e^{ika}\left\{Au(0)+Bv(0)\right\}}^{a\le x\le 2a} \\[1em] Au'(a)+Bv'(a) = e^{ika}\left\{Au'(0)+Bv'(0)\right\} \end{cases}$$

Óhliðrað jöfnuhneppi fyrir A og B hefur aðeins lausn ef ákveða þess hverfur

$$\rightarrow \begin{pmatrix} u(a)-e^{ika}u(0) & v(a)-e^{ika}v(0) \\ u'(a)-e^{ika}u'(0) & v'(a)-e^{ika}v(0) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = 0$$

$$\boxed{\begin{array}{l} \rightarrow \left\{u(a)-e^{ika}u(0)\right\}\left\{v'(a)-e^{ika}v'(0)\right\} \\ \qquad = \left\{u'(a)-e^{ika}u'(0)\right\}\left\{v(a)-e^{ika}v(0)\right\} \end{array}}$$

þessa jöfnu má umskrifa sem

$$\cos ka = \frac{\{u(0)v'(a)+u(a)v'(0)\} - \{v(0)u'(a)+v(a)u'(0)}{2\{u(0)v'(0)-v(0)u'(0)\}}$$

↑ þessi jafna ákvarðar möguleg gildi á k

Tökum nú víst dæmi

$$V(x) = \frac{\hbar^2}{m}\Omega\sum_{n=-\infty}^{+\infty}\delta(x+na)$$

og skoðum orkurófið

schrödinger jafnan er

$$-\frac{\hbar^2}{2m}\psi'' + V(x) = E\psi \quad , \quad E \geq 0$$

ef $x \neq an$ þá gildir

$$\psi'' + \frac{2mE}{\hbar^2}\psi = 0 \quad \rightarrow \text{ ef } q^2 \equiv \frac{2mE}{\hbar^2}$$

því reynum við á bilinu $(0,a)$

$$u(x) = e^{iqx} \quad \text{og} \quad v(x) = e^{-iqx}$$

$$\rightarrow \quad \psi(x) = Ae^{iqx} + Be^{-iqx}$$

og á bilinu $(a,2a)$ verður

$$\psi(x) = e^{ika}\left\{Ae^{iq(x-a)} + Be^{-iq(x-a)}\right\}$$

ψ ~~er~~ er samfellt

$$\hookrightarrow \boxed{\psi(a^+) = \psi(a^-)} \quad ①$$

Hvað gildir um afleiðuna ?

Athugum, heildum báðar hliðar schrödingerjöfnunnar rétt um $x = a$

$$\int_{a-\epsilon}^{a+\epsilon} dx\left\{-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x)\right\} = E\int_{a-\epsilon}^{a+\epsilon} dx\,\psi(x)$$

⑧

Samfelt

$$\int_{a-\epsilon}^{a+\epsilon} dx \left\{ -\frac{\hbar^2}{2m}\psi''(x) + \frac{\hbar^2}{m}\Omega\,\delta(x-a)\psi \right\} = E\left\{\psi(a+\epsilon) - \psi(a-\epsilon)\right\} = 0$$

$$\rightarrow \frac{\hbar^2}{m}\left\{ -\frac{1}{2}\left(\psi'(a+\epsilon) - \psi'(a-\epsilon)\right) + \Omega\psi(a) \right\} = 0$$

$$\rightarrow \boxed{\psi'(a^+) - \psi'(a^-) = 2\Omega\psi(a)} \quad ②$$

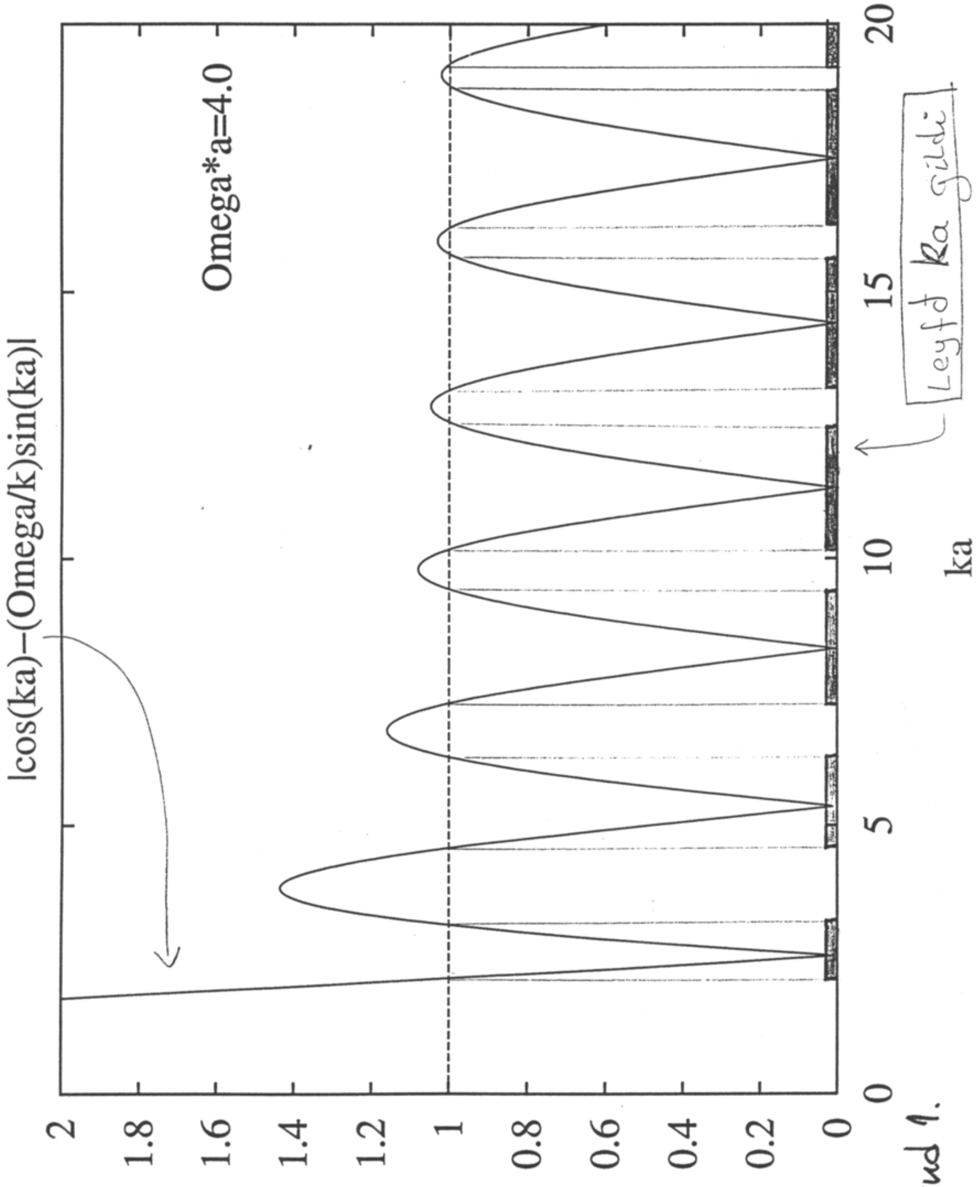
Setjum inn í ① og ②

$$① \rightarrow e^{ika}(A+B) = Ae^{iqa} + Be^{-iqa}$$

$$② \rightarrow iq\,e^{ika}(A-B) = iq(Ae^{iqa} - Be^{-iqa}) + 2\Omega(Ae^{iqa} + Be^{iqa})$$

ákveðan verður við hvør ta

$$\rightarrow \boxed{\cos ka = \cos qa + \frac{\Omega}{q}\sin qa} \quad ③$$



mynd 1.

Jafna ③ ákveður orkuróf eindarinnar

$$|\cos ka| \le 1$$

$$\to \left|\cos qa + \frac{\Omega a}{qa}\sin qa\right| \le 1$$

mynd 1 sýnir því að aðeins viss qa-gildi eru leyfileg í jöfnunni $E = \frac{\hbar^2}{2ma^2}(qa^2)$

Orkugildi rafeindar (eindar) hafa safnast saman í borða

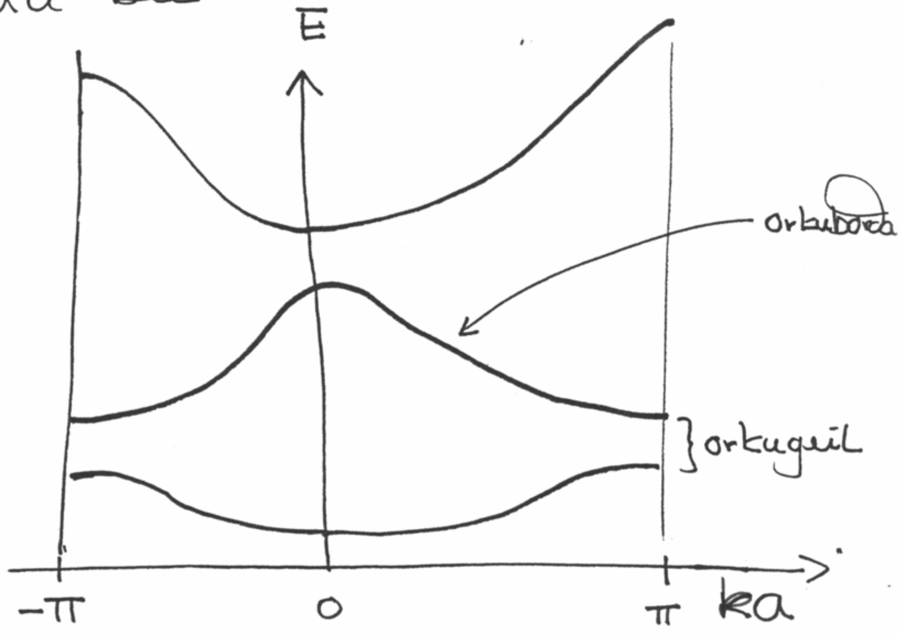
{ ekki strjál orkustig og heldur ekki alveg samfeld }

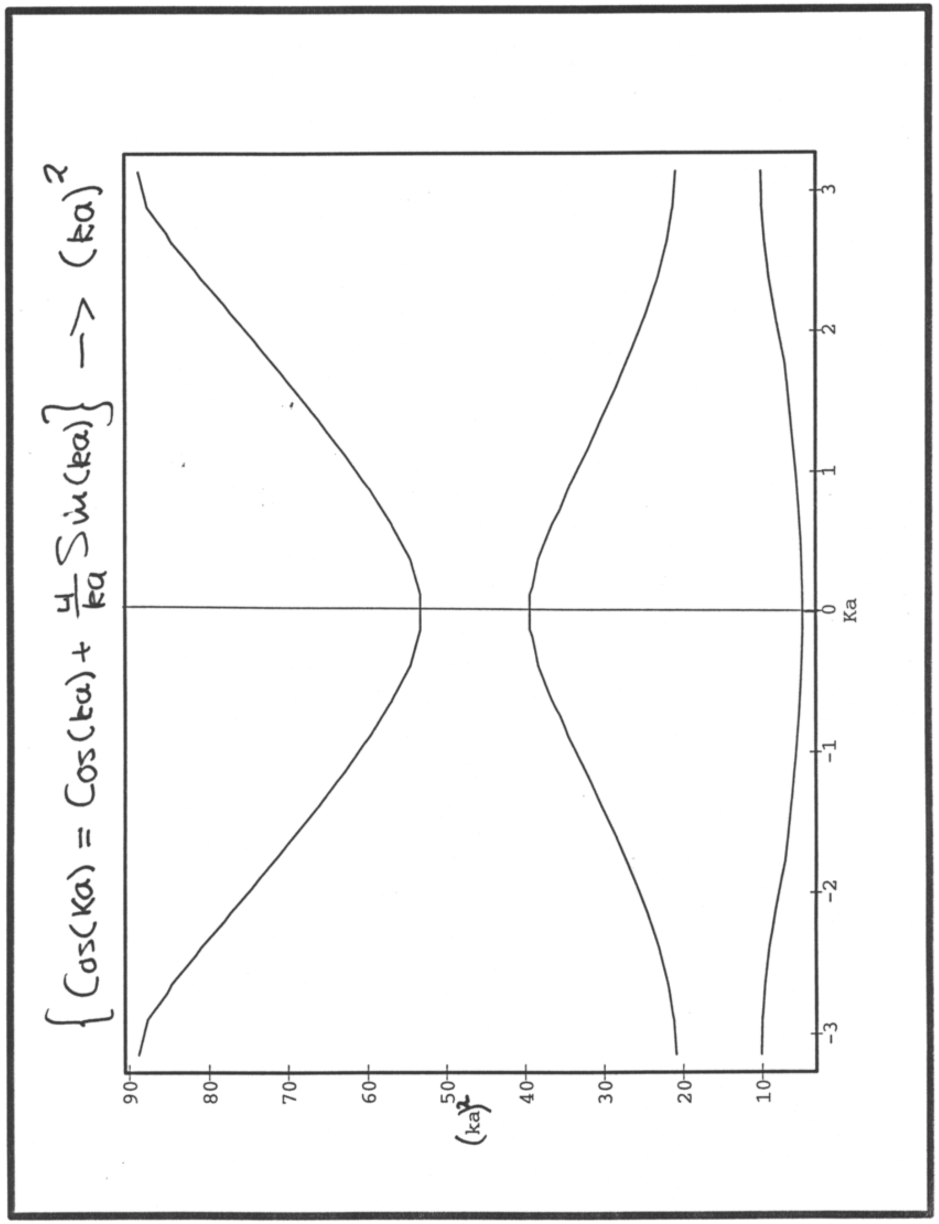
Við höfðum takmarkað k þ.a.

$$\boxed{-\pi \le ka \le \pi}$$

því þarf að leysa óbeinu jöfnuna ③ fyrir qa þegar ka tekur eitthvert gildi á þessu bili.

Fyrir hvert ka finnast óendanlega margar lausnir fyrir qa, því qa er ekki takmarkað við þetta bil





$$\left\{\cos(Ka) = \cos(ka) + \frac{4}{ka}\sin(ka)\right\} \longrightarrow (ka)^2$$

```
> with(plots):
> cos(Ka)=cos(ka)+(4/ka)*sin(ka);
```

$$\cos(Ka) = \cos(ka) + 4\,\frac{\sin(ka)}{ka}$$

```
> cos(Ka)=cos(sqrt(ka))+(4/sqrt(ka))*sin(sqrt(ka));
```

$$\cos(Ka) = \cos\left(\sqrt{ka}\right) + 4\,\frac{\sin\left(\sqrt{ka}\right)}{\sqrt{ka}}$$

```
> implicitplot(cos(Ka)=cos(sqrt(ka))+(4/sqrt(ka))*sin(sqrt(ka)), Ka=-Pi..Pi, ka
  =0..9*Pi^2);
>
```

Rafeindirnar í þessum „einvíða kristalli" rekast því ekki á jónirnar. Heldur geta einungis rafeindabylgjur með vissa skriðþunga borist um kristallinn.

Ástanda þéttleiki borða

Höfum oft

$$Q = 2\sum_{n\bar{k}} Q_n(\bar{k})$$

$$\rightarrow \quad q = \lim_{V\to\infty} \frac{Q}{V} = 2\sum_n \int_{P.C.} \frac{d\bar{k}}{(2\pi)^3}\, \underset{\uparrow}{Q_n(\bar{k})}$$

aðeins háð $n\bar{k}$ í gegnum $\varepsilon_{n\bar{k}}$

$$= \int d\varepsilon\, g(\varepsilon)\, Q(\varepsilon)$$

á borða

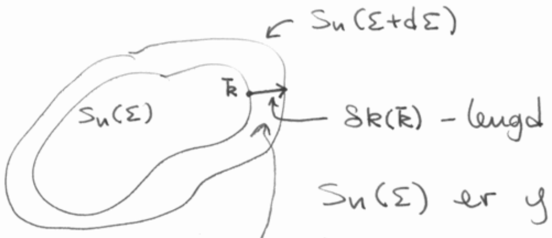
með $$g(\varepsilon) = \sum_n g_n(\varepsilon)$$

og $$g_n(\varepsilon) = \int_{P.C.} \frac{d\bar{k}}{4\pi^3}\, \delta(\varepsilon - \varepsilon_n(\bar{k}))$$

því $$\int d\varepsilon\, g(\varepsilon) Q(\varepsilon) = \int d\varepsilon \sum_n \int \frac{d\bar{k}}{4\pi^3}\, \delta(\varepsilon - \varepsilon_n(\bar{k})) Q(\varepsilon)$$

$$= 2\sum_n \int \frac{d\bar{k}}{(2\pi)^3}\, Q(\varepsilon_n(\bar{k}))$$

$$= 2\sum_n \int \frac{d\bar{k}}{(2\pi)^3}\, Q_n(\bar{k})$$



$S_n(\Sigma)$ er yfirborðið $\Sigma(\bar{k})=\Sigma$
innan P.C. (frumgr. ein.)

$$\to g_n(\Sigma)d\Sigma = 2\int_{S_n(\Sigma)} \frac{dS}{(2\pi)^3}\,\delta k(\bar{k})$$

fjöldi ástanda í skel

$\frac{(2\pi)^3}{V}$ rúmmál um punkt í k-grind

$$\Sigma + d\Sigma = \Sigma + |\bar{\nabla}\Sigma_n(\bar{k})|\delta k(\bar{k})$$

$$\to \delta k(\bar{k}) = \frac{d\Sigma}{|\bar{\nabla}\Sigma_n(\bar{k})|}$$

Svo $$g_n(\Sigma) = 2\int_{S_n(\Sigma)} \frac{dS}{(2\pi)^3}\frac{1}{|\bar{\nabla}\Sigma_n(\bar{k})|}$$

$\Sigma_n(\bar{k})$ er lotubundið í $\bar{k}$
→ takmarkað að ofan og neðan

→ til punktar með $|\nabla\Sigma| = 0$

í 3D eru sérstöðup. heildanlegir

---

en valda ósamfellu í afleiðu

Van Hove sérstöðupunktar

Í 2D eða 1D eru punktarnir verri

Áhrif þeirra koma fram í
flutningsfræðum - - - - -

Næstum frjálsar rafeindir

Tilraunir: margir málmar
s og p rafeindir utan lokaðra
hvela

Bloch

$$\psi_{k}(\bar r) = e^{i\bar k\cdot\bar r}\,u(\bar r)$$

$$u(\bar r+\bar R) = u(\bar r)$$

næstum frjálsar -> sléttar bylgjur

fourier umm. lotubundins falls

reynum

$$u(\bar r) = \boxed{\sum_{\bar K} C_{\bar k-\bar K}\, e^{-i\bar K\cdot\bar r}}$$

↑ sést frá Schr.-jöfnu

$$\psi_{\bar k}(\bar r) = \sum_{\bar K} C_{\bar k-\bar K}\, e^{i(\bar k-\bar K)\cdot\bar r}$$

Hreyfijafnan er

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + U(\bar r)\right\}\psi = \varepsilon\psi$$

reynum innsetningu

$U(\bar r)$ er lotubundið í $\bar R$ og má því skrifa sem Fourierröð

$$U(\bar r) = \sum_{K} U_{\bar K}\, e^{i\bar K\cdot\bar r}$$

með

$$U_{\bar K} = \frac{1}{V}\int_{\text{eining}} d\bar r\, e^{-i\bar K\cdot\bar r}\, U(\bar r)$$

->

$$\sum_{\bar K}\left\{\left(\frac{\hbar^2}{2m}(\bar k-\bar K)^2-\varepsilon\right)C_{\bar k-\bar K}\, e^{i(\bar k-\bar K)\cdot\bar r} + \underbrace{\left(\sum_{\bar K'} U_{\bar K'}\, e^{i\bar K'\cdot\bar r}\right)C_{\bar k-\bar K}\, e^{i(\bar k-\bar K)\cdot\bar r}}\right\} = 0$$

$$\sum_{\bar K'\bar K} U_{\bar K'}\, e^{i(\bar k-(\bar K-\bar K'))\cdot\bar r}\, C_{\bar k-\bar K} \qquad \bar K \to \bar K'+\bar K$$

$$\sum_{\bar K'\bar K} U_{\bar K'}\, e^{i(\bar k-\bar K)\cdot\bar r}\, C_{\bar k-(\bar K+\bar K')}$$

því er hreyfijafnan

$$\sum_{\bar{K}} e^{i(\bar{k}-\bar{K})\cdot\bar{r}} \Big\{ \Big(\frac{\hbar^2}{2m}(\bar{k}-\bar{K})^2 - \Sigma\Big) C_{\bar{k}-\bar{K}}$$

$$+ \sum_{\bar{K}'} U_{\bar{K}'} C_{\bar{k}-(\bar{K}+\bar{K}')} \Big\} = 0$$

breytum síðari summunni

$$\bar{K}' \to \bar{K}' - \bar{K}$$

þá fæst:

$$\sum_{K} e^{i(\bar{k}-\bar{K})\cdot\bar{r}} \Big\{ \Big(\frac{\hbar^2}{2m}(\bar{k}-\bar{K})^2 - \Sigma\Big) C_{\bar{k}-\bar{K}}$$

$$+ \sum_{\bar{K}'} U_{\bar{K}'-\bar{K}} C_{\bar{k}-\bar{K}'} \Big\} = 0$$

fullkominn grunnur sem uppfyllir jaðarst.

því gildir fyrir sérhvern bylgjuvigur $\bar{k}-\bar{K}$

$$\boxed{\Big(\frac{\hbar^2}{2m}(\bar{k}-\bar{K})^2 - \Sigma\Big) C_{\bar{k}-\bar{K}} + \sum_{\bar{K}'} U_{\bar{K}'-\bar{K}} C_{\bar{k}-\bar{K}'} = 0}$$

$\vec{k} \in$ 1. Brillouin $\quad \vec{K} \in \mathcal{R}$

Frjálsar rafeindir fyrir ástand $|\bar{k}\rangle$ gildir

$$U_{\bar{K}} = 0$$

$$\to \Big(\frac{\hbar^2}{2m}(\bar{k}-\bar{K})^2 - \Sigma\Big) C_{\bar{k}-\bar{K}} = 0$$

$$\big(\Sigma^0_{\bar{k}-\bar{K}} - \Sigma\big) C_{\bar{k}-\bar{K}} = 0$$

→ fyrir sérhvert $\bar{K}$ gildir: annaðhvort er

$$C_{\bar{k}-\bar{K}} = 0 \quad \text{eða} \quad \Sigma = \Sigma^0_{\bar{k}-\bar{K}} \quad (*)$$

tveir möguleikar

① (*) gerist aðeins fyrir eitt $\bar{K}$

einföld ástönd

$$\Sigma = \Sigma^0_{\bar{k}-\bar{K}}, \quad \psi_{\bar{k}} \sim e^{i(\bar{k}-\bar{K})\cdot\bar{r}}$$

② (*) gerist fyrir $\bar{K}_1 \ldots \bar{K}_m$ gefa öll sömu orku

m-föld lausn, sérhver samantekt m-lausna (frjáls $C_{\bar{k}-\bar{K}}$) er líka lausn

Veikt lotubundið mætti

„ $U_{\bar K} \neq 0$ en mjög smá "

① ~~Næstum~~ einföld ástönd

Veljum $\bar k$ og athugum $\bar K_1$ þ.a.

$$\left| \Sigma^0_{\bar k - \bar K_1} - \Sigma^0_{\bar k - \bar K} \right| >> U \quad \forall \; \bar K \neq \bar K_1$$

Viljum finna áhrif U á frjálsa ástandið gefið með

$$\Sigma = \Sigma^0_{\bar k - \bar K_1}, \qquad C_{\bar k - \bar K} = 0, \; \bar K \neq \bar K_1$$

hreyfijafnan er

$$(\Sigma - \Sigma^0_{\bar k - \bar K_1}) C_{\bar k - \bar K_1} = \sum_{\bar K \neq \bar K_1} U_{\bar K - \bar K_1} C_{\bar k - \bar K} \qquad (1)$$

$$\underbrace{U_{\bar K} = 0 \quad \text{fyrir } \bar K = 0}_{\text{(fasti lagður við mættið)}}$$

Ef nú $\bar K \neq \bar K_1$ þá getur hreyfijafnan

$$C_{\bar k - \bar K} = \frac{U_{\bar K_1 - \bar K} C_{\bar k - \bar K_1}}{\Sigma - \Sigma^0_{\bar k - \bar K}} + \sum_{\bar K' \neq \bar K_1} \frac{U_{\bar K' - \bar K} C_{\bar k - \bar K'}}{\Sigma - \Sigma^0_{\bar k - \bar K}}$$

Stærri liður vegna $C_{\bar k - \bar K_1}$ sem er stærst

línulegt í U ef nefnarinn verður aldrei lítill vegna margfeldni

$$C_{\bar k - \bar K} = \frac{U_{\bar K_1 - \bar K} C_{\bar k - \bar K_1}}{\Sigma - \Sigma^0_{\bar k - \bar K}} + O(U^2)$$

notum í (1)

$$(\Sigma - \Sigma^0_{\bar k - \bar K_1}) C_{\bar k - \bar K_1} = \sum_{\bar K} \frac{U_{\bar K - \bar K_1} U_{\bar K_1 - \bar K}}{\Sigma - \Sigma^0_{\bar k - \bar K}} C_{\bar k - \bar K_1}$$

$$+ O(U^3)$$

leysum fyrir Σ upp til annarrar gráðu í U
(í nefnara $\Sigma \to \Sigma_{\bar k-\bar k_1}$)

$$\Sigma = \Sigma^0_{\bar k-\bar k_1} + \sum_{\bar k} \frac{|U_{\bar k-\bar k'}|^2}{\Sigma^0_{\bar k-\bar k_1}-\Sigma^0_{\bar k-\bar k}} + O(U^3)$$

$\uparrow$

* U kemur fyrst inn í annars stigs truflun

* Fráhrinding orkustiga

$\Sigma^0_{\bar k-\bar k} > \Sigma^0_{\bar k-\bar k_1}$ veldur lækkun Σ

$\Sigma^0_{\bar k-\bar k} < \Sigma^0_{\bar k-\bar k_1}$ veldur hækkun Σ

---

② næstum margfalt ástand

Veljum $\bar k$ þá eru til $\bar k_1 \ldots \bar k_m$

þ.a. $|\Sigma^0_{\bar k-\bar k} - \Sigma^0_{\bar k-\bar k_j}| >> U \quad j=1,\ldots,m$

$\bar k \neq \bar k_1 \ldots \bar k_m$

Öll önnur stig eru fjarri m.v. U

þá má sanna (lesa sjálf) að

$$(\Sigma-\Sigma^0_{\bar k-\bar k_i})C_{\bar k-\bar k_i} = \sum_{j=1}^{m} U_{\bar k_j-\bar k_i}C_{\bar k-\bar k_j}$$

$i = 1, \ldots, m$

①

Bragg flötur (slétta)

von Laue skilyrði fyrir speglun röntgen geisla frá kristalli var

$$\bar{R}\cdot(\bar{k}-\bar{k}') = 2\pi m, \quad m\in\mathbb{Z}$$
$$\forall\, \bar{R}\in\mathcal{B}$$

$\rightarrow$ $\bar{q} = \bar{k}'-\bar{k}$ er vigur í $\mathcal{R}$
einnig $-\bar{q}$

fjaðrandi árekstur $\rightarrow$ $\underbrace{|\bar{k}| = |\bar{k}'|}$

$$k = |\bar{k}'-\bar{q}|$$

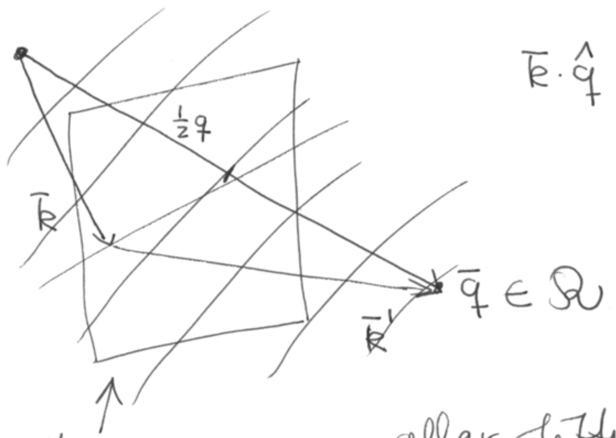
$\rightarrow$ $k^2 = (k')^2 - 2\bar{q}\cdot\bar{k}' + q^2$

$\rightarrow$ $k^2 = k^2 - 2\bar{q}\cdot\bar{k}' + q^2$

$\rightarrow$ $q^2 = 2\bar{q}\cdot\bar{k}'$ eða á sama hátt
$q^2 = 2\bar{q}\cdot\bar{k}$

$\rightarrow$ $\boxed{\bar{k}\cdot\hat{q} = \frac{1}{2}q}$

②



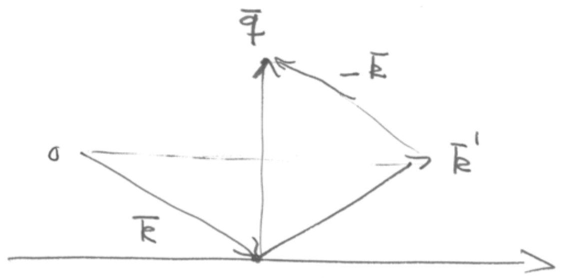
$\bar{k}\cdot\hat{q} = \frac{1}{2}q$

~~sléttan sem~~

allar sléttur þ. skilgreindar kallast **Bragg sléttur**

Umorðun á Laue skilyrðinu er

x-geisli speglast ef og aðeins ef bylgju vigur geislans $\bar{k}$ snertir Braggsléttu



Orkugildi nærri Bragg sléttu

↑ skýrist seinna

Um tvö frjáls orkugildi $\Sigma^0_{\bar{k}-\bar{K}_1}$ og $\Sigma^0_{\bar{k}-\bar{K}_2}$ gildir að þau eru nærri hvort öðru en U og <u>fjarri</u> öllum öðrum gildum $\Sigma^0_{\bar{k}-\bar{K}_i}$ með $i \neq 1,2$

þá gildir

$$\begin{cases} (\Sigma - \Sigma^0_{\bar{k}-\bar{K}_1})C_{\bar{k}-\bar{K}_1} = U_{\bar{K}_2-\bar{K}_1} C_{\bar{k}-\bar{K}_2} \\ (\Sigma - \Sigma^0_{\bar{k}-\bar{K}_2})C_{\bar{k}-\bar{K}_2} = U_{\bar{K}_1-\bar{K}_2} C_{\bar{k}-\bar{K}_1} \end{cases}$$

breytum rithætti

$$\bar{q} \equiv \bar{k}-\bar{K}_1 \quad \text{og} \quad \bar{K} = \bar{K}_2 - \bar{K}_1$$

$$\to (\Sigma - \Sigma^0_{\bar{q}})C_{\bar{q}} = U_{\bar{K}} C_{\bar{q}-\bar{K}}$$

$$(\Sigma - \Sigma^0_{\bar{q}-\bar{K}})C_{\bar{q}-\bar{K}} = U_{-\bar{K}} C_{\bar{q}} = U^*_{\bar{K}} C_{\bar{q}}$$

$$\Sigma^0_{\bar{q}} \simeq \Sigma^0_{\bar{q}-\bar{K}}, \quad |\Sigma^0_{\bar{q}} - \Sigma^0_{\bar{q}-\bar{K}'}| >> U$$

$$\text{ef } \bar{K}' \neq \bar{K}, \bar{0}$$

$\bar{K} \in \mathcal{R}$

$\Sigma_{\bar{k}} = \Sigma_{\bar{k}+\bar{K}}$: er lotubundið, en

$\Sigma^0_{\bar{q}} = \Sigma^0_{\bar{q}-\bar{K}}$ aðeins ef $\underbrace{|\bar{q}| = |\bar{q}-\bar{K}|}$

→ <u>skilyrði fyrir því að $|\bar{q}|$ snerti Bragg-sléttu</u>

þess vegna er skilyrðið að

$\Sigma^0_{\bar{q}} = \Sigma^0_{\bar{q}-\bar{K}'}$ aðeins fyrir $\bar{K}' = \bar{K}$

Krafa um að $\bar{q}$ snerti aðeins þetta eina Bragg-plan

→ næstum tvöfalt ástand jafngildir því að $\Sigma_{\bar{q}}$ sé nærri því að <u>Bragg dreifast</u>

Veikt lotubundið mætti hefur því aðeins áhrif á rafeindir sem hafa bylgjuvigur sem næstum uppfyllir Bragg skilyrðin

Skoðum hreyfijöfnurnar

Óhliðrað jöfnuhneppi -> ákveða = 0

$$\begin{pmatrix} \Sigma - \Sigma^0_{\bar{q}} & -U_{\bar{K}} \\ -U^*_{\bar{K}} & \Sigma - \Sigma^0_{\bar{q}-\bar{K}} \end{pmatrix} \begin{pmatrix} C_{\bar{q}} \\ C_{\bar{q}-\bar{K}} \end{pmatrix} = 0$$

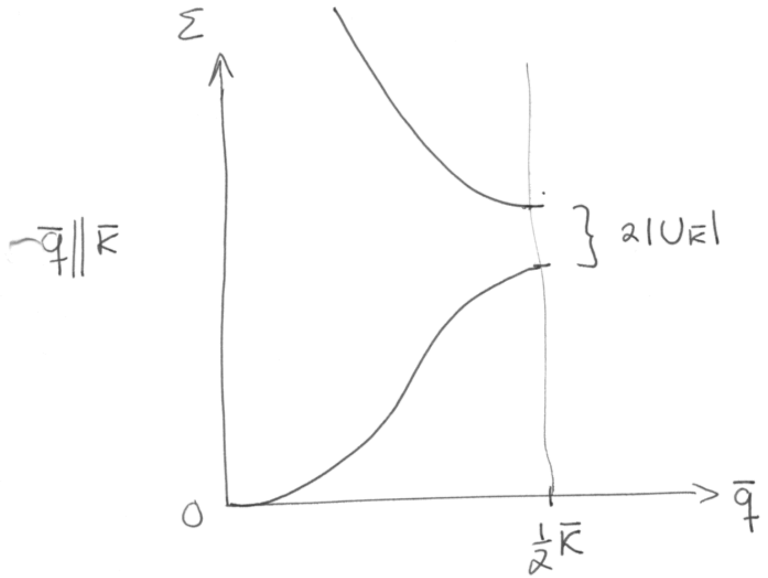
~~með~~ $$AC = 0$$

$\det A = 0$ gefur tvær lausnir

$$\Sigma = \frac{1}{2}\left(\Sigma^0_{\bar{q}} + \Sigma^0_{\bar{q}-\bar{K}}\right) \pm \left\{ \left(\frac{\Sigma^0_{\bar{q}} - \Sigma^0_{\bar{q}-\bar{K}}}{2} \right)^2 + |U_{\bar{K}}|^2 \right\}^{1/2}$$

Í Bragg sléttu gildir $\Sigma^0_{\bar{q}} = \Sigma^0_{\bar{q}-\bar{K}}$

$\rightarrow \Sigma = \Sigma^0_{\bar{q}} \pm |U_{\bar{K}}|$ f. q á Bragg sl.



Í Bragg-sléttunni gildir

yfirborð fastrar orku eru hornrétt á Braggsléttur

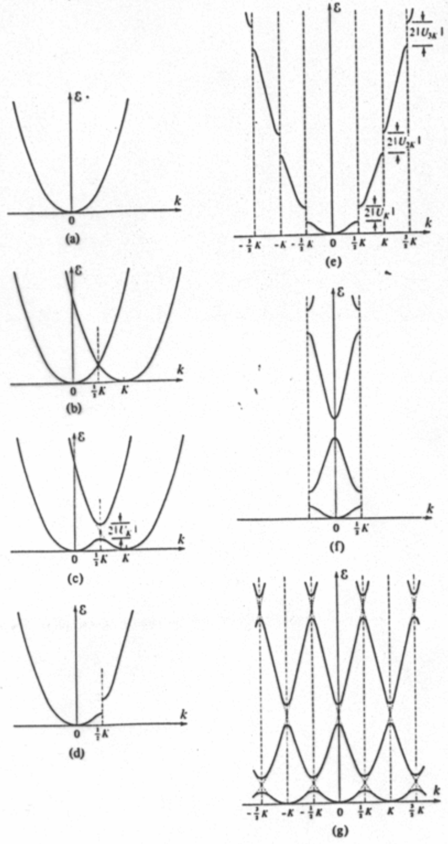


Figure 9.4
(a) The free electron ε vs. k parabola in one dimension. (b) Step 1 in the construction to determine the distortion in the free electron parabola in the neighborhood of a Bragg "plane," due to a weak periodic potential. If the Bragg "plane" is that determined by K, a second free electron parabola is drawn, centered on K. (c) Step 2 in the construction to determine the distortion in the free electron parabola in the neighborhood of a Bragg "plane." The degeneracy of the two parabolas at $K/2$ is split. (d) Those portions of part (c) corresponding to the original free electron parabola given in (a). (e) Effect of all additional Bragg "planes" on the free electron parabola. This particular way of displaying the electronic levels in a periodic potential is known as the *extended-zone scheme*. (f) The levels of (e), displayed in a *reduced-zone scheme*. (g) Free electron levels of (e) or (f) in a *repeated-zone scheme*.

ūtvittad
extended
zone
scheme

reduced
skert

repeated
endurbtein

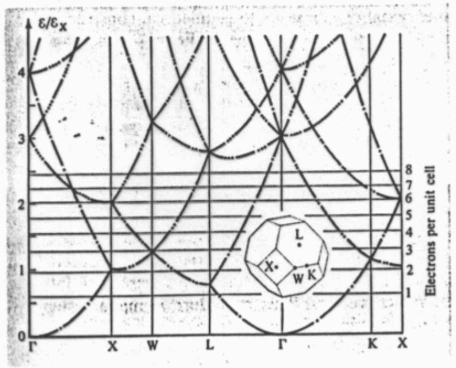


Figure 9.5
Free electron energy levels for an fcc Bravais lattice. The energies are plotted along lines in the first Brillouin zone joining the points $\Gamma(\mathbf{k} = 0)$, K, L, W, and X. $\mathcal{E}_x$ is the energy at point X ($[\hbar^2/2m][2\pi/a]^2$). The horizontal lines give Fermi energies for the indicated numbers of electrons per primitive cell. The number of dots on a curve specifies the number of degenerate free electron levels represented by the curve. (From F. Herman, in *An Atomistic Approach to the Nature and Properties of Materials*, J. A. Pask, ed., Wiley, New York, 1967.)

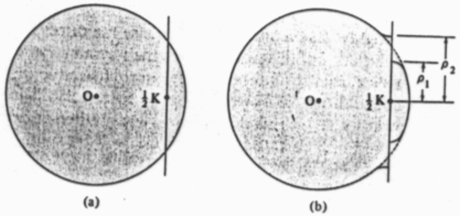


Figure 9.6
(a) Free electron sphere cutting Bragg plane located at $\frac{1}{2}\mathbf{K}$ from the origin ($U_{\mathbf{K}} = 0$). (b) Deformation of the free electron sphere near the Bragg plane when $U_{\mathbf{K}} \neq 0$. The constant-energy surface intersects the plane in two circles, whose radii are calculated in Problem 1.

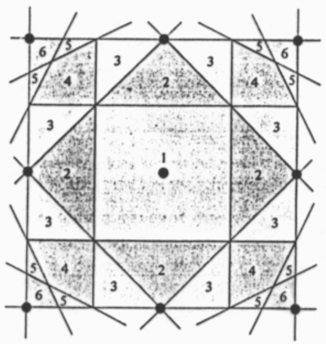


Figure 9.7
Illustration of the definition of the Brillouin zones for a two-dimensional square Bravais lattice. The reciprocal lattice is also a square lattice of side b. The figure shows all Bragg planes (lines, in two dimensions) that lie within the square of side $2b$ centered on the origin. These Bragg planes divide that square into regions belonging to zones 1 to 6. (Only zones 1, 2, and 3 are entirely contained within the square, however.)

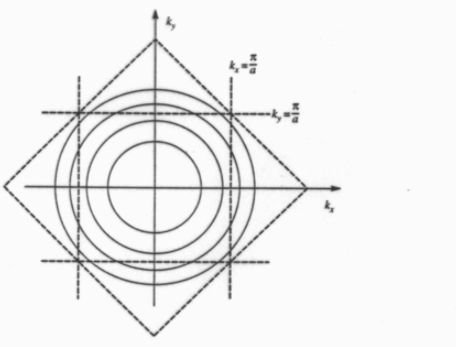


Fig. 5.18 Circular constant-energy contours (at equal energy intervals) for a free-electron gas in the empty-lattice approximation superimposed on the boundaries of the first two Brillouin zones of the 2D square real-space lattice.

the energy contours bend outwards from the free-electron circles towards the zone boundary. Likewise, the increase in energy for $\boldsymbol{k}$-values just above the zone boundary causes the constant-energy contours to fall below the free-electron circular contours towards the zone boundary. The perturbed NFE contours meet the zone boundaries at *right angles*. Since the solutions of the Schrödinger equation at the zone boundaries are *standing waves* (eqn. (5.75)), the electron group velocity, $\partial\omega/\partial k = (1/\hbar)\nabla_k\mathscr{E}$, must vanish there. The gradient of $\mathscr{E}$ in $\boldsymbol{k}$-space must therefore be *parallel* to the zone boundary, and consequently the constant-energy contour is normal to the boundary.

The NFE constant-energy contours for the 2D square lattice, superimposed on the boundaries of the first three, and part of the fourth, Brillouin zones (cf. Fig. 2.41) are shown in Fig. 5.19. The discontinuities in the energy contours at the zone boundaries correspond to the bandgaps in the band-structure ($\mathscr{E}(\boldsymbol{k})$) representation (Fig. 5.17). Figure 5.19 corresponds to the *extended-zone scheme* (cf. Fig. 5.17a). The energy contours can also be represented in the *reduced-zone scheme* (cf. Fig. 5.17b) by translating contours from zones higher than the first back into the first zone by means of appropriate reciprocal-lattice vectors. This is illustrated for the second zone in Fig. 5.20. Periodic continuation in $\boldsymbol{k}$-space of these first and second zones (the contours already lying in the first zone in Fig. 5.19 and those translated into it from the second zone in Fig. 5.20, respectively) generates the *repeated-zone representation* (Fig. 5.21).

In general, of course, the most important energy contour to consider is that corresponding to the *Fermi energy*, $\mathscr{E}_F$, since it is electrons having this energy that control most of the electronic behaviour. A 2D example, for a square lattice containing four

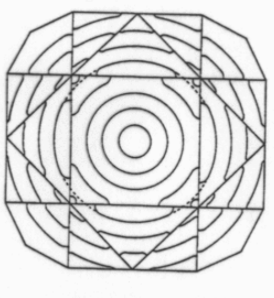


Fig. 5.19 Constant-energy contours for the NFE model applied to a 2D square lattice, superimposed on the boundaries of the first three, and part of the fourth, Brillouin zones in the extended-zone scheme. The dashed curves show one of the undistorted circular contours of the free-electron case.

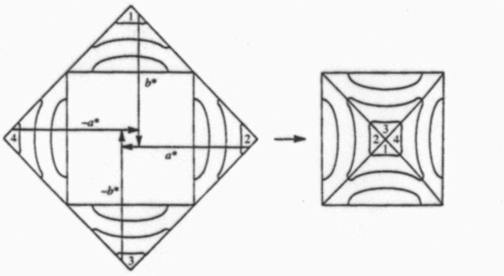


Fig. 5.20 Constant-energy contours from the second Brillouin zone in the extended-zone scheme (Fig. 5.19) represented in the reduced-zone scheme. The reciprocal-lattice vectors necessary to translate the segments from the second zone are indicated.

electrons per primitive unit cell in the free-electron approximation, is shown in Fig. 5.22a; the Fermi circle intersects four zones in this case. Those parts of higher zones that are occupied by electrons can be folded back into the first zone and periodically continued to generate repeated-zone representations, as in Figs. 5.22b–d. Note that there are two topologically distinct contours represented in Figs. 5.22b–d. In one,

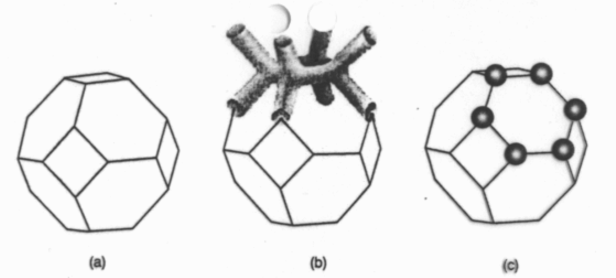


Fig. 5.24 The Fermi surface for an f.c.c. metal with four electrons per cell in the NFE approximation. (a) Second-zone hole-like surface. (b) Third-zone monster. (c) Four-zone electron-like surface.

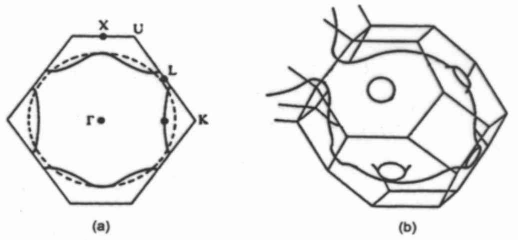


Fig. 5.25 The Fermi surface of Cu. (a) A (110) section through the first Brillouin zone. The dashed line represents the free-electron Fermi sphere. (b) The 3D Fermi surface inserted in the truncated octahedral Brillouin zone.

second and fourth zones are isolated and are hole-like and electron-like, respectively. However, the Fermi surface for the third zone is multiply connected in the repeated-zone scheme and cannot therefore be described as simply electron- or hole-like. Such topological forms for the Fermi surface are called, rather picturesquely, *monsters*.

For the monovalent alkali metals (Na, etc.), the Fermi wavevector is appreciably *less* than the shortest distance in reciprocal space to the first Brillouin-zone boundary (see Problem 5.1). Thus, NFE effects are negligible, and consequently the Fermi surface is simply a sphere lying within the first zone. Thus, such metals essentially behave like quantum free-electron systems. Cu also has one conduction electron per atom, and so the first Brillouin zone is also half-filled. However, k_F is rather close to the L-point in the first Brillouin zone (a truncated octahedron, since Cu has an f.c.c. structure), and so the electron energies in the ⟨111⟩ directions in $\boldsymbol{k}$-space are strongly perturbed, and 'necks' occur near the L-points (Fig. 5.25).

5.2.5 Metals versus insulators

We have noted previously that the simple free-electron model p
with part-filled electron shells should be *metals*, since the result
gas should be free to respond to an applied electric field at all
this picture is contrary to experience, since many materials are
insulators, i.e. they have a zero electrical conductivity at zero
tronic transport properties will be discussed thoroughly in
nonetheless, to mention briefly here how the NFE picture allow
to be distinguished.

It is instructive to consider at the outset a 1D crystal, for w
consists of a single band, with bandgaps at the zone boundaries,
the first Brillouin zone contains N states (where N is the number
length L), each of which can contain *two* electrons (because of t
the case of a monovalent chain (one conduction electron per ato
filled with electrons, and $\mathscr{E}_F$ lies in the middle of the band (Fig.

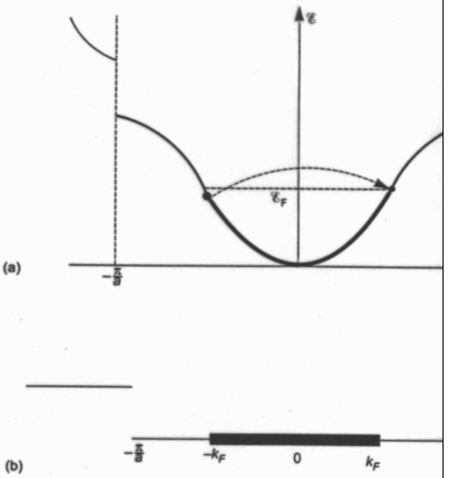
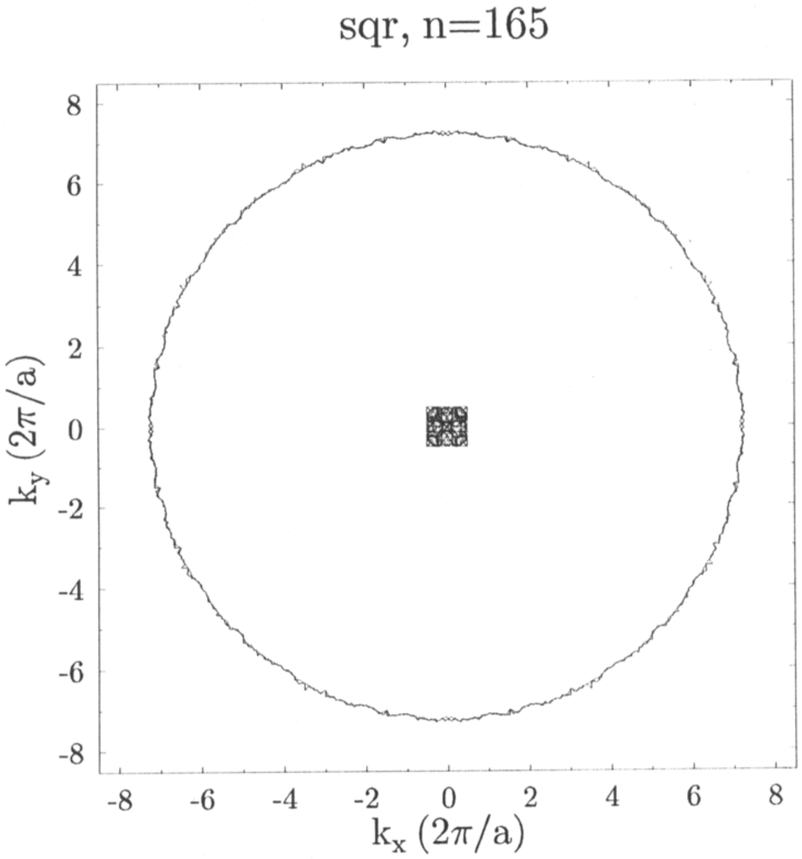
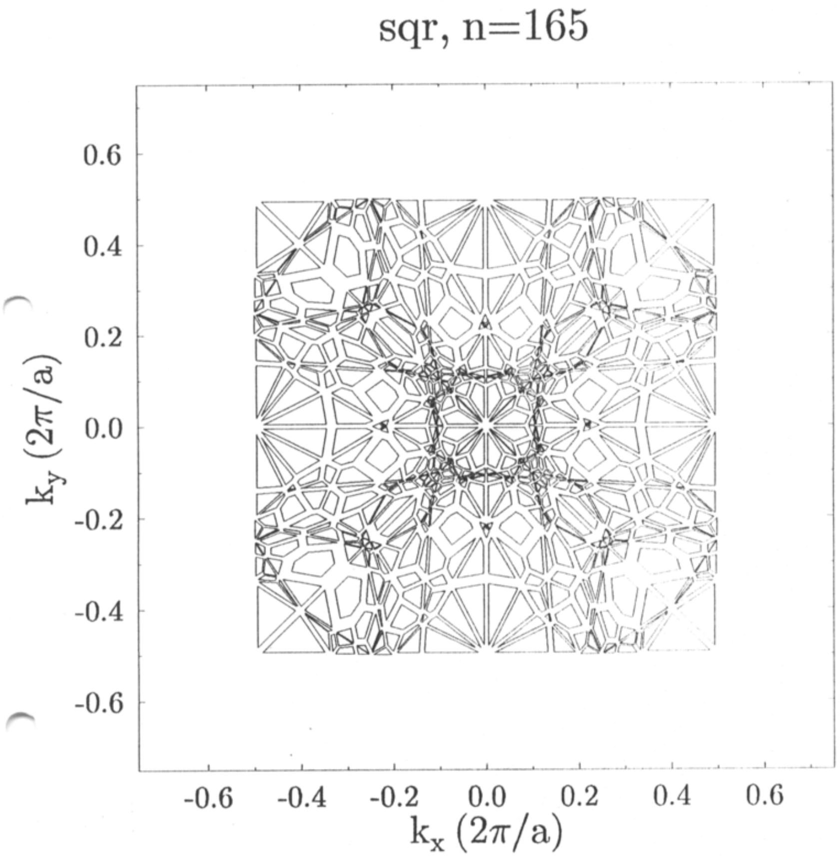
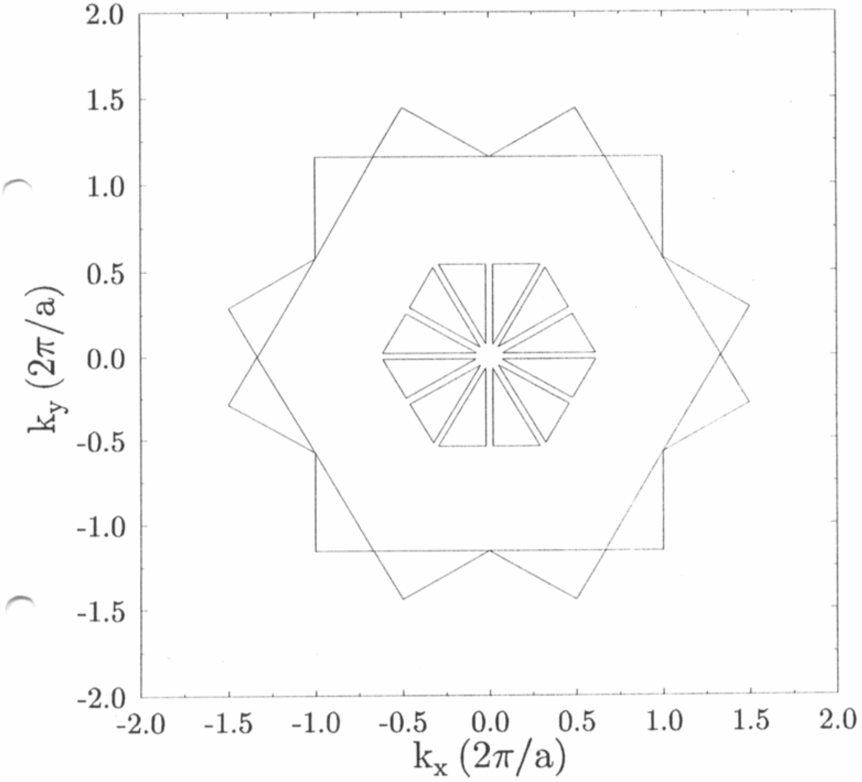


Fig. 5.26 (a) Band structure for a monovalent 1D crystal with periodi
shown by the bold curve. The system is metallic because the Fermi lev
band. A possible electronic transition, involving a change in momentu
to the finite electrical resistance, is indicated. (b) Schematic representat
for the 1D monatomic chain in the NFE approximation. There is a
boundaries, $\pm\pi/a$. If $|k_F| < \pi/a$, the electron distribution (shown by th
bodily in $\boldsymbol{k}$-space under an applied electric field and so gives a finite co
metallic behaviour is exhibited.


sqr, n=165

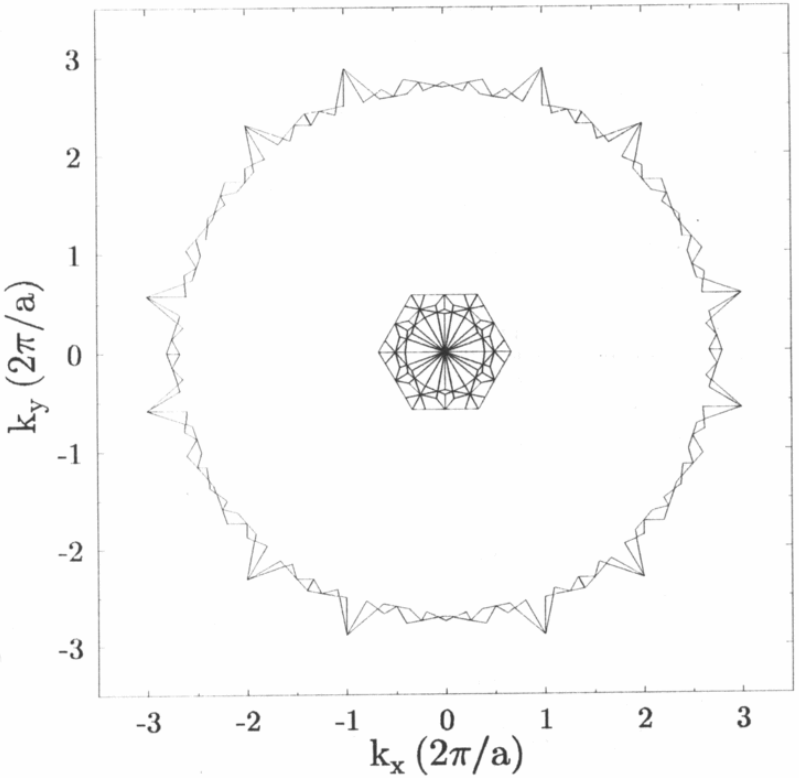

sqr, n=165

hex, n=5

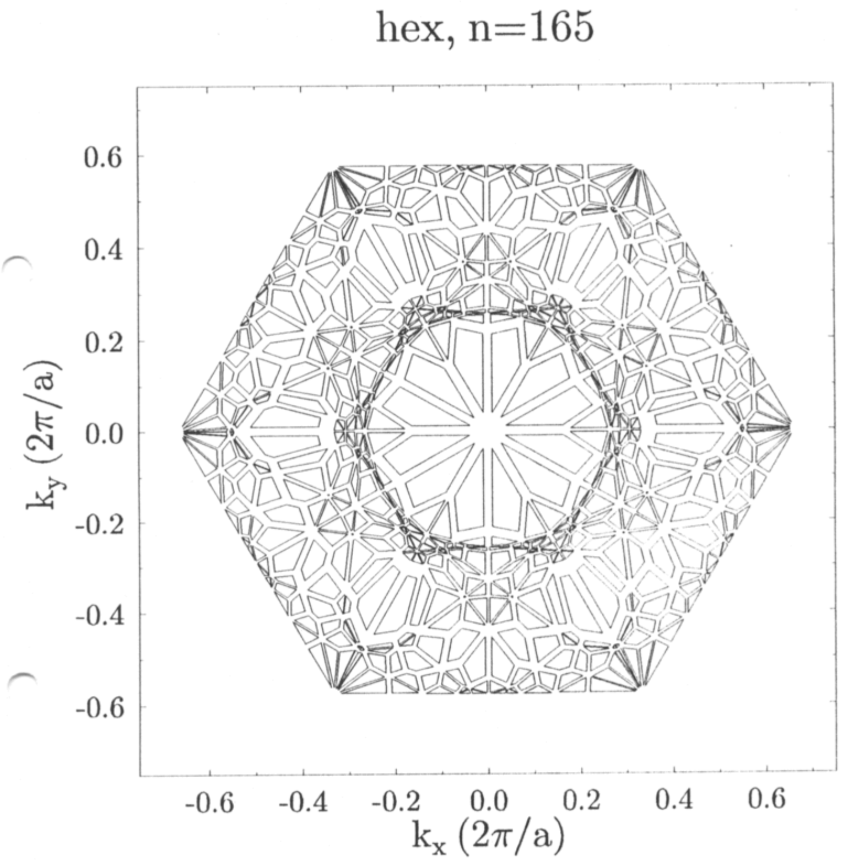


2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
k_y (2π/a)
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
k_x (2π/a)

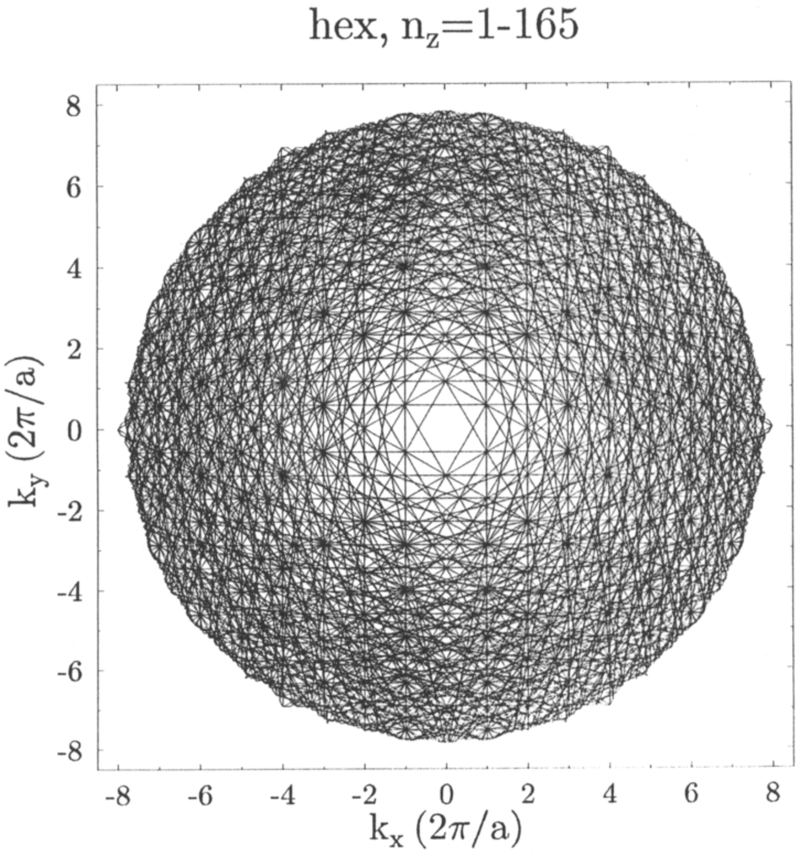
(n=21)



3
2
1
0
-1
-2
-3
k_y (2π/a)
-3
-2
-1
0
1
2
3
k_x (2π/a)



hex, n=165



hex, n_z=1-165

* Spunabrautar víxlverkun klýfur oft margfalda borða í háum samhverfupunktum.

10 – Þéttbundnar rafeindir

Gengur þegar litið má á grind atóma og finna rafeindaástönd kristalsins með truflanareikningi fyrir atómástönd.

Einangrar

Málmar með d-gildis rafeindir

* * *

Ef atómin eru þ. í grindinni að rafeindaástöndin truflast ekki vegna næstu granna þá gildir

$$H_{at}\psi_n = E_n\psi_n$$

fyrir eitt visst atóm

skörun bylgjufalla mismunandi atóma þarf að vera lítil (eða engin)

Ef skörun er þá þarf

$$H = H_{at} + \Delta U(\bar r)$$

allar leiðréttingar á atómmættinu til að lýsa lotubundna mætti grindar.

Ef $\Delta U = 0$ alltaf þegar $\psi_n(\bar r) \neq 0$ þá væri ψ_n líka lausn fyrir H.

Til að uppfylla Bloch: $\psi(\bar r+\bar R) = e^{i\bar k\cdot\bar R}\psi(\bar r)$
þá væri lausnin valin sem

$$\psi_{n\bar k}(\bar r) = \sum_{\bar R} e^{i\bar k\cdot\bar R}\phi_n(\bar r-\bar R) \qquad \uparrow \text{ má sanna}$$

($\bar k$ tekur N gildi á 1. Bs til að uppfylla BvK)

$\varepsilon_n(\bar k)$ væri óháð $\bar k$ vegna engrar skörunar bylgjufalla

Með skörum

Leitum lausnar

$$\psi(\bar r) = \sum_{\bar R} e^{i\bar k\cdot\bar R}\phi(\bar r-\bar R) \qquad (1)$$

þ.s. ϕ er ekki „atóm-fall" en verður að ákvarðast.

ϕ má liða í ψ_n: (LCAO)

$$\phi(\bar r) = \sum_n b_n\psi_n(\bar r) \qquad (2)$$

$$H\psi(\bar r) = (H_{at} + \Delta U(\bar r))\psi(\bar r) = \varepsilon(\bar k)\psi(\bar r)$$

innfalda með ψ_m og nota

$$\langle\psi_m|H_{at}|\psi\rangle = \int\psi_m^*(\bar r)\, H_{at}\psi(\bar r)\,d\bar r$$

$$= E_m\langle\psi_m|\psi\rangle$$

þá fæst

$$E_m\langle\psi_m|\psi\rangle + \langle\psi_m|\Delta U|\psi\rangle = \varepsilon(\bar k)\langle\psi_m|\psi\rangle$$

$$\rightarrow (\varepsilon(\bar k) - E_m)\langle\psi_m|\psi\rangle = \langle\psi_m|\Delta U|\psi\rangle$$

---

notum (1) og (2)

$$(\varepsilon(\bar k) - E_m)\underbrace{\sum_{\bar R} e^{i\bar k\cdot\bar R}\sum_n b_n\int d\bar r\,\psi_m^*(\bar r)\,\psi_n(\bar r-\bar R)}$$

$$= \sum_{\bar R} e^{i\bar k\cdot\bar R}\sum_n b_n\int d\bar r\,\psi_m^*(\bar r)\,\Delta U(\bar r)\,\psi_n(\bar r-\bar R)$$

Ef $\bar R = 0$ þá fæst $\langle\psi_m|\psi_n\rangle = \delta_{m,n}$

því er þetta

$$(\varepsilon(\bar k)-E_m)\,b_m = -(\varepsilon(\bar k)-E_m)\sum_n\left\{\sum_{\bar R\neq 0}\int d\bar r\,\psi_m^*(\bar r)\,\psi_n(\bar r-\bar R)\cdot e^{i\bar k\cdot\bar R}\right\}b_n$$

$$+\sum_n\left\{\int\psi_m^*(\bar r)\,\Delta U(\bar r)\,\psi_n(\bar r)\,d\bar r\right\}b_n$$

$$+\sum_n\left\{\sum_{\bar R\neq 0}\int\psi_m^*(\bar r)\,\Delta U(\bar r)\,\psi_n(\bar r-\bar R)\,e^{i\bar k\cdot\bar R}\,d\bar r\right\}b_n$$

~~$(\varepsilon(\bar k)-E_m)\,b_m = \{-(\varepsilon(\bar k)-E_m)\,\alpha(\bar R)$~~

Notum líkanið þegar rafeindaástönd eru staðbundin þ.a. liðir með

$$\int d\bar{r}\, \psi_m^*(\bar{r})\, \psi_n(\bar{r}-\bar{R}) \qquad (\text{störum})$$

eru smáir m.v. 1

Eins er búist við að

$$\int d\bar{r}\, \psi_m^*(\bar{r}) \Delta U(\bar{r})\, \psi_n(\bar{r})$$

sé smár liður, ψ_n er lítið þ.s. ΔU er ekki hverfandi

$(\Sigma(\bar{k}) - E_m) b_m$ er lítið

t.d. fyrir $m=0$

$\rightarrow \Sigma(\bar{k}) \simeq E_0 , \; b_m \simeq 0$ nema $E_m \simeq 0$

Með í liðum á ψ þarf að taka ástönd sem nærri liggja í orku

s-borði vegna eins s-ástands atóms

$$(\Sigma(\bar{k}) - E_s) b_s = -(\Sigma(\bar{k}) - E_s) \sum_{\bar{R} \neq 0} \int d\bar{r}\, \psi_s^*(\bar{r}) \psi_s(\bar{r}-\bar{R}) e^{i\bar{k}\bar{R}} b_s$$

$$+ \int d\bar{r}\, |\psi_s^*(\bar{r})|^2 \Delta U(\bar{r})\, b_s$$

$$+ \sum_{\bar{R} \neq 0} \int d\bar{r}\, \psi_s^*(\bar{r}) \Delta U(\bar{r}) \psi_s(\bar{r}-\bar{R})\, b_s$$

Umskrifum sem:

$$(\Sigma(\bar{k}) - E_s) = -(\Sigma(\bar{k}) - E_s) \sum_{\bar{R} \neq 0} \alpha(\bar{R}) e^{i\bar{k}\cdot\bar{R}}$$

$$- \beta - \sum_{\bar{R} \neq 0} \gamma(\bar{R}) e^{i\bar{k}\cdot\bar{R}}$$

eða

$$(\Sigma(\bar{k}) - E_s)\left(1 + \sum_{\bar{R} \neq 0} \alpha(\bar{R})\right) = -\beta - \sum_{\bar{R} \neq 0} \gamma(\bar{R})$$

$$\rightarrow \quad \Sigma(\bar{k}) = E_s - \frac{\beta + \sum_{\bar{R} \neq 0} \gamma(\bar{R}) e^{i\bar{k}\cdot\bar{R}}}{1 + \sum_{\bar{R} \neq 0} \alpha(\bar{R}) e^{i\bar{k}\cdot\bar{R}}}$$

$\psi_s(\bar r) \in \mathbb{R}$ og aðeins háð $|\bar r|$

$$\rightarrow \alpha(-\bar R) = \alpha(\bar R)$$

$$\Delta U(-\bar r) = \Delta U(\bar r) \leftarrow$$ speglunarsamhv. grindar

$$\gamma(-\bar R) = \gamma(\bar R)$$

Næstu grannar   nefnari $\rightarrow 1$ $\frac{1}{2}\{e^{i\bar k\cdot\bar R} + e^{-i\bar k\cdot\bar R}\}$

$$\downarrow$$

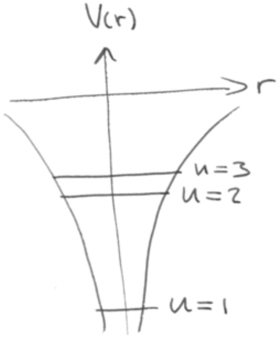
$$\rightarrow \mathcal{E}(\bar k) = E_s - \beta - \sum_{n.n.} \gamma(R) \cos(\bar k\cdot\bar R)$$

fcc (sc)

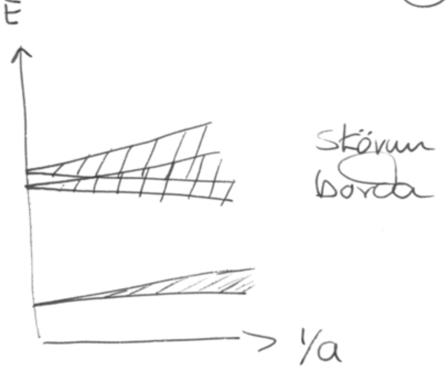
$$\bar R = \frac{a}{2}(\pm 1, \pm 1, 0),\ \frac{a}{2}(\pm 1, 0, \pm 1),\ \frac{a}{2}(0, \pm 1, \pm 1)$$

$$\mathcal{E}(\bar k) = E_s - \beta - 4\gamma \Big\{ \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right) + \cos\left(\frac{k_z a}{2}\right)\cos\left(\frac{k_x a}{2}\right) \Big\} \quad (*)$$

$\uparrow$ fleygboga háð k fyrir lítil $\bar k$



atóm



kristallur

fyrir $ka \ll 1$

$$\mathcal{E}(\bar k) \simeq E_s - \beta - 4\gamma \Big\{ \left(1 - \left(\frac{k_x a}{2}\right)^2 \frac{1}{2}\right)\left(1 - \frac{1}{2}\left(\frac{k_y a}{2}\right)^2\right) + \left(1 - \frac{1}{2}\left(\frac{k_y a}{2}\right)^2\right)\left(1 - \frac{1}{2}\left(\frac{k_z a}{2}\right)^2\right) + \left(1 - \frac{1}{2}\left(\frac{k_z a}{2}\right)^2\right)\left(1 - \frac{1}{2}\left(\frac{k_x a}{2}\right)^2\right) \Big\}$$

$$\simeq E_s - \beta - 4\gamma \left\{ 3 - \frac{k^2 a^2}{8} \cdot 2 \right\}$$

$$= E_s - \beta - 12\gamma + \gamma k^2 a^2$$

$\uparrow$

jafnorkufletir um $\bar k \simeq 0$ eru kúlusamhverfir.

* $\gamma_{ij}(\bar{R}) = -\int d\bar{r}\, \psi_i^*(\bar{r}) \Delta U(\bar{r}) \psi_j(\bar{r}-\bar{R})$

Stýrir bandbreidd borða

-> störum ⇔ borðabreidd.

* Block-ástönd -> rafeind er ekki staðbundin í kristallinum

sést líka þá $\bar{v}(\bar{k}) = \frac{1}{\hbar}\bar{\nabla}_k \varepsilon(\bar{k})$

mjórri borðar -> minni hraði

* Spuna-Brautar víxlverkun er nauðsynleg þegar ástönd eru næstum margföld.

* fjöleindahrif a -> ∞ leiðni minnka hægt og rólega

en í Raun þekkist Mott-breytingin

Lesa sjálf um Wannier

bls 187 - 188

Borðareikningar

Tvær atferðir:

1) Næstum frjálsar rafeindir s,p-málmar
2) þéttbundnar rafeindir d-málmar einangrarar

↑ Tvö markgildi á sitthvorum jaðri „rófs"
Ekki alveg ljóst hví þær verka frekar vel!

Fleiri atferðir

Til að ráða við fleiri tilfelli

fjöleindakerfi <-> fjöleindaatferðir

↓

Nálgun

↓

Ein eind í virku mætti

↑ lýst með $\psi(\bar{r})$

Safn frjálsra einda $\psi_\alpha(\bar{r})$
hver í virku mætti $V(\bar{r})$ ← sem er háð öllum öðrum ψ_α

Ólínulegar jöfnur -> ítrun lausna

Ástönd gildisrafeinda

Ástönd á innri hvelum eru staðbundin
$\psi \to 0$ fjær kjarna ψ tekur miklum breytingum nærri kjarna

Ástönd á „gildisborða" eru ekki staðbundin

Öll ástöndin eru hornrétt
—> jafnvel gildisástönd breytast hratt í kringum kjarna
↓
Ekki hægt að lýsa með næstum frjálsum ástöndum, nema mjög stór grunnur sé notaður

↓ vegna þessa og af öðrum ástöndum

Aðrar aðferðir

Einingaraðferð
-> brauðkolla form
-> viðhengdar sléttar bylgjur (APW)
-> Greensfalla aðferð (KKR)

Leiðréttar flatar bylgjur
↳ sýndarmætti

Einingaraðferð (grindareining)

uppfyllir Bloch skilyrðið

$$\boxed{\psi_{\bar{k}}(\bar{r}+\bar{R}) = e^{i\bar{k}\cdot\bar{R}}\psi_{\bar{k}}(\bar{r})}$$

Schrödinger jafnan er leyst innan aðeins einnar frumgrindareiningar

Mættið er einfaldað þ.a. aðeins ein jón ákvarðar það

Jaðarskilyrði

$$\boxed{\begin{aligned} \psi(\bar{r}) &= e^{-i\bar{k}\cdot\bar{R}}\psi(\bar{r}+\bar{R}) \\ \hat{n}(\bar{r})\cdot\bar{\nabla}\psi(\bar{r}) &= -e^{-i\bar{k}\cdot\bar{R}}\hat{n}(\bar{r}+\bar{R})\cdot\bar{\nabla}\psi(\bar{r}+\bar{R}) \end{aligned}}$$

$$\psi(\bar{r},\varepsilon) = \sum_{lm} A_{lm} Y_{lm}(\theta,\varphi)\,\chi_{l,\varepsilon}(\bar{r})$$

(almennt ekki eiginástönd L^2)

Vandi Erfitt að uppfylla jaðarsk. í flókinni einingu
Einöngruð jón í grindareiningu

④

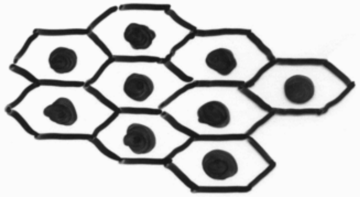
Brauðkollaform (muffin tin) (APW, KKR)

Innan einingar:

$U(\vec r) = V(|\vec r - \vec R|)$ ef $|\vec r - \vec R| < r_0$ jón
$= V(r_0) = 0$ ef $|\vec r - \vec R| > r_0$ milli

r_0 < fjarlægð næstu granna

(gæti gerst v. stýlingar)



APW Viðbættar sléttar bylgjur

Millisvæði: $\phi_{\vec k,\varepsilon}(\vec r) = e^{i\vec k\cdot\vec r}$

$\vec k, \varepsilon$ eru óháð, engin Schrödinger jafna

Atómsvæði: $\phi_{\vec k,\varepsilon}$ uppfyllir

$$-\frac{\hbar^2}{2m}\nabla^2\phi_{\vec k,\varepsilon}(\vec r) + V(|\vec r - \vec R|)\phi_{\vec k,\varepsilon}(\vec r) = \varepsilon\phi_{\vec k,\varepsilon}(\vec r)$$

$|\vec r - \vec R| < r_0$

---

⑤

Jafnan ber ekkert $\vec k$

$\vec k$ ákvarðast af jaðarskilyrðinu að $\phi_{\vec k,\varepsilon}$ sé samfellt fyrir $|\vec r| = r_0$

$$\psi_{\vec k}(\vec r) = \sum_{\vec K} C_{\vec K}\,\phi_{\vec k+\vec K,\varepsilon(\vec k)}(\vec r)$$

uppfyllir Bloch en er ekki m. samfelda afleiðu fyrir $|\vec r| = r_0$

↓

því er

$$\boxed{E[\psi] = \frac{\int\left(\frac{\hbar^2}{2m}|\nabla\psi|^2 + U(\vec r)|\psi|^2\right)d\vec r}{\int|\psi|^2 d\vec r}}$$

Lágmarkað (ákvarðar $C_{\vec K}$ og $\varepsilon(\vec k)$)

Hvikareikningur
(stórt í tölulegum reikn)

⑥

Greensfallaaðferð Korringa, Kohns og Rostokers (KKR)

Schrödinger jafnan er skrifuð á heildisformi

$$\boxed{\psi_{\bar k}(\bar r) = \int d\bar r' G_{\Sigma(E)}(\bar r-\bar r')U(\bar r')\psi_{\bar k}(\bar r')}$$

$$G_\Sigma(\bar r-\bar r') = -\frac{e^{iK|\bar r-\bar r'|}}{4\pi|\bar r-\bar r'|}$$

$K = \sqrt{2m\Sigma/\hbar^2}$ ef $\Sigma > 0$

$= i\sqrt{2m(-\Sigma)/\hbar^2}$ ef $\Sigma < 0$

notum $U(\bar r) = \sum_{\bar R} V(|\bar r-\bar R|)$ muffin tin

setjum $\bar r'' = \bar r' - \bar R$

$$\psi_{\bar k}(\bar r) = \sum_{\bar R}\int d\bar r'' G_\Sigma(\bar r-\bar r''-\bar R)V(\bar r'')\psi_{\bar k}(\bar r''+\bar R)$$

Bloch -> $\psi_{\bar k}(\bar r''+\bar R) = e^{i\bar k\cdot\bar R}\psi_{\bar k}(\bar r'')$

---

⑦

því fæst

$$\psi_{\bar k}(\bar r) = \int d\bar r' \mathcal{G}_{\bar k,\Sigma(E)}(\bar r-\bar r')V(r')\psi_{\bar k}(\bar r''+\bar R)$$

með $\mathcal{G}_{\bar k,\Sigma}(\bar r-\bar r') = \sum_{\bar R} G_\Sigma(\bar r-\bar r'-\bar R)e^{i\bar k\cdot\bar R}$

allar upplýsingar um kristallsuppbygg. og áhrif $\bar k$ eru í $\mathcal{G}$ sem er óháð U

reyna mism. U

óhliðruð jafna -> ákveða = 0

$$\Big\downarrow$$

$$\boxed{\Sigma(\bar k)}$$

Ráða aðeins kosti heildisjafna

Leiðréttar sléttar bylgjur   OPW

jón ↔ millisvæði

$$\phi_{\bar{k}} = e^{i\bar{k}\cdot\bar{r}} + \sum_c b_c \psi^c_{\bar{k}}(\bar{r})$$

gildisástönd

innri hvel
fengin frá
öðrum reikn.

Krefjumst að gildis og ástönd innri hvela séu hornrétt

$$\int d\bar{r}\, \psi^{*c}_{\bar{k}}(\bar{r})\, \phi_{\bar{k}}(\bar{r}) = 0$$

$$\Downarrow$$

$$b_c = -\int d\bar{r}\, \psi^{*c}_{\bar{k}}(\bar{r})\, e^{i\bar{k}\cdot\bar{r}}$$

Kostir

* Jafnvel ϕ_k breytast hratt nærri jón

* Leiðrétting á sléttum bylgjum er lítil á milli jóna

Sýndarmætti   Pseudopotential

útvíkkun OPW

$$\phi^v_{\bar{k}}(\bar{r}) = \sum_{\bar{K}} C_K e^{i(\bar{k}+\bar{K})\cdot\bar{r}}$$

$$\psi^v_{\bar{k}}(\bar{r}) = \phi^v_{\bar{k}}(\bar{r}) - \sum_c \left(\int d\bar{r}'\, \psi^{c*}_{\bar{k}}(\bar{r}')\, \phi^v_{\bar{k}}(\bar{r}') \right) \cdot \psi^c_{\bar{k}}(\bar{r})$$

Hægt er að umskrifa

$$H\psi^v_{\bar{k}} = \varepsilon^v_k \psi^v_{\bar{k}}$$

sem

$$(H + V^R)\phi^v_k = \varepsilon^v_k \phi^v_k$$

með

$$V^R\psi = \sum_c (\varepsilon^v_{\bar{k}} - \varepsilon_c)\left(\int d\bar{r}'\, \psi^{c*}_{\bar{k}} \psi \right) \psi^c_k$$

Sýndarmættið er skilgreint sem

$$H + V^R = -\frac{\hbar^2}{2m}\nabla^2 + V^{pseudo}$$

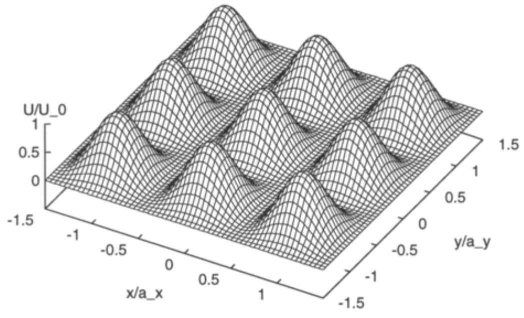
óstaðbundið

2 Lýsing kerfis

Við leggjum til grundvallar eftirfarandi andpunkta-mætti til lýsingar á virku mætti kristallsins í sléttunni:

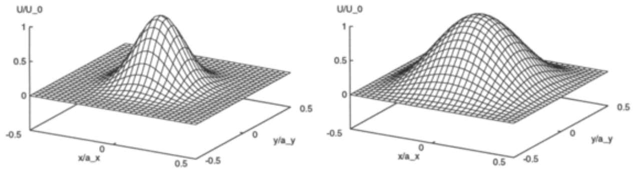
$$U(x,y) = U_0 \left[cos(\frac{\pi}{a_x}x) cos(\frac{\pi}{a_y}y) \right]^{2\alpha} . \tag{1}$$

Hér veljum við grindarfastana $a_x = a_y = 100$ nm og mættishæðina U_0 á stærðarþrepinu meV. Þessar stærðir eru í samræmi við þau GaAs kerfi sem hægt er að búa til á tilraunastofum með núverandi tækni (sjá [7]). Andpunktarnir í jöfnu (1) mynda ferningslaga Bravais-grind eins og sýnt er á mynd 1.



Mynd 1: Ferningsgrind andpunkta samkvæmt jöfnu (1). Hér er $\alpha = 1$.

Við munum skoða Bravais-grindina nánar hér á eftir en beinum nú sjónum okkar að eiginleikum andpunktanna (1). Breidd punktanna ákvarðast af veldisvísinum α. Af þessum vísi ræðst því hversu vel aðgreindir andpunktarnir eru, hver frá öðrum, og þar með hversu breiðar "rásir" liggja á milli þeirra. Þetta er sýnt á mynd 2



Mynd 2: Vel einangraður andpunktur (a) og breiður andpunktur með skörun (b). Í (a) er $\alpha = 3$ en fyrir (b) er $\alpha = 1$. Sýnd er ein frumeining í ferningsgrindinni.

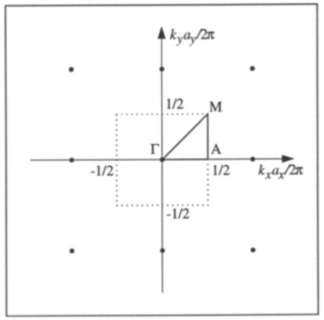
---

4 Útreikningar á orkuborðum

Samkvæmt grein 3 gefur lausn jöfnuhneppisins (25) okkur orku og eiginástönd rafeindar í andpunkta-mættinu (1). Við endurritum hér jöfnuhneppið til hægðarauka:

$$\left(\frac{\hbar^2}{2m} (\mathbf{k}+\mathbf{K})^2 - E \right) c_{\mathbf{k}+\mathbf{K}} + \sum_{\mathbf{K}' \in \mathcal{K}} \hat{U}(\mathbf{K}-\mathbf{K}') c_{\mathbf{k}+\mathbf{K}'} = 0, \;\; \forall\, \mathbf{K} \in \mathcal{K}. \tag{27}$$

Hér er $\mathcal{K} = \{\mathbf{K} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 \,|\, m_1, m_2 \in \mathrm{Z}\}$ þar sem $\mathbf{b}_1, \mathbf{b}_2$ eru grunnvigrar nykurgrindarinnar eins og þeir voru skilgreindir í kafla 2. Við munum skoða lausnirnar innan fyrsta Brillouin svæðisins og höfum sérstaklega áhuga á orkuborðunum á samhverfuásum í nykurgrindinni. Þessir ásar eru ΓA, AM og MΓ og eru þeir sýndir á mynd 4 (nafngiftir eru hér í samræmi við [7]). Ef við



Mynd 4: Fyrsta Brillouin svæðið fyrir andpunkta-grindina. Mikilvægustu samhverfupunktar ásamt nafngiftum eru sýndir.

skilgreinum einingarlausu stikana t_x og t_y þannig

$$t_x \;:=\; \frac{a_x}{2\pi}k_x \tag{28}$$

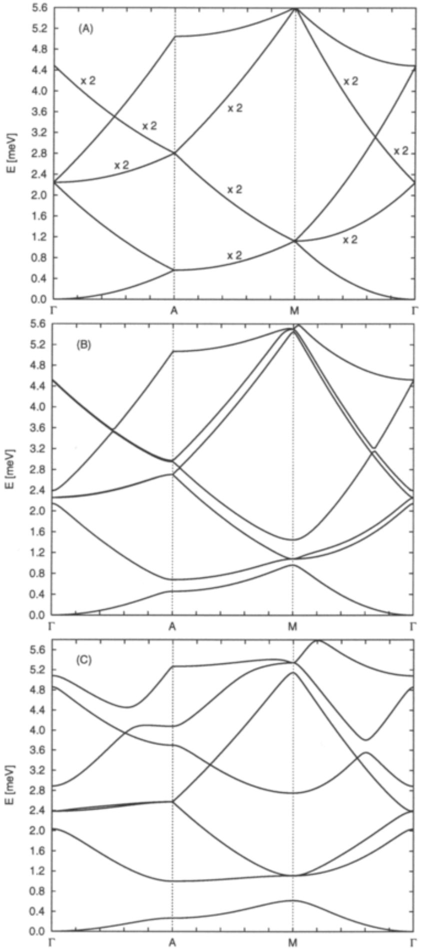
$$t_y \;:=\; \frac{a_y}{2\pi}k_y \tag{29}$$

þá má rita fyrsta Brillioun svæðið sem mengið $[-1/2, 1/2] \times [-1/2, 1/2]$. Þetta er sýnt á mynd 4. Við munum notast við þessa framsetningu svæðisins héðan í frá.

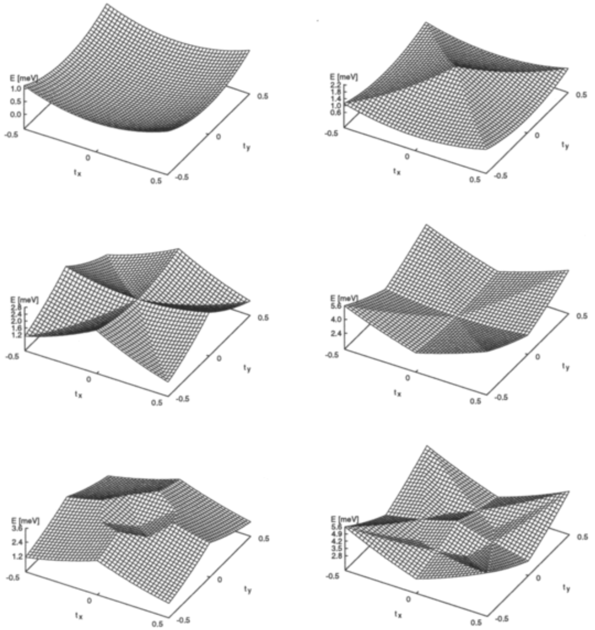
Í næstu greinum munum við leysa jöfnu (27) fyrir tvö tilvik. Annars vegar fyrir frjálsar rafeindir í umræddri grind og hins vegar fyrir rafeindir sem víxlverka við andpunkta í grindinni (sjá kafla 2).

4.1 Frjálsar rafeindir

Strangt til tekið þá hafa frjálsar rafeindir ekki orkuborða eins og lýst var í kafla 3. Þetta sést á því að víxlverkunarmættið er $U(\mathbf{r}) = 0$ fyrir frjálsar agnir



Mynd 9: Orkuborðar rafeinda í ferningsgrind andpunkta með mættishæð $U_0 = 0$ meV (A), 1 meV (B) og 5 meV (C). Borðarnir eru sýndir á samhverfuásum nykurgrindarinnar. Tvöfaldir borðar eru auðkenndir með “x 2”.



Mynd 7: Lægstu orkustig frjálsra rafeinda í ferningslaga grind. Orkustigin hafa verið flokkuð í sex “borða”.

þar sem fallið f er

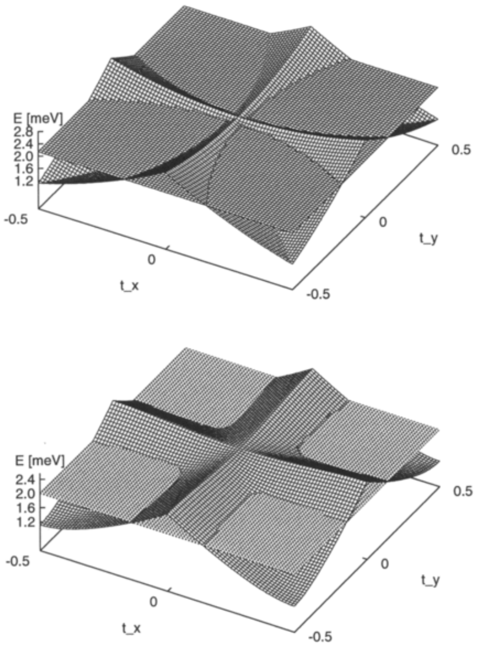
$$f(z) := 2e^{-i\frac{1}{2}z}\sin\left(\frac{1}{2}z\right)\left[\frac{2z^2-(2\pi)^2}{z(z^2-(2\pi)^2)}\right]. \tag{35}$$

Athugum nú að $\mathbf{K} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2$ og

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}. \tag{36}$$

Jöfnu (34) má því rita

$$\hat{U}(\mathbf{K}(m_1, m_2)) = \frac{U_0}{4}f(2\pi m_1)f(2\pi m_2) \tag{37}$$



Mynd 16: Skurður Fermi-orku við 3. orkuborða. Efri myndin sýnir tvívítt rafeindagas en sú neðri rafeindir í grind andpunkta. Hér er agnaþéttleikinn $n = 6 \times 10^{10}$ cm^{-2} og andpunktarnir hafa mættishæð $U_0 = 5$ meV og $\alpha = 1$.

skera plönin. Síðarnefnda atriðið er afleiðing af breyttri borðabyggingu. Eins og sést á myndum 14 og 15 þá eru orkuborðarnir í þessum tveimur kerfum töluvert ólíkir, t.d. liggur fyrsti orkuborðinn mun neðar í andpunktakerfinu en rafeindagasinu. Sá fjöldi setinna ástanda sem virðist í fljótu bragði á vanta til að rafeindaþéttleikinn sé hinn sami í kerfunum er því veginn upp af meiri sætni í neðri orkuborðum andpunktakerfisins.

Auðvelt er að sýna að þéttefni með hálffyllta orkuborða hefur ætíð málmkennda eiginleika (sjá [6]). Á myndum 16 og 18 kemur greinilega fram að 3. orkuborðinn er aðeins fylltur að hluta við rafeindaþéttleikann $n = 6 \times 10^{10}$ cm^{-2} í andpunktagrindinni. Reyndar er svo við flestar aðstæður í kerfinu okkar; orkuborðar eru hálffylltir og kerfið því málmkennt.

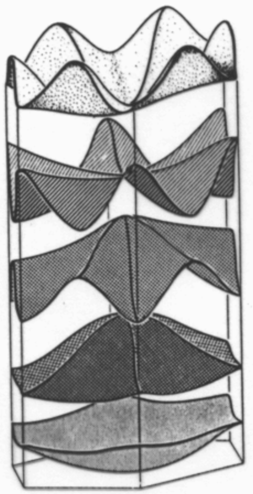


Fig. 2.17. The bands of Fig. 2.15b "smoothed" by the effect of a weak lattice potential.

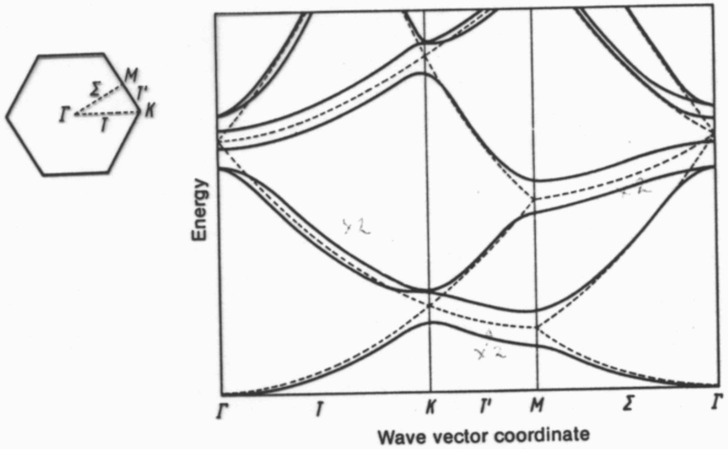
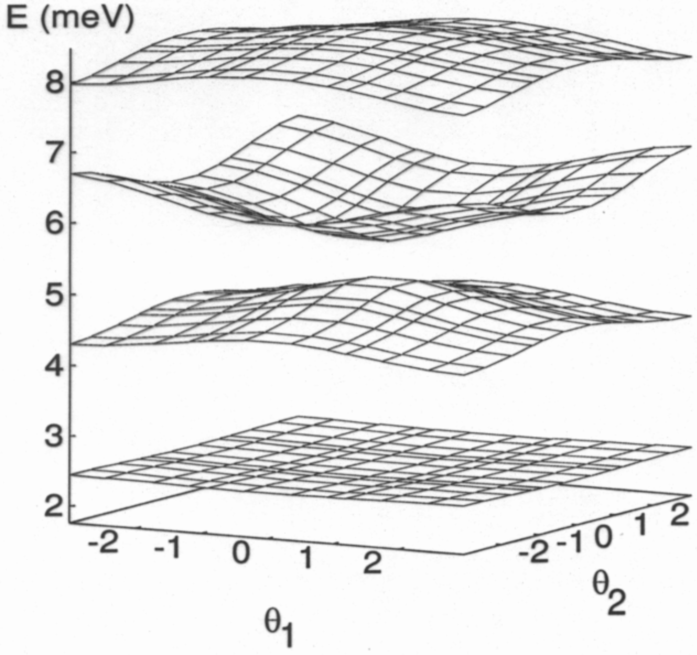
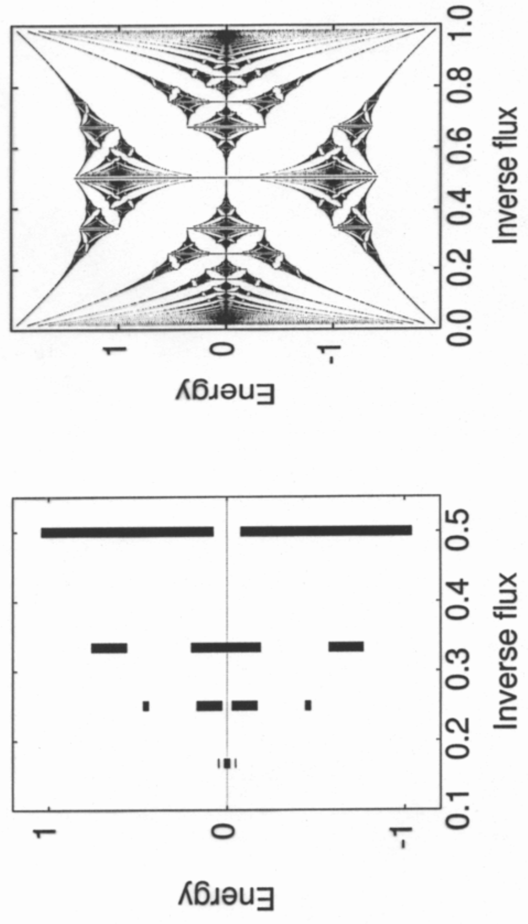


Fig. 2.18. The energy spectrum of Figs. 2.17 and 2.15b (dashed) along lines of symmetry in the Brillouin zone of the hexagonal lattice. Nomenclature of the lines of symmetry is explained at top left.

electrons were degenerate, that degeneracy has been removed by the periodic potential. At the same time the "kinks" in the bands are smoothed out and $E_n(\boldsymbol{k})$ thus becomes a smooth function there as well. Fig. 2.18 shows a section through the Brillouin zone of the previous illustration from the midpoint (Γ) to a corner of the hexagon (K), along one side to its midpoint (M), and back to Γ. The individual parabola segments are intersections of different paraboloids (centred on different $\boldsymbol{K}_m$) in the repeated zone scheme.



Gudmundsson, Fig. 1



Gudmundsson, Fig. 9

①

Hálf sígild hreyfing rafeinda í kristalli

Rafeindir í Bloch borðum:

ástönd: $|n,\bar{k}>$ $\hbar\bar{k}$: kristallsskriðþ.

$\bar{k} \in$ frumeiningu nykurgrindar
fjöldi takmarkast með B.v-K

Orkuborðar $\Sigma_n(\bar{k}+\bar{K}) = \Sigma_n(\bar{k})$

Hraði $\bar{v}_n(\bar{k}) = \frac{1}{\hbar}\bar{\nabla}\Sigma_n(\bar{k})$

Bylgjufall $\psi_{n\bar{k}}(\bar{r}) = e^{i\bar{k}\cdot\bar{r}}\, u_{n\bar{k}}(\bar{r})$

$$u_{n\bar{k}}(\bar{r}+\bar{R}) = u_{n\bar{k}}(\bar{r})$$

Óvissu lögmál: viljum geta tilgreint bylgjuvigur á Brillouin svæðinu

↳ Bylgjupakki sem í B nær yfir margar grindareiningar

---

②

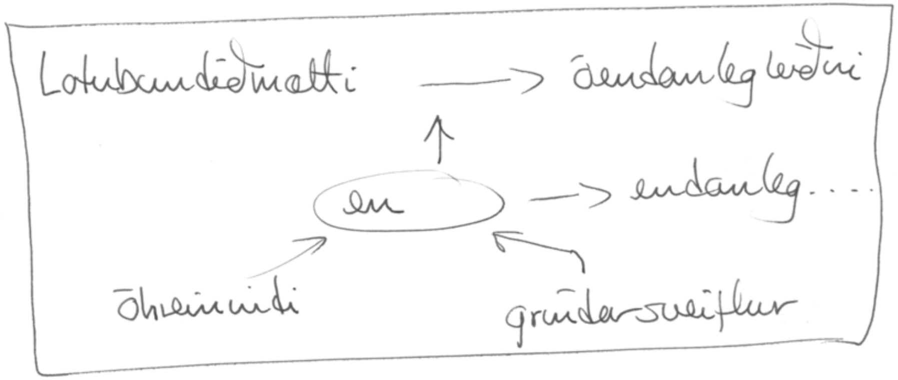
Ehrenfest gæti þá gefið:

$$\dot{\bar{r}} = \frac{\hbar\bar{k}}{m}$$

$$\hbar\dot{\bar{k}} = -e\left(\bar{E} + \frac{1}{c}\bar{v}\times\bar{H}\right)$$

Ástand $|n\bar{k}>$ hefur fastan hraða $\bar{v}_n(\bar{k})$

Engir árekstrar við jónir, en sterk víxlverkun möguleg. Kemur fram í $\Sigma_n(\bar{k})$



Líkan

Allar upplýsingar fást frá $\Sigma_n(\bar{k})$
(sem er fyrirfram gefið)

① Borðavísir ástands <u>n</u> er hreyfingarfasti

② Hreyfijöfnur rafeinda í borða <u>n</u> eru:

$$\dot{\bar{r}} = \bar{v}_n(\bar{k}) = \frac{1}{\hbar}\bar{\nabla}_{\bar{k}}\Sigma_n(\bar{k})$$

$$\hbar\dot{\bar{k}} = -e\left\{\bar{E}(\bar{r},t) + \frac{1}{c}\bar{v}_n(\bar{k})\times\bar{H}(\bar{r},t)\right\}$$

③

Enginn munur er á ástandi

$$|\bar{r},n,\bar{k}\rangle \text{ og } |\bar{r},n,\bar{k}+\bar{K}\rangle$$

öll mismunandi $\bar{k}$ eru í einingu nyturgrindarinnar

Fermieindir

$$2f(\Sigma_n(\bar{k}))\frac{d\bar{k}}{(2\pi)^3} = \frac{2d\bar{k}/(2\pi)^3}{e^{(\Sigma_n(\bar{k})-\mu)/k_BT}+1}$$

---

fastur fjöldi rafeinda á borða
tómir borðar með $\Sigma_n(k) \gg \Sigma_F$ skipta ekki máli
munum sjá að borðar með $\Sigma_n(k) \ll \Sigma_F$,
fylltir borðar skipta heldur ekki máli

→ $\boxed{\text{borðar um } \Sigma_F \text{ stýra leiðni eiginleikum}}$

Líkanið gildir ef

$$eEa \ll \frac{\left(\overset{0,1\,\text{eV}}{\Sigma_{gap}(\bar{k})}\right)^2}{\Sigma_F}$$

$$\hbar\omega_c \ll \frac{\left(\Sigma_{gap}(\bar{k})\right)^2}{\Sigma_F}$$

↗

engar örvanir á milli borða

frekar sterk rafsvið möguleg
en segulsvið undir 1T

Lág tíðni nálgun $\hbar\omega \ll \Sigma_{gap}$

Lang bylgju nálgun $\lambda \gg a$

fullir borðar

$$\vec{j} = (-e)2\int_C \frac{d\bar{k}}{(2\pi)^3}\,\frac{1}{\hbar}\,\bar{\nabla}_k \Sigma_n(\bar{k})$$ rafstraumsþétt.

$$\vec{J}_\Sigma = 2\int_C \frac{d\bar{k}}{(2\pi)^3}\,\Sigma_n(\bar{k})\frac{1}{\hbar}\,\bar{\nabla}_k \Sigma_n(\bar{k}) = \int \frac{d\bar{k}}{(2\pi)^3}\,\frac{1}{\hbar}\,\bar{\nabla}_k\left(\Sigma_n(\bar{k})\right)^2$$

↑ orkustraumsþéttleiki

$\boxed{\text{C: frumgrindareining í nyturgrind.}}$

$\Sigma_n(\bar{k})$ lotubundið fall
vegna þess að borðinn er fylltur

Lotubundið fall á C: $f(\bar{k})$ App İ

$$I(\bar{k}') = \int_C d\bar{k}\, f(\bar{k}+\bar{k}')$$

er óháð $\bar{k}'$

$$\rightarrow 0 = \bar{\nabla}' I(\bar{k}') = \int_C d\bar{k}\, \bar{\nabla}' f(\bar{k}+\bar{k}')$$

$$= \int_C d\bar{k}\, \bar{\nabla} f(\bar{k}+\bar{k}')$$

$$\bar{\nabla}' I(\bar{k}')\Big|_{\bar{k}'=0} = \int_C d\bar{k}\, \bar{\nabla} f(\bar{k}) = 0$$

$\rightarrow$ $\vec{j} = 0$ og $\vec{J}_\Sigma = 0$ fyrir fullan borða

$\boxed{\text{Leiðni er aðeins vegna rafeinda í borða sem er að hluta setinn}}$

spurn: Hver borði hefur N·2 ástönd
þ.s. N er fjöldi grindareininga
(B.v.k)

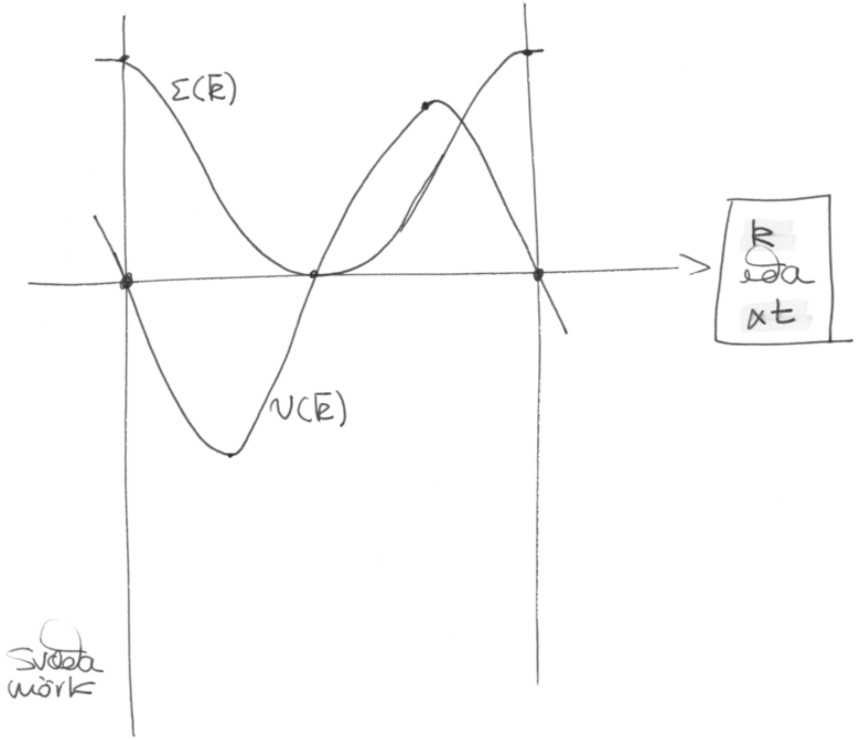
Allir borðar kristall geta verið fullir eða tómir $\Rightarrow$ fjöldi rafeinda á grindarein. er jöfn tala

Öfugt þarf ekki að vera rétt

DC-svið

$$\bar{k}(t) = \bar{k}(0) - \frac{e\bar{E}t}{\hbar}$$

$$\bar{v}(\bar{k}(t)) = \bar{v}\left(\bar{k}(0) - \frac{e\bar{E}t}{\hbar}\right)$$



$\mathcal{E}(\bar{k})$ lotubundið

Bragg speglun við Bragg sléttur

hröðun getur verið andstæð krafti

↑ $\boxed{\text{allt áhrif grindar}}$

Holur

① $$\bar{J} = (-e)2\int_{\text{setin}} \frac{d\bar{k}}{(2\pi)^3}\, \bar{v}(\bar{k}) \qquad (*)$$

$$0 = 2\int_{\text{svæði}} \frac{d\bar{k}}{(2\pi)^3}\, v(\bar{k}) = 2\int_{\text{setin}} \frac{d\bar{k}}{(2\pi)^3}\, \bar{v}(\bar{k}) + 2\int_{\text{ósetin}} \frac{d\bar{k}}{(2\pi)^3}\, \bar{v}(\bar{k})$$

því má endurrita (*) sem

$$\bar{J} = (+e)2\int_{\text{ósetin}} \frac{d\bar{k}}{(2\pi)^3}\, \bar{v}(\bar{k})$$

Straumur vegna vissra setinna rafeindaástanda er jafn straumi sem fengist með því að

tæma setin ástöndin

fylla tóm ástöndin með eindum með +e hleðslu

↑

holur

$\boxed{\text{aðeins mögulegt vegna borðamyndunar}}$

Í borða verður annaðhvort að notast
við rafeindir eða holur

---

(2) Sex hálf-sígildar hreyfijöfnur $\dot{\bar{r}} = \dots ,$
$\hbar\dot{\bar{k}} = \dots .$

fyrsta stigs jöfnur, nákvæmlega
uppfylla orsakar afleiðinga lögmál

Heimslínur agna hafa ekki sameiginlega
punkta

Í fasarúminu eru ~~ástönd~~ setin og
og ósetin ástönd aðgreind

→ ástönd þróast óháð því hvort þau
eru setin eða ekki

holur og rafeindir

(3) Svörun rafeinda við ytri áreitum

nægir
gildir líka
fyrir holur

Ósetin ástönd eru í jafnvægi (og næstum
jafnvægi) í efri hluta borða

$$\rightarrow \Sigma(\bar{k}) \simeq \Sigma(\bar{k}_0) - A(\bar{k}-\bar{k}_0)^2 , \quad A > 0$$

hágildi

línulega liðurinn
verður að hverfa

Venja er að skilgreina

$$\frac{\hbar^2}{2m^*} = A \qquad \underline{m^* > 0}$$

$$\longrightarrow \quad \bar{v}(\bar{k}) = \frac{1}{\hbar}\bar{\nabla}\varepsilon(\bar{k}) \approx -\frac{\hbar(\bar{k}-\bar{k}_0)}{m^*}$$

$$\longrightarrow \quad \bar{a} = d_t\bar{v}(\bar{k}) = -\frac{\hbar}{m^*}\dot{\bar{k}}$$

$\hbar\dot{\bar{k}} \sim \dot{\bar{p}} = F$

$\underbrace{\bar{a}}_{\text{hröðun}}$ er gagnstæð $\underbrace{\dot{\bar{k}} \leftarrow \text{samhliða krafti}}$

$\boxed{\text{það er því eins og rafeindin hafi neikvæðan massa } -m^* \text{ nærri } \bar{k}_0}$

en athugum þetta með hreyfijöfnunni

$$\hbar\dot{\bar{k}} = (-e)\left(\bar{E} + \frac{1}{c}\bar{v}\times\bar{H}\right) = -m^*\bar{a}$$

Jöfnuna má skrifa sem

$$m^*\bar{a} = (+e)\left(\bar{E} + \frac{1}{c}\bar{v}\times\bar{H}\right)$$

<u>jákvætt hlaðin eind</u> svarar á hefðbundinn hátt

<u>Svörun holu er eins og svörun rafeinda sem væri í tóma ástandinu</u>

$\boxed{\hookrightarrow \text{holur haga sér eins og eindir með jákvæðan massa og hleðslu}}$

hvort heppilegt sé að nota holu eða rafeinda hugtakið tengist því hvort hornið milli $\dot{\bar{k}}$ og $\bar{a}$ er á því svæði sem staðað er (hluti af borða)

$$\dot{\bar{k}}\cdot\bar{a} = \dot{\bar{k}}\cdot d_t\bar{v} = \dot{\bar{k}}\cdot d_t\frac{1}{\hbar}\bar{\nabla}\varepsilon(\bar{k})$$

$$= \frac{1}{\hbar}\sum_i \dot{k}_i\, d_t\left(\frac{\partial\varepsilon}{\partial k_i}\right) = \frac{1}{\hbar}\sum_i \dot{k}_i\left(\sum_j \frac{\partial^2\varepsilon}{\partial k_i\partial k_j}\frac{\partial k_j}{\partial t}\right)$$

$$= \frac{1}{\hbar}\sum_{ij}\dot{k}_i\frac{\partial^2\varepsilon}{\partial k_i\partial k_j}\dot{k}_j < 0$$

ef hornið milli $\dot{\bar{k}}$ og $\bar{a}$ er stærra en $\frac{\pi}{2}$

nærri hágildi á $\Sigma(\bar{k})$ gildir að

$$\sum_{ij} \Delta_i \frac{\partial^2 \Sigma}{\partial k_i \partial k_j} \Delta_j < 0 \quad f. \ \forall \ \bar{\Delta}$$

→ $\dot{\bar{k}} \cdot \bar{a} < 0$ nærri hágildi á $\Sigma(\bar{k})$

Venjan að skilgreina

$$\left[M^{-1}(\bar{k}) \right]_{ij} = \overset{\text{lággildi}}{\underset{\text{hágildi}}{\pm}} \frac{1}{\hbar^2} \frac{\partial^2 \Sigma(\bar{k})}{\partial k_i \partial k_j}$$

$$\dot{\bar{k}} \cdot \bar{a} = \frac{1}{\hbar} \sum_{ij} \dot{k}_i \frac{\partial^2 \Sigma}{\partial k_i \partial k_j} \dot{k}_j = \sum_i \dot{k}_i a_i$$

$$\rightarrow \quad a_i = \frac{1}{\hbar^2} \sum_j \frac{\partial^2 \Sigma}{\partial k_i \partial k_j} \hbar \dot{k}_j$$

$$\rightarrow \quad \boxed{\bar{a} = \pm M^{-1}(\bar{k}) \hbar \dot{\bar{k}}} \quad \begin{matrix} \text{lággildi} \\ \text{hágildi} \end{matrix}$$

Virki massa þinurinn er skilgreindur til að hreyfijöfnur líkist jöfnunum fyrir frjálsar eindir og áhrif grinda felist öll í $M^{-1}(\bar{k})$

Fast segulsvið

$$\bar{E} = 0 \, , \quad \bar{H} \neq 0$$

$$\dot{\bar{r}} = \bar{v}(\bar{k}) = \frac{1}{\hbar} \bar{\nabla} \Sigma(\bar{k})$$

$$\hbar \dot{\bar{k}} = (-e) \frac{1}{c} \bar{v}(\bar{k}) \times \bar{H}$$

↓

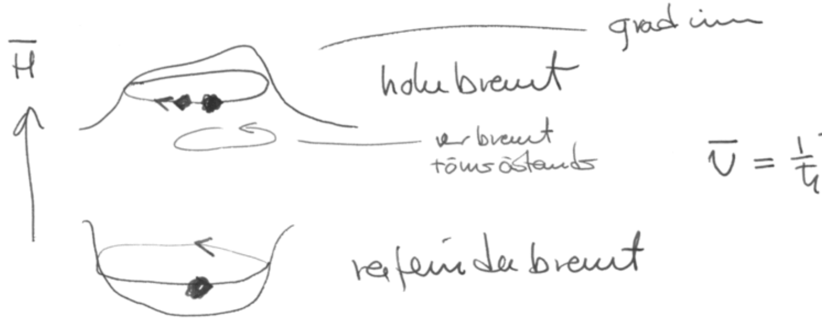
þáttur $\bar{k}$ samhliða $\bar{H}$ er hreyfingarfasti

$\Sigma(\bar{k})$ er hreyfingafasti, því krafturinn er alltaf hornréttur á $\bar{v}$

Braut eindar í k-rúminu er ákveðin af skurðferli sléttu ⊥ á $\bar{H}$ og jafnorku fleti $\Sigma(\bar{k})$ = fasti

stefnan ákveðst af hægri handar reglu

⑥



$$\bar{v} = \frac{1}{\hbar}\bar{\nabla}\varepsilon(\bar{k})$$

Rafeind

(ath í bók)

↳ tölum um holur í eftir dæminu

Í staðarrúmi

$$\hat{H} \times \hbar\dot{\bar{k}} = (-e)\frac{1}{c}\,\hat{H}\times\left(\bar{v}(\bar{k})\times\bar{H}\right)$$

$$= -\frac{eH}{c}\,\hat{H}\times\left(\bar{v}(\bar{k})\times\hat{H}\right)$$

$$= -\frac{eH}{c}\left\{\bar{v}\left(\hat{H}\cdot\hat{H}\right) - \hat{H}\left(\hat{H}\cdot\bar{v}\right)\right\}$$

$$= -\frac{eH}{c}\left\{\dot{\bar{r}} - \hat{H}\left(\hat{H}\cdot\dot{\bar{r}}\right)\right\} = -\frac{eH}{c}\,\dot{\bar{r}}_{\perp}$$

heildast sem

$$\bar{r}_{\perp}(t) - \bar{r}_{\perp}(0) = -\underbrace{\frac{\hbar c}{eH}}_{\ell^2 :\ \text{segullengd}}\,\hat{H}\times\left(\bar{k}(t) - \bar{k}(0)\right)$$

⑦

$\bar{k}$ liggur í sléttu $\perp$ á $\bar{H}$

→ $\bar{r}$-braut liggur í sömu sléttu en snúin um $\pi/2$

$$\boxed{\text{Brautir þurfa ekki að vera lokaðar frekar en jafnorkufletir}}$$

lesa framhald lauslega

①

Yfirborðshrif

Lausleg yfirferð hér, Lesa sjálf.

Mikilvægi .... Ekki farið í hér.

Mættið frá Wigner-Seitz grindareiningu

$$U(\vec{r}) = -e\int_C d\vec{r}\,' \frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}$$

fellur eins og r^{-5} ef einingin er óhlaðin, grindin hefur punktsamhverfu og tenings samhverfu

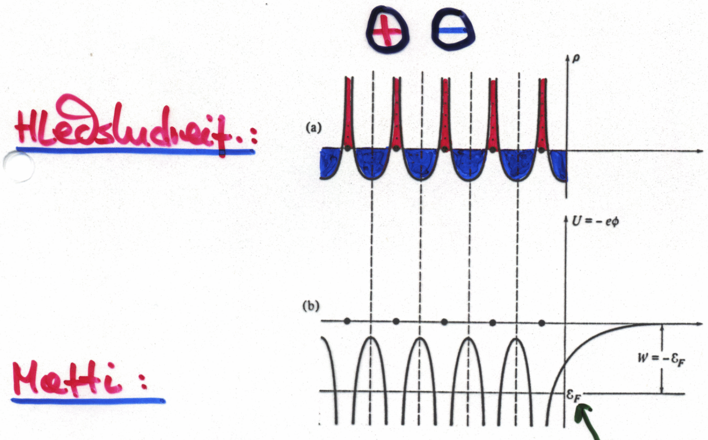
Mættið deyr mjög hratt út
Oft nægir víxlverkun við næstu granna.

Ef þessir eiginleikar óendanlegs kristalls gilda einnig í endanlegum kristalli þá gæti mætti við yfirborð litið út á eftirfarandi hátt:

---

②

Engin endurröðun við yfirborðið, engin söfnun hleðslu.



Fermi orka
Efnamætti μ
Næstum sama
ef $T_F >>> T$

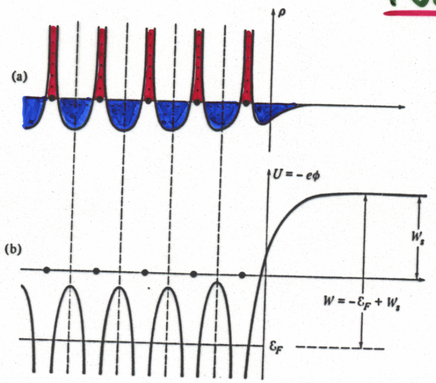
Minnsta orka sem þarf til að fjarlægja eina rafeind væri

$$W = 0 - \varepsilon_F = -\varepsilon_F \geq 0$$

Vinnufall Lokaástand upphafsástand

En, Grindin breytist við yfirborðið, fjarlægðir breytast, endurröðun atóma. Hleðsludreifing breytist.

Einfalt líkan -> túlka sem yfirborðslag tvískauta



ekki bara tvískautalag
↓
Yfirborðslag -> rafsvið $\bar{E}$, viðbótarorka sem þarf

$$W_s = e\int d\bar{l}\cdot\bar{E}$$

Vinnufallið verður

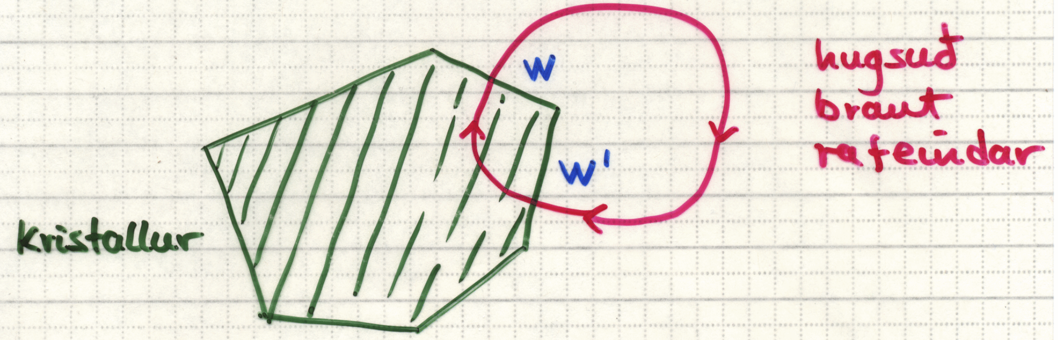
Lokaástand

upphafsást.

$$\rightarrow W = W_s - \Sigma_F$$

Spennumunur yfirborða sama kristalls

Endurröðun, eða hleðsludreifing getur verið mismunandi fyrir mism. yfirborð



Mismunandi yfirborð -> mism. vinnuföll

Geyminn kraftur -> vinnan fyrir hringinn = 0

en $W \neq W'$ -> yfirborðin verða að vera undir mismunandi spennu

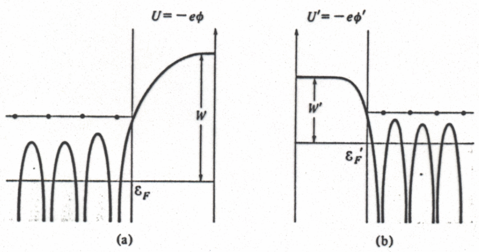
$$-e(\phi - \phi') = W - W'$$

Vinnufall er skilgreint sem lægsta orka sem þarf til að fjarlægja rafeind

↓

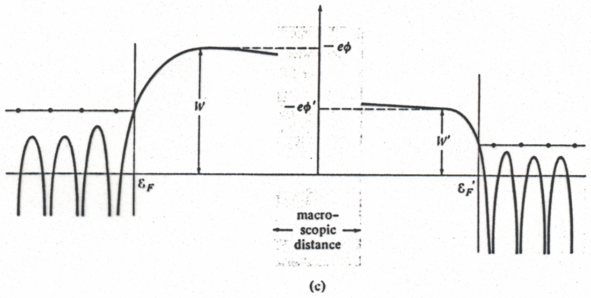
Leiðir til snertispennu

Snertispenna



(a) (b)

engin snerting



(c)

Snerting

Snerting í jafnvægi → $\mu = \mu'$

↑ næst með færslu rafeinda á milli hluta

↓

ekki lengur óhlaðnir → yfirborðshleðsla

↓

Snertispenna

Lesa afgang kaflans lauslega sjálf

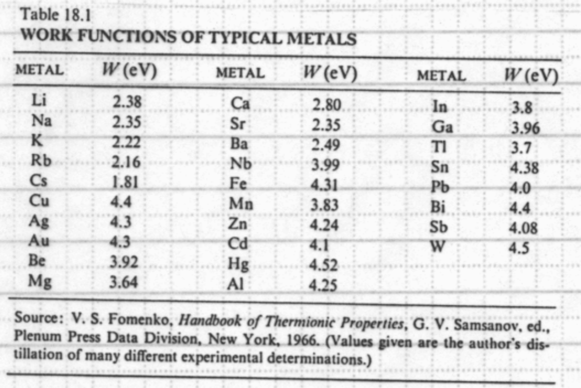


Table 18.1
WORK FUNCTIONS OF TYPICAL METALS

METAL	W (eV)	METAL	W (eV)	METAL	W (eV)
Li	2.38	Ca	2.80	In	3.8
Na	2.35	Sr	2.35	Ga	3.96
K	2.22	Ba	2.49	Tl	3.7
Rb	2.16	Nb	3.99	Sn	4.38
Cs	1.81	Fe	4.31	Pb	4.0
Cu	4.4	Mn	3.83	Bi	4.4
Ag	4.3	Zn	4.24	Sb	4.08
Au	4.3	Cd	4.1	W	4.5
Be	3.92	Hg	4.52		
Mg	3.64	Al	4.25		

Source: V. S. Fomenko, *Handbook of Thermionic Properties*, G. V. Samsanov, ed., Plenum Press Data Division, New York, 1966. (Values given are the author's distillation of many different experimental determinations.)

Flokkun kristallaðs efnis

Lesa að mestu sjálf

Algerlega lotubundinn kristallur
T = 0

tómir borðar
fylltir borðar
↓
Einangrarar

tómir borðar
borðar, að hluta tómir
fylltir borðar
↓
málmar

T ≠ 0, orkugeil
ekki breið

veilur
← hálfleiðarar

flokkun samkvæmt ástandarúmi
(bylgjuvigra)

Í staðarrúminu er flokkun ekki
eins einföld,
en skörun bylgjufalla segir sögu

Einangrarar

Samgildur kristallur (Covalent)

Bylgjuföll þurfa ekki að vera staðbundin
við jónir

allir borðar fullir eða tómir

Rafeindahleðsla milli jóna venjul.
ekki einsleit <> efnatengi

Demantur $E_g = 5.5 eV$

Sameindakristallur

þéttbundnar rafeindir

veikir kraftar
tvístaut-tvístaut
spanað tvístaut

Ne, Ar, Kr, Xe, H_2, N_2 ....

$-r^{-6}$
$+r^{-12}$

Jónakristallur

þéttbundnar rafeindir, en oft ólíkt
upphaflegum atómum
Rafeindir safnast í kringum vissar jónir

NaCl

sterkir kraftar

Kristallur m. vetnistengjum

Málmar

frekar jöfn dreifing næstum frjálsra rafeinda

Næstum frjálsar rafeindir oft

víxlverkun milli rafeinda (fermíeinda) dofnar með vaxandi þéttleika rafeinda

$n_s \sim 1/r_s^3$ $n_s \uparrow$ $r_s \downarrow$

$E_{kin} \sim \frac{1}{r_s^2}$ fermíeindir

$E_{pot} \sim \frac{1}{r_s}$

$\hookrightarrow E_{kin} > E_{pot}$

Jellium Model of Metallic Nanocohesion

C. A. Stafford,[1,*] D. Baeriswyl,[1] and J. Bürki[1,2]
[1]*Institut de Physique Théorique, Université de Fribourg, CH-1700 Fribourg, Switzerland*
[2]*Institut Romand de Recherche Numérique en Physique des Matériaux, CH-1015 Lausanne, Switzerland*

(Received 17 March 1997)

A unified treatment of the cohesive and conducting properties of metallic nanostructures in terms of the electronic scattering matrix is developed. A simple picture of metallic nanocohesion in which conductance channels act as delocalized chemical bonds is derived in the jellium approximation. Universal force oscillations of order ε_F/λ_F are predicted when a metallic quantum wire is stretched to the breaking point, which are synchronized with quantized jumps in the conductance. [S0031-9007(97)04243-9]

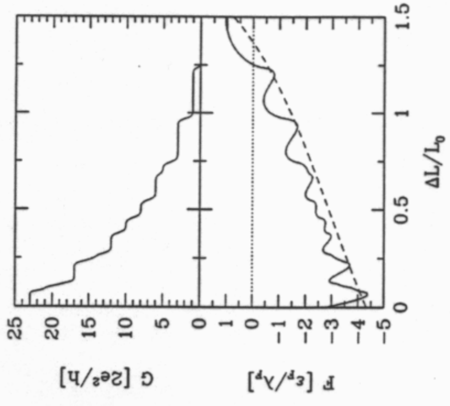


FIG. 2. Electrical conductance G and tensile force F of a cosine constriction in a cylindrical quantum wire of radius $k_F R = 11$ versus the elongation $\Delta L/L_0$. For the calculation of G, an initial length $k_F L_0 = 50$ was assumed. The dashed line indicates the contribution to the force due to the macroscopic surface tension $F_S = -\sigma \partial S/\partial L$, where S is the surface area of the system and $\sigma = \varepsilon_F k_F^2/16\pi$. F_S determines the overall

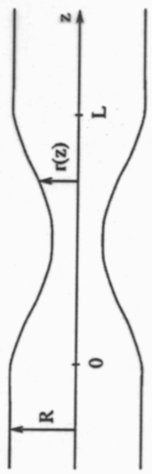


FIG. 1. Schematic diagram of a constriction in a cylindrical quantum wire. Electrons are confined along the z axis by a hard-wall potential at $r = r(z)$. Two different geometries are considered: $r(z) = (R + R_{\min})/2 + (R - R_{\min})\cos(2\pi z/L)/2$ (cosine constriction) and $r(z) = R_{\min} + (R - R_{\min})(2z/L - 1)^2$ (parabolic constriction), with $r(z) = R$ for $z < 0$ and $z > L$. The minimum radius of the neck $R_{\min}$ as a function of the elongation $\Delta L/L_0$ is determined by a constant volume constraint $\int_0^L r(z)^2\,dz = R^2 L_0$.

Samloðun

Mikilvægi → sögulegt

→ upphaf bandareikn.

→ Orkustig veilna (mikilvægi íbótar)

Sameindakristallar (atómkristallar) Ne, Ar, Kr, Xe

veikt mætti milli atóma (sameinda)

lítil breyting á rafeindadreifingu

↕

Víxlverkun ↔ spanað tvískaut

aðdráttarkraftur $\sim -r^{-6}$ ← truflanareikn.

fráhrinding, Pauli … $\sim +r^{-12}$ ←

Stikun mættis

(engin ástæða fyrir einföldum lið)

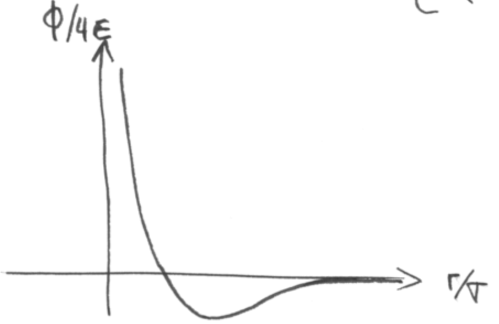
Lennard-Jones 6-12 mætti

$$\phi(r) = 4\epsilon\left\{\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right\}$$

$$\sigma = \left(\frac{B}{A}\right)^{1/6}$$

$$\epsilon = \frac{A^2}{4B}$$

↗ mátunar stikar



mjög veikir kraftar fyrir eðalgösin $\epsilon \sim 1\,\text{meV}$

Heildarorka kristalls

stöðuorka eins atóms í miðju hnitakerfis

$$\sum_{R \neq 0} \phi(\bar{R})$$

← engin sjálfsvíxlv.

margfaldað með N gefur tvisvar heildarorku kristalls. (hvert par atóma tvítalið) ->

● heildarorka á atóm

$$u = \frac{1}{2}\sum_{\bar{R}\neq 0} \phi(\bar{R})$$

Setjum $\bar{R} = \alpha(\bar{R})\, r$

víddarlaus tala

fjarlægð næstu granna

$$\to \quad u = 4\epsilon\left\{\frac{1}{2}\sum_{\bar{R}\neq 0}\frac{1}{\alpha(\bar{R})^{12}}\left(\frac{\sigma}{r}\right)^{12} - \frac{1}{2}\sum_{\bar{R}\neq 0}\frac{1}{\alpha(\bar{R})^{6}}\left(\frac{\sigma}{r}\right)^{6}\right\}$$

$$= 2\epsilon\left\{A_{12}\left(\frac{\sigma}{r}\right)^{12} - A_6\left(\frac{\sigma}{r}\right)^{6}\right\}$$

með

$$A_n = \sum_{\bar{R}\neq 0} \alpha(\bar{R})^{-n}$$

Tafla 20.2 gefur A_n fyrir

SC, BCC og FCC

og $n \geq 4$

Alklassískir reikn., engin núllpunktsorka

-> gæti lýst þungum atómum

(engin ónumhreyfing atóma)

Jafnvægisþættir

r má finna frá $\frac{\partial u}{\partial r} = 0$

$$\frac{\partial u}{\partial r} = 2\epsilon\left\{A_{12}\sigma\, 12\left(\frac{\sigma}{r}\right)^{11} - A_6\sigma 6\left(\frac{\sigma}{r}\right)^{5}\right\} = 0$$

$$\to \quad A_{12}2\left(\frac{\sigma}{r}\right)^{6} - A_6 = 0$$

$$\to \quad r_0 = \left(\frac{2A_{12}}{A_6}\right)^{1/6}\sigma = 1{,}09\sigma$$

Passar vel við mæld gildi f. þung. atóm

$$U_0 = U(r_0) = 2\epsilon\left\{A_{12}\left(\frac{A_6}{2A_{12}}\right)^2 - A_6\left(\frac{A_6}{2A_{12}}\right)\right\}$$

$$= 2\epsilon\left\{\frac{A_6^2}{4A_{12}} - \frac{A_6^2}{2A_{12}}\right\} = -\frac{\epsilon A_6^2}{2A_{12}}$$

$$= -8{,}6\,\epsilon$$

Passar vel við mælingar

Nú er einnig hægt að reikna

fjaðurstuðul $B = -V\left(\frac{\partial P}{\partial V}\right)_T$

því $B = v\frac{\partial}{\partial v}\left(\frac{\partial u}{\partial v}\right)$, $v = \frac{V}{N}$

Passar vel f. Xe og Kr en
illa fyrir léttari efnin

↳ væntanlega núllpunktsorka

Jónakristallar

Sterk Coulomb víxlverkun

↳ heildar kristallaorka á jónapar

$$U(r) = U_{coul}(r) + U_{core}(r)$$

↑ fráhrinding

Jónapar:

$\frac{a}{2}$

{ neikvæð anjón í $\bar{R} \in \mathcal{B}$
og jákvæð katjón hliðruð $\bar{d}$ frá $\bar{R}$

t.d. fcc Bravais grind fyrir NaCl

$r = \frac{a}{2}$ $(=|d|)$ fjarlægð næstu granna

$$|\bar{R}| = \alpha(\bar{R})\,r$$
$$|\bar{R}+\bar{d}| = \alpha(\bar{R}+\bar{d})\,r$$

Stærsti hlutinn kemur frá U_{coul}

heildarorka einnar jónar (katjónar)

$$-\frac{e^2}{r}\left\{\frac{1}{\alpha(\bar{d})}+\sum_{\bar{R}\neq 0}\left(\frac{1}{\alpha(\bar{R}+\bar{d})}-\frac{1}{\alpha(\bar{R})}\right)\right\}$$

og því eins og áður

$$U_{coul}(r)=-\frac{e^2}{r}\left\{\frac{1}{\alpha(\bar{d})}+\sum_{\bar{R}\neq 0}\left(\frac{1}{\alpha(\bar{R}+\bar{d})}-\frac{1}{\alpha(\bar{R})}\right)\right\}$$

↑

Stærðfræðilega ekki vel skilgreind röð

umröðun -> hvaða svar sem er!

Hver er eðlisfræðilega merkingin?

Er hún til?

Summu röð <-> mism. yfirborð

↓

mism. yfirborðshleðsla

↑

Stærsta fyrir N -> ∞

Magar leiðir út

Summa óhlaðna eininga sem víxlverka veikt + ...

Fasti Madelungs →

$$U_{coul}(r)=-\alpha\frac{e^2}{r}$$

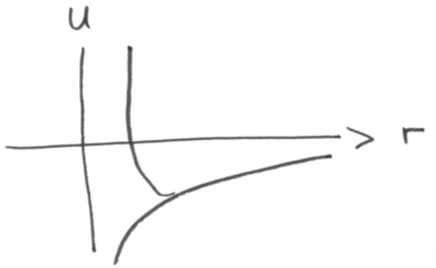
Niðurstaða reiknings fyrir ~~víxlverkun~~ heildar víxlverkunarorkuna á jóna par

CsCl	$\alpha = 1,7627$
NaCl	$\alpha = 1,7476$ ....

Stöðugleiki kristallsins fæst með U_{core}

↳ stikuð oft með

$$U(r)=-\frac{\alpha e^2}{r}+\frac{c}{r^m}$$



Samgildir kristallar

Mikil breyting á rafeindadreifingu
↳ engin einföld algild líkön
↳ Borðareitir.

Málmar með næstum frjálsar rafeindir

Hér skiptir rafeindagasið mestu
(Sterk skýling á jóna mætti)

Sígild hreyfing kristalls

Af hverju? tilraunaniðurstöður

Jafnvægi

- Eðlisvarmi, lítill hluti er vegna rafeindakerfis
- Þéttni, samloðun vantar núllpunkts hreyf.
- Hitaþensla
- Bráðnun

Flutningseiginleikar
- rafleiðni
- hitaleiðni
- ofurleiðni BCS

Víxlverkun við geislun röntgen
⋮

① Jafnvægis staðsetn jóna er $\bar{R}$

Meðalgildi staðsetn er $\bar{R}$

② sveifla jóna er lítil m.v. a

lýsir ekki bráðnun, sveimi .....

<u>Hreintónanálgun</u> (Harmonic)

Til eru mikilvægir eiginleikar sem skýrast með hærri nálgun (anharmonic)

② Er ekki rétt lýsing á He-kristalli

"skammta storka"

núllp. útslag er að sömu stærðargráðu eins og a

Staðsetn. jóna

$$\bar{r}(\bar{R}) = \bar{R} + \bar{u}(\bar{R})$$

Jafnvægis p. meðalgildi

breyting m.v. $\bar{R}$

Heildarorka kristalls (sígild ef hreyfiorku. er sleppt)

$$U = \frac{1}{2}\sum_{\bar{R}\,\bar{R}'} \phi(\bar{R}-\bar{R}') = \frac{N}{2}\sum_{\bar{R}\neq 0} \phi(\bar{R}) \,.$$

forðast tvítalin.

summa allra parvíxlv.

En tillit þarf að taka til hreyfinga

$$U = \frac{1}{2}\sum_{\bar{R}\,\bar{R}'} \phi(\bar{r}(\bar{R}) - \bar{r}(\bar{R}'))$$

málið er háð breytunum $\bar{u}(\bar{R})$

þurfum að skoða eiginleika kerfis sem lýst er með

$$H = \sum_{\bar{R}} \frac{\bar{P}(\bar{R})^2}{2M} + U$$

Hreintóna nálgun

Mættið ϕ er oft mjög flókið

$\rightarrow$ nálgun, lítið útslag

↳ notum Taylor liðun

$$f(\bar{r}+\bar{a}) = f(\bar{r}) + \bar{a}\cdot\bar{\nabla} f(\bar{r}) + \frac{1}{2}(\bar{a}\cdot\bar{\nabla})^2 f(\bar{r}) + \cdots$$

notum þetta fyrir U þ.a.

$$U = \frac{N}{2}\sum \phi(\bar{R}) + \frac{1}{2}\sum_{\bar{R}\bar{R}'}(\bar{u}(\bar{R}) - \bar{u}(\bar{R}'))\cdot\bar{\nabla}\phi(\bar{R}-\bar{R}')$$

$$+ \frac{1}{4}\sum_{\bar{R}\bar{R}'}\left\{(\bar{u}(\bar{R}) - \bar{u}(\bar{R}'))\cdot\bar{\nabla}\right\}^2 \phi(\bar{R}-\bar{R}') + \cdots$$

Línulegi liðurinn

$$\frac{1}{2}\sum_{\bar{R}\bar{R}'}\left\{\bar{u}(\bar{R}) - \bar{u}(\bar{R}')\right\}\cdot\bar{\nabla}\phi(\bar{R}-\bar{R}')$$

$$= \frac{1}{2}\sum_{\bar{R}} u(\bar{R}) \underbrace{\sum_{\bar{R}'} \bar{\nabla}\phi(\bar{R}-\bar{R}')} + \frac{1}{2}\sum_{\bar{R}'} u(\bar{R}') \underbrace{\sum_{\bar{R}} \bar{\nabla}\phi(\bar{R}-\bar{R}')}$$

summa allra krafta

↳ $-F$ sem verkar á $\bar{R}$ eða $\bar{R}'$

$\bar{R}$ og $\bar{R}'$ eru jafnvægisstöður $\rightarrow$ $\underline{F = 0}$

Eftir standa

$\longrightarrow$ $U^{eq} = \frac{N}{2}\sum \phi(\bar{R})$ fasti

sem oft má sleppa

(ekki þ. heildarorka skiptir máli, þéttleika, samleðu ...)

og

$$U^{harm} = \frac{1}{4}\sum_{\substack{\bar{R}\bar{R}' \\ \mu,\nu = x,y,z}} \left\{u_\mu(\bar{R}) - u_\mu(\bar{R}')\right\} \phi_{\mu\nu}(\bar{R}-\bar{R}') \left\{u_\nu(\bar{R}) - u_\nu(\bar{R}')\right\}$$

með $$\phi_{\mu\nu}(\bar{r}) = \frac{\partial^2 \phi(\bar{r})}{\partial r_\mu \partial r_\nu}$$

Almennara form er

$$U^{harm} = \frac{1}{2}\sum_{\substack{\bar{R}\bar{R}' \\ \mu\nu}} u_\mu(\bar{R}) D_{\mu\nu}(\bar{R}-\bar{R}') u_\nu(\bar{R}') .$$

og í okkar sértilfelli er

$$D_{\mu\nu}(\bar{R}-\bar{R}') = \delta_{\bar{R},\bar{R}'} \sum_{\bar{R}''} \phi_{\mu\nu}(\bar{R}-\bar{R}'') - \phi_{\mu\nu}(\bar{R}-\bar{R}')$$

athugum með innsetningu

$$U^{harm} = \frac{1}{2}\sum_{\substack{\bar{R}\bar{R}' \\ \mu\nu}} u_\mu(\bar{R}) \delta_{\bar{R}\bar{R}'} \sum_{\bar{R}''} \phi_{\mu\nu}(\bar{R}-\bar{R}'') u_\nu(\bar{R}')$$

$$- \frac{1}{2}\sum_{\substack{\bar{R},\bar{R}' \\ \mu\nu}} u_\mu(\bar{R}) \phi_{\mu\nu}(\bar{R}-\bar{R}') u_\nu(\bar{R}')$$

$$= \frac{1}{2}\sum_{\substack{\bar{R}\bar{R}' \\ \mu\nu}} u_\mu(\bar{R}) \phi_{\mu\nu}(\bar{R}-\bar{R}') u_\nu(\bar{R}')$$

röð skiptir ekki máli

$$- \frac{1}{2}\sum_{\substack{\bar{R}'\bar{R} \\ \mu\nu}} u_\mu(\bar{R}') \phi_{\mu\nu}(\bar{R}'-\bar{R}) u_\nu(\bar{R})$$

$$= \frac{1}{4}\sum_{\bar{R}\bar{R}'} \left\{u_\mu(\bar{R}) - u_\mu(\bar{R}')\right\} \phi_{\mu\nu}(\bar{R}-\bar{R}') \left\{u_\nu(\bar{R}) - u_\nu(\bar{R}')\right\}$$

því krossliðir geta

$$\sum_{\bar{R}'} \phi_{\mu\nu}(\bar{R}-\bar{R}') = \frac{\partial^2}{\partial R_\mu \partial R_\nu} \overbrace{\sum_{\bar{R}'} \phi(\bar{R}-\bar{R}')}^{\text{óháð } \bar{R}} = 0$$

Jóna-jóna víxlverkunin er ekki almennt ekki summa parvíxlverkana

rafeindahreyfingin tengist inn

Tveir mismunandi tímastuðlar

$\tau_{\text{raf}} << \tau_{\text{jón}}$

þ.a. líta má svo á að á hverju augnabliki í hreyfingu jónar sé rafeindakerfið strax búið að finna jafnvægisstöðu

síðan koma leiðréttingaliðir

adiabatísk nálgun

nálgun einangraðs kerfis

Sígildur kristallur

Sígild safneðlisfræði: þéttleiki varmaorku

$$u = -\frac{1}{V}\frac{\partial}{\partial\beta}\ln\int d\Gamma\, e^{-\beta H}$$

með $\beta = \frac{1}{k_B T}$ og $d\Gamma = \prod_{\bar{R}} d\bar{u}(\bar{R})\, d\bar{P}(\bar{R})$

↑ fasarúms eining.

β má skala út úr heildinu

$$\bar{u}(\bar{R}) = \beta^{-1/2}\,\bar{\bar{u}}(\bar{R})$$

$$\bar{P}(\bar{R}) = \beta^{-1/2}\,\bar{\bar{P}}(\bar{R})$$

$$d\bar{u}(\bar{R}) = du_i(\bar{R})\,du_j(\bar{R})\,du_k(\bar{R})$$

$$\rightarrow d\bar{u}(\bar{R}) = \beta^{-3/2}\,d\bar{\bar{u}}(\bar{R})$$

$$d\bar{P}(\bar{R}) = \beta^{-3/2}\,d\bar{\bar{P}}(\bar{R})$$

$$\int d\Gamma\, e^{-\beta H} = \int d\Gamma \exp\left\{-\beta\left(\sum \frac{\bar{P}(\bar{R})^2}{2M} + U^{eq} + U^{harm}\right)\right\}$$

$$= \underbrace{e^{-\beta U^{eq}}}_{} \beta^{-3N}\left\{\int \prod_{\bar{R}} d\bar{u}(\bar{R})\, d\bar{\bar{P}}(\dot{\bar{R}}) \cdot \exp\left[-\sum\frac{\bar{\bar{P}}^2(\bar{R})}{2M} - \frac{1}{2}\sum \bar{\bar{u}}_\mu(\bar{R}) D_{\mu\nu}(\bar{R}-\bar{R}')\, \bar{\bar{u}}_\nu(\bar{R}')\right]\right\}$$

fasti sem taka má út fyrir heildið

Heildið er óháð β, því sést að

$$u = -\frac{1}{V}\frac{\partial}{\partial\beta}\ln\left\{e^{-\beta U^{eq}}\beta^{-3N}\times \text{fasti}\right\}$$

$$= -\frac{1}{V}(-1)\frac{\left\{U^{eq}\beta^{-3N}\times\text{fasti}\bullet e^{-\beta U^{eq}} + e^{-\beta U^{eq}}\times\text{fasti}\cdot\beta^{-3N-1}3N\right\}}{e^{-\beta U^{eq}}\beta^{-3N}\times\text{fasti}}$$

$$= \frac{U^{eq}}{V} + \frac{3N}{V\beta} = \frac{U^{eq}}{V} + \frac{3N}{V}k_BT$$

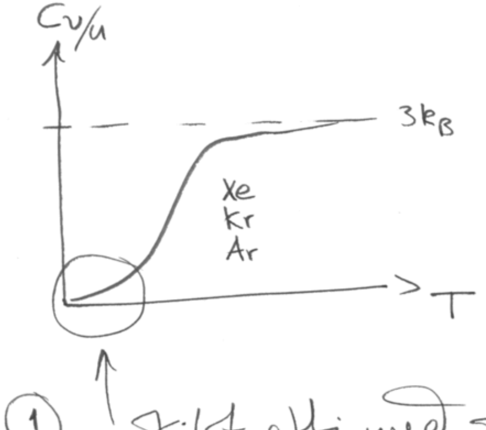
$$\rightarrow \quad \boxed{u = u^{eq} + 3nk_BT}$$

mjög lítil breyting með T,

Öll hreyfing frýs við T = 0

$$C_v = \frac{\partial u}{\partial T} = 3nk_B \qquad \boxed{\text{Dulong og Petit}}$$

bera illa saman við mælingar sérstaklega við lágt hitastig



① Skilst ekki með sígildri lýsingu

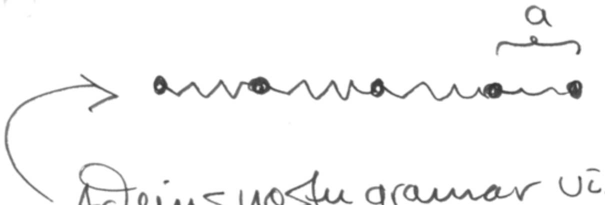
② Klassískt má skilja frá vik frá D og P við hátt T, vegna liða sem sleppt er í hreintóna nálguninni

H-virkinn er á þreningsformi.

Margir eiginleikar þess erfast yfir í skammtafræði

-> Athugum sígilt líkan

Sveifluhættir einsatóma keðju



$K = \phi''(a)$

ϕ mætti milli atóma

Aðeins næstu grannar víxlverkast

$$\rightarrow \quad U^{harm} = \frac{1}{2} K \sum_n \left[u(na) - u((n+1)a) \right]^2$$

Notum B v-K jaðarskilyrði, N-atóm

$$u((N+1)a) = u(a)$$
$$u(0) = u(Na)$$

hreyfijöfnur:

$$M\ddot{u}(na) = -\frac{\partial U^{harm}}{\partial u(na)}$$

hvar kemur u(na) fyrir í U^{harm} ?

$$U^{harm} = \frac{1}{2} K \left\{ \cdots + (u((n-1)a) - u(na))^2 + (u(na) - u((n+1)a))^2 + \cdots \right\}$$

$$\rightarrow \quad -\frac{\partial U^{harm}}{\partial u(na)} = -K \Big\{ -(u((n-1)a) - u(na)) + (u(na) - u((n+1)a)) \Big\}$$

$$\rightarrow \quad \boxed{M\ddot{u}(na) = -K \left\{ 2u(na) - u((n-1)a) - u((n+1)a) \right\}}$$

reyna lausnir á forminu

$$u(na,t) \sim e^{i(kna - \omega t)}$$

jaðarskilyrði $\quad u(0) = u(Na)$

$$\rightarrow \quad e^{-i\omega t} = e^{i(kNa - \omega t)}$$

$$\rightarrow \quad kNa = 2\pi n \qquad n \in \mathbb{Z}$$

$$\rightarrow \quad k = \frac{2\pi n}{Na}$$

Lausnirnar eru óbreyttar með hliðrun $k \rightarrow k + \frac{2\pi}{a}$

því eru aðeins N k-gildi sem við getum valið til að vera á bilinu

$$\left(-\frac{\pi}{a}, \frac{\pi}{a}\right)$$

Setjum lausnir inn í hreyfijöfnu

$$-M\omega^2 e^{i(kna-\omega t)} = -K\left\{2-e^{-ika}-e^{ika}\right\}e^{i(kna-\omega t)}$$

$$= -2K\left(1-\cos(ka)\right)e^{i(kna-\omega t)}$$

því verður að gilda

$$\omega(k) = \sqrt{\frac{2K(1-\cos(ka))}{M}}$$

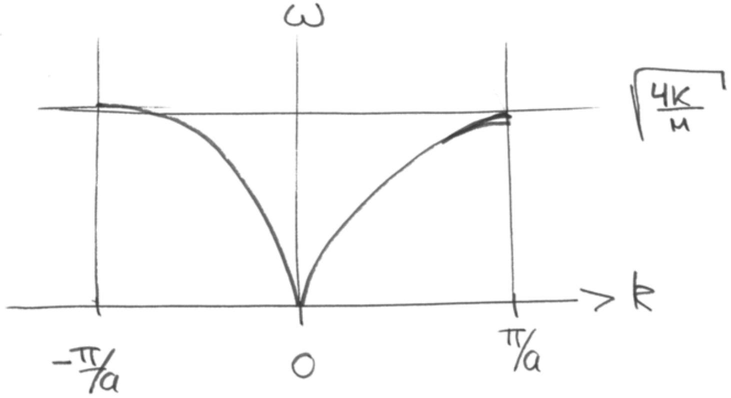
ω er jafnstætt fall af k því nægir jákvæða rótin því hliðranir atómanna

$$\cos(kna-\omega t)$$
$$\sin(kna-\omega t)$$

eru óbreyttar eða jafngildar fyrir

$\boxed{k \text{ og } -\omega(k)}$ og $\boxed{-k \text{ og } \omega(-k) = \omega(k)}$

2N óháðar lausnir, <u>en N sveifluhættir</u>



$$\boxed{\text{tvístursamband} \quad \omega = \omega(k)}$$

fasahraði $c = \frac{\omega}{k}$

grúpuhraði $v = \frac{\partial \omega}{\partial k}$ $\to 0$ v. $k = \pm\frac{\pi}{a}$

aðeins jafnir fyrir $k \sim 0$ þegar $\omega(k)$ er línulegt

$$\omega = \left(a\sqrt{\frac{K}{M}}\right)|k|$$

Keðja með grunni

Veljum

$$\boxed{\begin{matrix} K \geq G \\ d \leqslant \frac{a}{2} \end{matrix}}$$

u_1 lýsir jónum við $R = na$

u_2 —||— $R = na + d$

Aðeins víxlverkun næstu granna

$$U^{\text{harm}} = \frac{K}{2} \sum_n \left[u_1(na) - u_2(na)\right]^2$$

$$+ \frac{G}{2} \sum_n \left[u_2(na) - u_1((n+1)a)\right]^2$$

Notum B-vK jaðarskilyrði

---

tengdar hreyfijöfnur fyrir u_1 og u_2

$$M\ddot{u}_1(na) = -K\left\{u_1(na) - u_2(na)\right\} - G\left\{u_1(na) - u_2((n-1)a)\right\}$$

$$M\ddot{u}_2(na) = -K\left\{u_2(na) - u_1(na)\right\} - G\left\{u_2(na) - u_1((n+1)a)\right\}$$

leitað lausna

$$u_1(na) = \epsilon_1 e^{i(kna - \omega t)}$$

$$u_2(na) = \epsilon_2 e^{i(kna - \omega t)}$$

innsetning gefur

$$\begin{pmatrix} M\omega^2 - (K+G) & K + Ge^{-ika} \\ K + Ge^{ika} & M\omega^2 - (K+G) \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} = 0$$

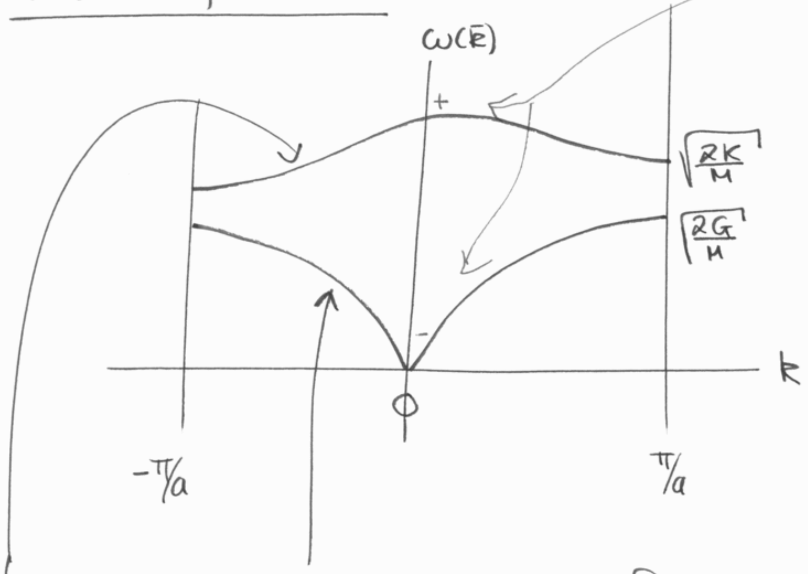
tvístursamband fæst með því að krefjast að ákveðan hverfi

$$\omega^2 = \frac{K+G}{M} \pm \frac{1}{M}\sqrt{K^2+G^2+2KG\cos(ka)}$$

einnig má finna

$$\frac{\epsilon_2}{\epsilon_1} = \mp \frac{K+Ge^{ika}}{|K+Ge^{ika}|}$$

2N sveifluhættir



acoustical branch: hljóðlag grein

optical branch: ljóslag grein

Hvers konar sveifluhættir ?

Athugum $\boxed{k \ll \frac{\pi}{a}}$

$$\rightarrow \quad \cos(ka) \simeq 1 - \frac{(ka)^2}{2}$$

Ljóslag

$$\omega^2 \simeq \frac{K+G}{M} + \frac{1}{M}\left(K^2+G^2+2KG\left(1-\frac{(ka)^2}{2}\right)\right)^{1/2}$$

$$\omega \simeq \sqrt{\frac{2(K+G)}{M}} - O(ka)^2$$

hljóðlag

$$\omega^2 \simeq \frac{K+G}{M} - \frac{1}{M}\left(K^2+G^2+2KG\left(1-\frac{(ka)^2}{2}\right)\right)^{1/2}$$

$$\simeq \frac{K+G}{M} - \frac{1}{M}\left((K+G)^2 - KG(ka)^2\right)^{1/2}$$

$$\simeq \frac{(K+G)}{M} - \frac{(K+G)}{M}\left(1 - \frac{KG(ka)^2}{(K+G)^2}\right)^{1/2}$$

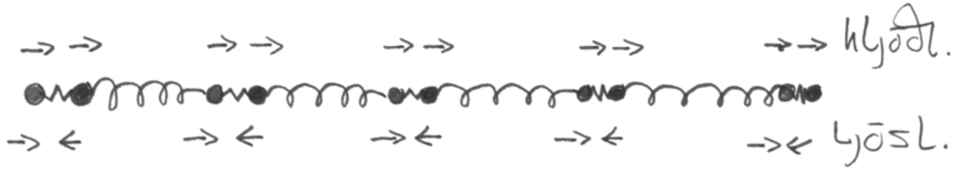
$$\simeq \frac{KG}{2M(K+G)}(ka)^2$$

$$\to \boxed{\omega \simeq \sqrt{\frac{KG}{2M(K+G)}}\,|ka|}$$

$$\frac{\epsilon_2}{\epsilon_1} = \mp \frac{K+Ge^{ika}}{|K+Ge^{ika}|} \simeq \pm 1 \quad \text{þ.} \quad \boxed{ka \to 0}$$

$\epsilon_2 = \epsilon_1 \Leftarrow$ hljóðlog grein

$\epsilon_2 = -\epsilon_1 \Leftarrow$ ljóslog grein



$K > G$

$\boxed{k = \pi/a}$ $k \to \frac{\pi}{a}$

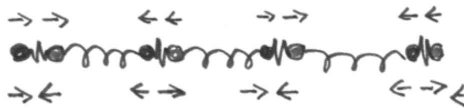
bara G-gormur sveiflast

$$\omega^2 \simeq \frac{K+G}{M} - \frac{1}{M}\left((K-G)^2\right)^{1/2} = \frac{2G}{M}$$

$$\omega^2 \simeq \frac{K+G}{M} + \frac{1}{M}\left((K-G)^2\right)^{1/2} = \frac{2K}{M}$$

hljóðl. →

$\epsilon_1 = +\epsilon_2$



ljósl.

$\epsilon_1 = -\epsilon_2$

---

hljóðlog grein

Jónir innan grundareininga sveiflast í fasa

tíðni ræðst af víxlverkun milli grundareininga → lág tíðni

ljóslog grein

Jónir innan grundareininga sveiflast í andfasa

Hátíðni sveiflur sameinda

q

breikka í bönda vegna víxlverkun á milli grundareininga

Rafsegulsvið getur örvað ljóslogu..

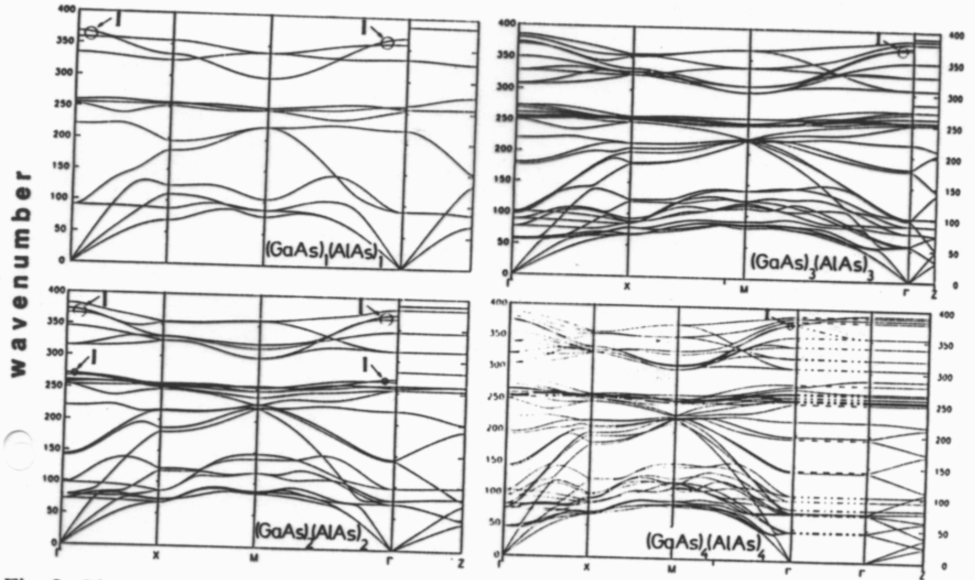
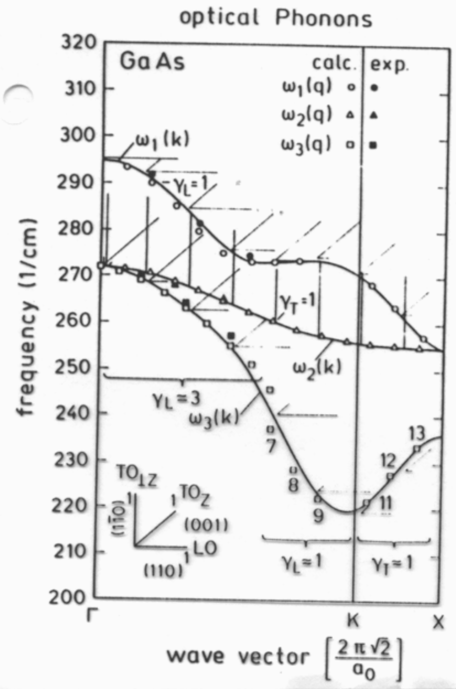
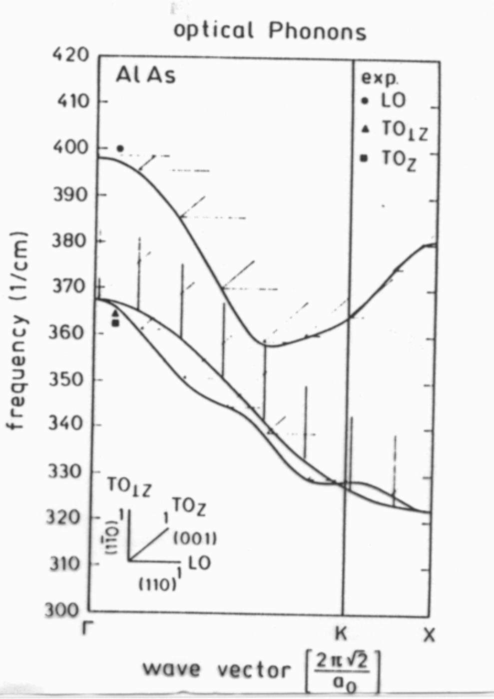


Fig. 2. Phonon dispersion relations of four GaAs/AlAs superlattices with interface modes labelled "I". From Ref. 10.





Sveifluhættir í 3D

lesa að mestu sjálf

Aðalatriði :

hreyfingajafna í fylkjatáknum

$$M\ddot{\bar{u}}(\bar{R}) = -\sum_{\bar{R}'} D(\bar{R}-\bar{R}')\,\bar{u}(\bar{R}')$$

með lausnum

$$\bar{u}(\bar{R},t) = \bar{\epsilon}\, e^{i(\bar{k}\cdot\bar{R}-\omega t)}$$

pólunar eða skautunar vigur

B.-vK. - jaðarskilyrði

-> $\bar{k}$ tekur gildin $\bar{k} = \frac{n_1}{N_1}\bar{b}_1 + \frac{n_2}{N_2}\bar{b}_2 + \frac{n_3}{N_3}\bar{b}_3$

$$\bar{b}_i\cdot\bar{a}_j = 2\pi\delta_{ij}$$

nykurgrindarvigrar

Nægir að líta á $k \in$ 1. Brillouin svæði

3-skautanir -> 3N sveifluhættir

Í einsátta (jafnátta) efni er ein grein ~~sam~~ með skautun samsíða $\bar{k}$ og tvær með skautun þvert á $\bar{k}$

-> 1 langs sveifluháttur
2 þver sveifluhættir

Sjá Mynd 22.13

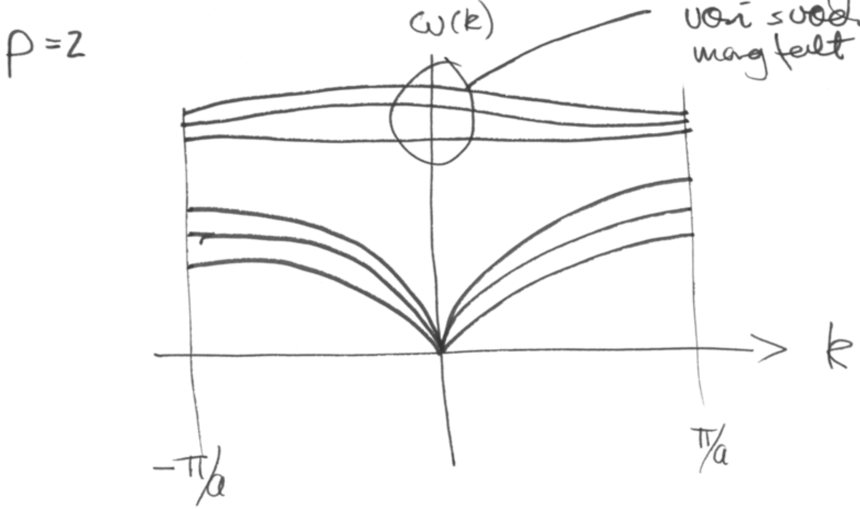
3D grind með grunni

p: fjöldi jóna í grunni

fyrir hvert $\bar{k}$ eru 3p sveifluhættir (3Np sveifluhættir alls)

3 af 3p sveifluháttum eru hljóðlíkir

3(p-1) eru ljóslegir



fyrir háa samhverfu væri svæðið margfelt

①

Skammtafræði kristallahreyfinga

Getur skammtafræði skýrt

$$C_v \xrightarrow[T\to 0]{} \begin{cases} T^3 & : \text{einangrarar} \\ AT+BT^3 & : \text{málmar} \end{cases}$$

Sígild eðlisfræði getur:

Dulong + Petit, C_v er fasti

í stað þéttleika varmaorkunnar er litið á meðalorkuþéttleika í skammtasafni ~~rafeinda~~ ~~atóma~~ einda

$$u = \frac{1}{V}\frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} \qquad \beta = \frac{1}{k_B T}$$

E_i er orka i.-sístæða ástands kristallsins. summan er yfir öll slík ástönd

②

Kristallinum í hreintónanálgun er lýst með

$$H^{harm} = \sum_{\bar{R}} \frac{\bar{P}(\bar{R})^2}{2M} + \frac{1}{2}\sum_{\bar{R}\bar{R}'} u_\mu(\bar{R}) D_{\mu\nu}(\bar{R}-\bar{R}') u_\nu(\bar{R}')$$

Sem má skammta → N-jóna kristallur verður sem 3N-óháðir hreintónasveiflar

Heildarorka einhvers sístæðs ástands kristallsins er

$$E = \underbrace{\sum_{\bar{k},s} \left(n_{\bar{k},s} + \frac{1}{2}\right)\hbar\omega_s(\bar{k})}_{\text{summuð upp orka hvers sveifils}}$$

$\bar{k}$ er summað yfir N-nykurvigra nykurgrindar. p-sveifluhættir fyrir hvern vigur $\bar{k}$. p- greinar.

$$n_{\bar{k},s} \in \{0, 1, 2, \ldots\ldots\}$$

Hljóðeindir

Með hliðstæðu við rafsegulsvið (skammtað) í holrúmi er eftirfarandi gert

$\Downarrow$

„Örvunartala, $n_{\bar{k}s}$, sveifluháttar með bylgjuvigur $\bar{k}$ í grein s

$\Updownarrow$ jafngilt

$n_{\bar{k}s}$ hljóðeindir af tegund s með bylgjuvigur $\bar{k}$

↑ einfaldara til umfjöllunar

Varmarýmd kristalls

Meðalorku þéttleiki

$$u = -\frac{\partial f}{\partial \beta}$$

með

$$f = \frac{1}{V}\ln\left(\sum_i e^{-\beta E_i}\right)$$

$$\sum_i e^{-\beta E_i} = \sum_i \exp\left\{-\beta\sum_{\bar{k},s}\left(n^i_{\bar{k}s}+\tfrac{1}{2}\right)\hbar\omega_s(\bar{k})\right\}$$

$$= \prod_{\bar{k},s}\Big(\underbrace{e^{-\beta\hbar\omega_s(\bar{k})/2} + e^{-3\beta\hbar\omega_s(\bar{k})/2} + \cdots\cdots}_{\text{hægt að summa}}\Big)$$

$$= \prod_{\bar{k},s}\left\{\frac{e^{-\beta\hbar\omega_s(\bar{k})/2}}{1-e^{-\beta\hbar\omega_s(\bar{k})}}\right\}$$

$$\rightarrow\ u = -\frac{1}{V}\frac{\partial}{\partial\beta}\ln\prod_{\bar{k},s}\left\{\frac{e^{-\beta\hbar\omega_s(\bar{k})/2}}{1-e^{-\beta\hbar\omega_s(\bar{k})}}\right\}$$

$$u = -\frac{1}{V}\frac{\partial}{\partial\beta}\sum_{\bar{k}s} \ln\left\{\frac{e^{-\beta\hbar\omega_s(\bar{k})/2}}{1-e^{-\beta\hbar\omega_s(\bar{k})}}\right\}$$

$$= -\frac{1}{V}\frac{\partial}{\partial\beta}\sum_{\bar{k}s}\left\{\ln e^{-\beta\hbar\omega_s(\bar{k})/2} - \ln(1-e^{-\beta\hbar\omega_s(\bar{k})})\right\}$$

$$= \frac{1}{V}\sum_{\bar{k},s}\left\{\frac{1}{2} + \frac{e^{-\beta\hbar\omega_s(\bar{k})}}{1-e^{-\beta\hbar\omega_s(\bar{k})}}\right\}\hbar\omega_s(\bar{k})$$

$$= \frac{1}{V}\sum_{\bar{k},s}\hbar\omega_s(\bar{k})\left\{n_s(\bar{k}) + \frac{1}{2}\right\}$$

ef $n_s(\bar{k}) = \dfrac{1}{e^{\beta\hbar\omega_s(\bar{k})}-1}$

↑

miðal fjöldi hljóðeinda af gerð $\bar{k},s$
við hitastigið T

bóseindir ⇐ bósedreifing.

Orkuþéttleikin er

$$u = u^{eq} + \frac{1}{V}\sum_{\bar{k}s}\hbar\omega_s(\bar{k})\left\{n_s(\bar{k}) + \frac{1}{2}\right\}$$

sama og fyrir
klassiskan kristall

Hér kemur T fyrir
$n_s(\bar{k}) \xrightarrow[T\to 0]{} 0$

núllpunkts-
orka ekki
háð T

Varmarýmd

$$C_V = \frac{1}{V}\sum_{\bar{k},s}\left\{\frac{\partial}{\partial T}n_s(\bar{k})\right\}\hbar\omega_s(\bar{k})$$

athugum markgildi fyrir hátt og lágt T

Hátt T

þ.e. $k_B T >> \hbar\omega_s(\bar{k})$ f. $\forall\ \bar{k}, s$

Mikill fjöldi hljóðeinda af öllum gerðum.

$$x = \frac{\hbar\omega}{k_B T} << 1$$

$$\frac{1}{e^x - 1} = \frac{1}{x + \frac{x^2}{2} + \frac{x^3}{6} + \cdots} = \frac{1}{x}\left(1 - \frac{x}{2} + \frac{x^2}{12} + O(x^3)\right)$$

fyrsti liðurinn

$$n_s(\bar{k}) \approx \frac{k_B T}{\hbar\omega_s(\bar{k})} \to u = u^{eq} + \frac{1}{V}\sum_{\bar{k},s} k_B T + \cdots$$

$$= u^{eq} + \frac{3N}{V} k_B T + \cdots$$

$$\to \boxed{C_V = 3nk_B}$$ Dulong + Petit

Línulegi liðurinn vegur upp núllpunktsorkuna nákvæmlega

Næstu liðir eru því leiðrétting á Dulong + Petit.

Anharmonic-liðir gefa leiðréttingu með sömu stærðargráðu

Lágt T

eða hljóðeindir

Allir hættir með $\hbar\omega_s(\bar{k}) >> k_B T$ skipta ekki máli (eru frosnir út)

En eftir lifa alltaf einhverjar hljóðeindir, hljóðlagir hættir með $k \to 0$

Nálgun

① Einungis hljóðlagir hættir skipta máli

② Langbylgjunálgun $\to \omega = c_s(\hat{k})\, k$

③ Heildun yfir 1. B-svæðir er breytt í heildun yfir allt $\bar{k}$-rúmið
$n_s(\bar{k}) \to 0$ ef $\bar{k} \not\to 0$

$$C_v = \frac{1}{V}\sum_{\bar{k}s}\left\{\frac{\partial}{\partial T} n_s(\bar{k})\right\}\hbar\omega_s(\bar{k})$$

nota
$$\frac{1}{V}\sum_{\bar{k},s} \rightarrow \int\frac{d\bar{k}}{(2\pi)^3}\sum_s$$

$$\rightarrow C_v = \frac{\partial}{\partial T}\sum_s\int\frac{d\bar{k}}{(2\pi)^3} n_s(\bar{k})\hbar\omega_s(\bar{k})$$

$$\simeq \frac{\partial}{\partial T}\sum_s\int\frac{d\bar{k}}{(2\pi)^3}\frac{\hbar C_s(\hat{k})k}{e^{\hbar C_s(\hat{k})k/k_BT}-1}$$

breytuskipti
$$\beta\hbar C_s(\hat{k})k = x$$

$$\rightarrow C_v = \frac{\partial}{\partial T}\frac{(k_BT)^4}{\hbar^3}\int_0^\infty\frac{x^3dx}{e^x-1}\frac{4\pi}{(2\pi)^3}\overbrace{3\frac{1}{3}\int\frac{d\Omega}{4\pi}\frac{1}{C_s(\hat{k})^3}}^{\frac{1}{c^3}}$$

$$= \frac{\partial}{\partial T}\frac{(k_BT)^4}{(\hbar c)^3}\frac{3}{2\pi^2}\int_0^\infty\frac{x^3dx}{e^x-1}$$

$$\int_0^\infty\frac{x^3dx}{e^x-1} = \frac{\pi^4}{15}$$

$$\rightarrow \boxed{C_v \simeq \frac{2\pi^2}{5}k_B\left(\frac{k_BT}{\hbar c}\right)^3}$$

Tvö líkön fyrir hljóðeindir
við „milli-hitastig“

Debye-líkanið

þrjár greinar, hver með tvístrs.

$$\omega = ck$$

Í stað 1. Brillouin svæðisins er notuð kúla með geisla k_D sem er valinn þ.a. N gildi bylgjuvigra sé innan hennar.

rúmmál á bylgjuvigur k í k-rúminu er $(2\pi)^3/V$

$$\downarrow$$

$$\frac{(2\pi)^3}{V}\cdot N = \frac{4\pi}{3}k_D^3$$

$$\rightarrow \boxed{n = \frac{k_D^3}{6\pi^2}}$$

þéttleiki jóna

$$\rightarrow C_V = \frac{\partial}{\partial T}\frac{3\hbar c}{2\pi^2}\int_0^{k_D}\frac{k^3dk}{e^{\beta\hbar ck}-1}$$

Skilgreinum

$$\omega_D = k_D c$$

$$k_B\Theta_D = \hbar\omega_D = \hbar c k_D$$

k_D : tengist andhverfi fjarlægð jóna

ω_D : hæsta hljóðeinda tíðni

Θ_D : fyrir ofan Θ_D eru allar hljóðeindir til staðar (fyrir neðan frjósa þær út)

Heildum með breytiskiptingu

$$\frac{\hbar ck}{k_BT} = x$$

$$\rightarrow C_V = 9nk_B\left(\frac{T}{\Theta_D}\right)^3\int_0^{\Theta_D/T}\frac{x^4e^xdx}{(e^x-1)^2}$$

$$= \frac{12\pi^4}{5} nk_B \left(\frac{T}{\theta_D}\right)^3 \leftarrow \text{NB} \qquad \text{fyrir } T << \theta_D$$

gildir best hér því aðeins hljóðlaga greinar eru teknar með

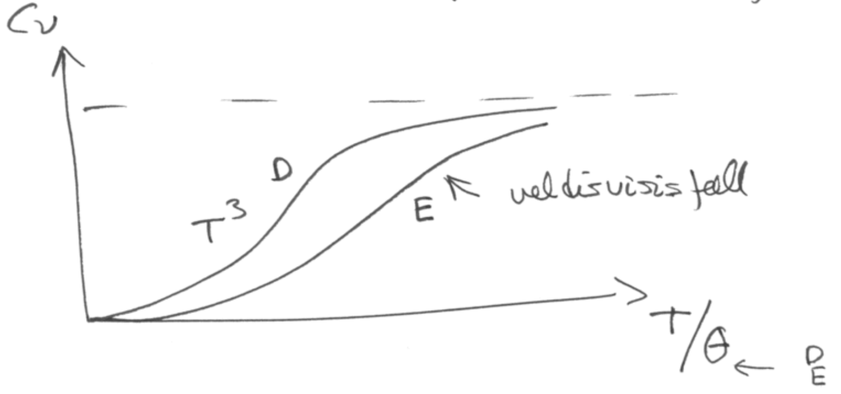
Einstein líkanið

Hver ljóslæg grein hefur tvístursambandið

$$\omega = \omega_E$$

fyrir p-greinar fast

$$C_V^{opt} = pnk_B \frac{\left(\frac{\hbar\omega_E}{k_BT}\right)^2 e^{\hbar\omega_E/k_BT}}{\left(e^{\hbar\omega_E/k_BT} - 1\right)^2}$$



Kristallar með rafeindum

$T \to 0$

$$C_V \sim aT + bT^3$$

(Jónir) hljóðeindir bóseindir

rafeindir, fermíeindir

finna má hitastigið þegar liðirnir eru jafnstórir

$$T_0 = 0.145 \left(\frac{Z\theta_D}{T_F}\right)^{1/2} \theta_D$$

~ örfáar gráður Kelvin

$$n_e = Z n_i$$

Ástandaþéttleiki

$$\frac{1}{V}\sum_{\bar{k}s} Q(\omega_s(\bar{k})) = \sum_s \int \frac{d\bar{k}}{(2\pi)^3}\, Q(\omega_s(\bar{k}))$$

$$= \int d\omega\, \overset{\text{ástandaþ.}}{g(\omega)}\, Q(\omega)$$

$$\rightarrow g(\omega) = \sum_s \int \frac{d\bar{k}}{(2\pi)^3}\,\delta(\omega - \omega_s(\bar{k}))$$

eins og fyrir rafeinda ástandaþéttleika má umskrifa

$$g(\omega) = \sum_s \int \frac{dS}{(2\pi)^3}\,\frac{1}{|\bar{\nabla}\omega_s(\bar{k})|}$$

Van-Hove sérstöðupunktar

---

fyrir Debye-líkanið fast.

$$g_D(\omega) = 3\int_{k<k_D} \frac{d\bar{k}}{(2\pi)^3}\,\delta(\omega - ck)$$

$$= \frac{3}{2\pi^2}\int_0^{k_D} k^2 dk\,\delta(\omega - ck)$$

$$= \begin{cases} \dfrac{3}{2\pi^2}\dfrac{\omega^2}{c^3} & \omega < \omega_D = k_D c \\ 0 & \omega > \omega_D \end{cases}$$

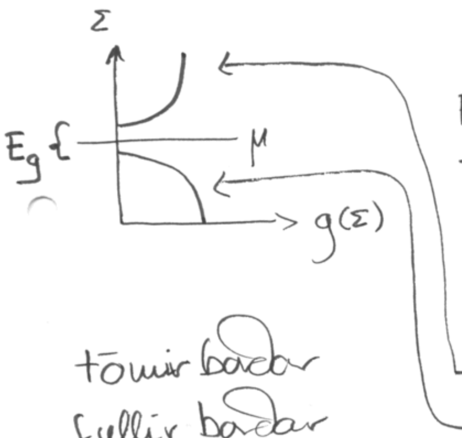
bera saman við mynd 23.6

①

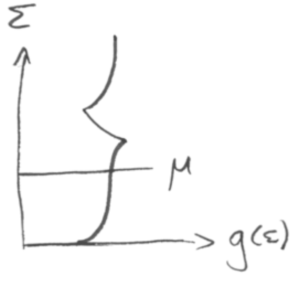
Hálfleiðarar

Einsleitur kristall

Einangrar   hálfleiðarar   Málmar



$E_g \lesssim 2eV$



tómir borðar
fullir borðar
Orkugeil

leiðniborði
gildisborði

borði að hluta fylltur

Í hálfleiðara eru hitaörvaðar rafeindir í leiðniborða og/eða holur í gildisborða

Hreinn hálfleiðari: hitaörvunin er frá gildis- yfir í leiðniborða

Íbættur hálfleiðari: hitaörvun getur verið frá eða í veilu ástand nærri öðrum eða báðum borðum

②

Íbót getur gerbreytt eiginleikum hálfleiðara.

leiðni eykst venjulega með vaxandi hitastigi, öfugt m.v. málma þ.s. leiðnin minnkar

$$\sigma = \frac{ne^2\tau}{m}$$

vegna aukinna árekstra við hljóðeindir (τ minnkar með vaxandi T)

Gerist líka í hálfleiðara, en hitaörvunin vex miklu hraðar með T

→ breyting um stuðul 10^3 getur breytt leiðni um einn tug stærðargráðna

intrinsic : eigin, eiginleiðni ... hreins hálfleiðara

extrinsic : íbótar, íbótarleiðni ...

Hvaða efni?

Um mitt lotukerfið, Si, Ge, C, B, Se, Te...

samsetningar SiGe, GaAs, PbTe InAs
InP, GaP, AlSb . . . . .

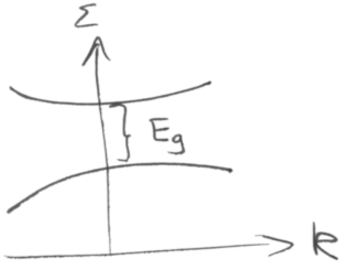
III - V, II - VI

samgildir

skautaðir + samg.

Beinir hálfleiðarar

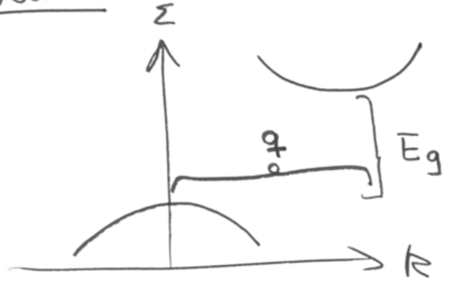
lágmark leiðniborða er fyrir sama k og hámark gildisborða



Orkulægsta forslan er bein ljósforsla

$$\omega = \frac{E_g}{\hbar}$$

Óbeinir



Orkulægsta forslan er óbein forsla með aðstoð hljóðeindar

$$\omega = \frac{E_g}{\hbar} - \omega(q)$$

---

k fyrir ljósið er svo lítið samanborið við vigra í nyturgrindinni
munurinn er nokkrar stærðargráður

Borðabygging

Orkan í kringum lágmark eða hámark er á forminu

$$\Sigma(\bar{k}) = \Sigma_C + \hbar^2\left(\frac{k_1^2}{2m_1} + \frac{k_2^2}{2m_2} + \frac{k_3^2}{2m_3}\right)$$

fyrir rafeindir

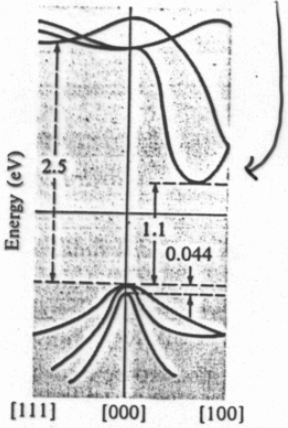
og

$$\Sigma(k) = \Sigma_v - \hbar^2\left(\frac{k_1^2}{2m_1} + \frac{k_2^2}{2m_2} + \frac{k_3^2}{2m_3}\right)$$

fyrir holur

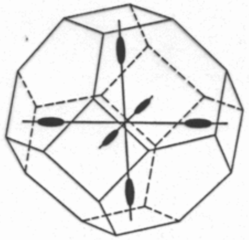
massa gildin eru mismunandi og háð borðum

C: $m_L = 1,0m$ $m_T = 0,2m$ Si



0,49m , 0,16m

fyrsta Brillouin svæðið

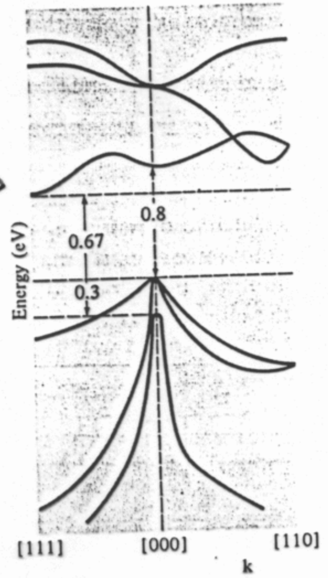


6× margfeldni sporvölur

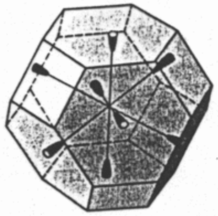
(walley deg.)

margfeldnin minnkar við skilfleti

$m_L = 1,6m$ $m_T = 0,08m$ Ge



0,28m , 0,044m



8× eða 4× margfeldni

Γ: þungar og léttar holur , spuna-brautar klofnun

Massarnir eru mældir með hringhraðalhermu

Hreyfijafna

$$\hat{M}\frac{d\bar{v}}{dt} = \mp\frac{e}{c}\bar{v}\times\bar{H}$$

Segulsvið $\vec{H} = H\hat{z}$ leiðir til virks massa

$$m^* = \left(\frac{|\hat{M}|}{M_{zz}}\right)^{1/2}$$

$\hat{M}$ er samhverfur rauntölu þinur

→ finna má höfuðása þ.a.

$$m^* = \sqrt{\frac{m_1 m_2 m_3}{\hat{H}_1^2 m_1 + \hat{H}_2^2 m_2 + \hat{H}_3^2 m_3}}$$

þættir [illegible] $\frac{\bar{H}}{H}$ samsíða Höfuðásunum

Með vali á stefnum má mæla m_1, m_2 eða m_3

$\omega\tau \gg 1$ ⟨ hreint kerfi
málmur skinndýpt lítil
hálfl. fáar rafeindir en sést inn í allt kerfið

Fjöldi hleðslubera í varmajafnvægi

Íbótarástönd breyta ekki $g_c(\varepsilon)$ eða $g_v(\varepsilon)$

ástandaþ. leiðnib. gildisb.

því þau lenda innan geilar

fermid.

$$n_c(T) = \int_{\varepsilon_c}^{\infty} d\varepsilon \, g_c(\varepsilon) \frac{1}{e^{(\varepsilon-\mu)/k_BT}+1}$$

líkur á setni rafeindar

$$p_v(T) = \int_{-\infty}^{\varepsilon_v} d\varepsilon \, g_v(\varepsilon) \left[1 - \frac{1}{e^{(\varepsilon-\mu)/k_BT}+1}\right]$$

sætafjöldi

líkur á tómu ástandi rafeinda = setni holu

þéttleiki rafeinda

Íbót ræður n_c og p_v og sérstaklega μ

en ef

$$\varepsilon_c - \mu \gg k_BT$$

$$\mu - \varepsilon_v \gg k_BT$$

þá er talað um rafberana sem hlýgas

Fermidreifingin innan leiðnibandsins er aðeins hali dreifingarinnar sem lýsa má sem Bolzmanns dr. sígilt gas <-> hlýgas

1-f hefur líka aðeins Bolzmanns-hala innan gildisborða <-> holurnar eru líka hlýgas

Ef μ er nær öðruhvorum borðanum eða innan hans er um kulgas að ræða sem lýsa verður með fermidreifingu.

Leiðsluberar – hlýgas

$$\Downarrow$$

$$\frac{1}{e^{(\varepsilon-\mu)\beta}+1} \simeq e^{-(\varepsilon-\mu)\beta} \qquad \underline{\varepsilon > \varepsilon_c}$$

$$1 - \frac{1}{e^{(\varepsilon-\mu)\beta}+1} \simeq e^{-(\mu-\varepsilon)\beta} \qquad \underline{\varepsilon < \varepsilon_v}$$

$$\rightarrow \boxed{\begin{aligned} n_c(T) &= N_c(T)\, e^{-(\varepsilon_c-\mu)\beta} \\ p_v(T) &= P_v(T)\, e^{-(\mu-\varepsilon)\beta} \end{aligned}}$$

hæg breyting með T

með

$$N_c(T) = \int_{\varepsilon_c}^{\infty} d\varepsilon\, g_c(\varepsilon)\, e^{-(\varepsilon-\varepsilon_c)\beta}$$

$$P_c(T) = \int_{-\infty}^{\varepsilon_v} d\varepsilon\, g_v(\varepsilon)\, e^{-(\varepsilon_v-\varepsilon)\beta}$$

föll sem breytast hægt með T

fyrir ástandaþéttleikann má nota

$$g_\alpha(\varepsilon) = \sqrt{2|\varepsilon-\varepsilon_\alpha|}\; \frac{m_\alpha^{3/2}}{\hbar^3\pi^2}$$

$$\alpha = c, v$$

$$\left(\text{og} \quad m^{3/2} = \sqrt{m_x m_y m_z}\right)$$

þá má heilda og fá

$$N_c(T) = \frac{1}{4}\left(\frac{2m_c k_B T}{\pi\hbar^2}\right)^{3/2} \qquad \text{með } c=\alpha$$

$$\left\{ N_v(T) = \frac{1}{4}\left(\frac{2m_v k_B T}{\pi\hbar^2}\right)^{3/2} \right\}$$

eða

$$N_\alpha(T) = 2.5\left(\frac{m_\alpha}{m}\right)^{3/2}\left(\frac{T}{300K}\right)^{3/2}\cdot 10^{19}\,\text{cm}^{-3}$$

→ <u>fyrir hálfleiðara m. hlýgasi</u>

<u>er $10^{18}-10^{19}$ hámark</u>

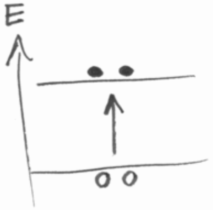
því veldisv. f. eru ≤ 1

massavirkni regla

Til að finna n_c og p_v þarf enn μ

en $\boxed{n_c p_v = N_c P_v e^{-E_g/k_BT}}$

Hreinn hálfleiðari



$$n_c(T) = p_v(T) \equiv n_i(T)$$

$$\rightarrow n_i = (n_c p_v)^{1/2} = \left(N_c(T) P_v(T)\right)^{1/2} e^{-E_g/2k_BT}$$

$$= p_v = P_v(T)\, e^{-(\mu-\varepsilon_v)/k_BT}$$

$\ln\ldots$ $\rightarrow$ $$\ln\left(\left\{N_c(T) P_v(T)\right\}^{1/2} e^{-E_g/2k_BT}\right)$$

$$= \ln\left(P_v(T)\, e^{-(\mu-\varepsilon_v)/k_BT}\right)$$

$$\rightarrow \frac{1}{2}\ln\left(N_c(T) P_v(T)\right) - \frac{E_g}{2k_BT} = + \ln\left(P_v(T)\right) - \frac{\mu-\varepsilon_v}{k_BT}$$

$$\rightarrow \left(\frac{1}{2}\ln\left(N_c(T)\right) + \frac{1}{2}\ln\left(P_v(T)\right) - \ln\left(P_v(T)\right)\right) k_BT$$

$$= \frac{E_g}{2} - \mu + \varepsilon_v$$ ~~$\frac{E_c - E_v}{2} - \mu + \varepsilon_v = E$~~

$$\rightarrow \mu = \varepsilon_v + \frac{E_g}{2} + \frac{1}{2} k_BT \ln\left(\frac{P_v(T)}{N_c(T)}\right)$$

$= \mu_i$ ← efnamættið fyrir hreinan hálfl.

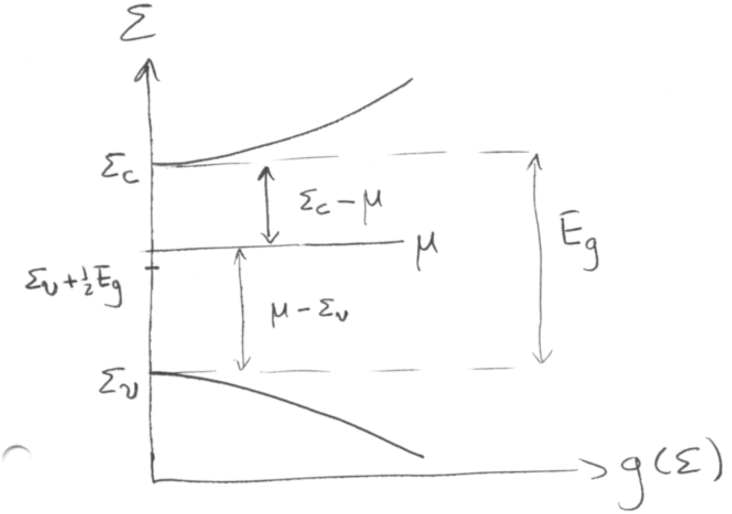
T styttist út

eins og sést.

$$\boxed{\mu_i = \varepsilon_v + \frac{E_g}{2} + \frac{3}{4} k_BT \ln\left(\frac{m_v}{m_c}\right)}$$

$T \rightarrow 0$ μ liggur í miðri geil

fyrir $k_BT << E_g$ fæst $(m_v \sim m_c)$ að μ liggur enn mjög nærri miðri geil.



Íbættur hálfleiðari

Ef leiðnirafeindir eða holur koma frá íbótar atómum er talað um íbættan....

$$\rightarrow n_c - p_v = \Delta n \neq 0$$

| reglan um massavirkni heldur því hún er óháð μ |

$$\rightarrow n_c p_v = n_i^2$$

$$n_c - p_v = \Delta n \rightarrow n_c = p_v + \Delta n$$

$$n_c p_v = n_i^2 \rightarrow p_v(p_v + \Delta n) = n_i^2$$

eða

$$p_v^2 + \Delta n p_v - n_i^2 = 0$$

$$\rightarrow p_v = -\tfrac{1}{2}\Delta n \pm \tfrac{1}{2}\sqrt{(\Delta n)^2 + 4n_i^2}$$

$$p_v \geqslant 0$$

$$\rightarrow p_v = \tfrac{1}{2}\sqrt{(\Delta n)^2 + 4n_i^2} - \frac{\Delta n}{2}$$

①

$$p_v = n_c - \Delta n$$

$$n_c(n_c - \Delta n) = n_i^2 \rightarrow n_c^2 - \Delta n p_v - n_i^2 = 0$$

$$n_c = \frac{\Delta n}{2} \pm \frac{1}{2}\sqrt{(\Delta n)^2 + 4n_i^2}$$

$$n_c \geqslant 0$$

②

$$\longrightarrow n_c = \frac{1}{2}\sqrt{(\Delta n)^2 + 4n_i^2} + \frac{\Delta n}{2}$$

viljum finna efnamættið μ fyrir
í báðum hálfleiðara og bera saman
v. hreinan (μ_i)

Hér má skilgreina μ með

$$\frac{n_c}{n_i} = e^{\beta(\mu-\mu_i)}$$

$$n_c p_v = n_i^2 \rightarrow p_v = e^{-\beta(\mu-\mu_i)} n_i$$

$$\Delta n = n_c - p_c = n_i \left(e^{\beta(\mu-\mu_i)} - e^{-\beta(\mu-\mu_i)}\right)$$

$$= n_i 2 \sinh\left(\beta(\mu-\mu_i)\right)$$

Sérlega sterkt fall af '$(\mu-\mu_i)\beta$'

-> jafnvel $\Delta n >> n_i$ þýðir samt $\mu \sim \mu_i$
<u>en hlýgas</u>

og frá (1+2) sést að þá er
annhvort $n_c \sim \Delta n$ eða $p_v \sim \Delta n$

$$\boxed{\text{Ríkjandi og víkjandi hleðslubera}}$$

$$\boxed{\text{p- eða n-efni}}$$

Hreinn hálfleiðari

$$n_i(T) = \left[N_c(T) P_v(T)\right]^{1/2} e^{-E_g/k_BT\cdot 2} \quad \leftarrow n_c = p_v$$

$$\mu_i(T) = \varepsilon_v + \frac{1}{2} E_g + \frac{3}{4} k_BT \ln\left(\frac{m_v}{m_c}\right)$$

Hálfl. með íbót

íbót ákveður n_c og p_v aðeins í gegnum μ

$$\rightarrow n_c p_v = n_i^2$$

$$\Delta n = n_c - p_v \; , \; \binom{n_c}{p_v} = \frac{1}{2}\left((\Delta n)^2 + 4n_i^2\right)^{1/2} \pm \frac{\Delta n}{2}$$

$$\frac{\Delta n}{n_i} = 2 \sinh \beta(\mu - \mu_i)$$

Hér þarf frekari upplýsingar um íbótina

$$n_c p_v = N_c P_v \cdot e^{-E_g\beta}$$

n_i og μ_i eru gildi fyrir hreinan hálfl.

Orkustig íbótaratóma

Úr lotutöflu

B	C	N
Al	Si	P
Ga	Ge	As
In	Sn	Sb

→ As í Ge-grind getur verið rafgjafi

5 gilt   4 gilt

aukarafeind losnar föst jákvæð hleðsla verður eftir

Ga í Ge-grind getur verið rafþegi

* ϵ í hálfleiðara stækkar með minnkandi E_g (er ∞ í málmum)

Orkuborðar -> virkur massi oft minni en m_e

-> bindiorka rafeinda við $\oplus$-hleðslunna í rafgjafa

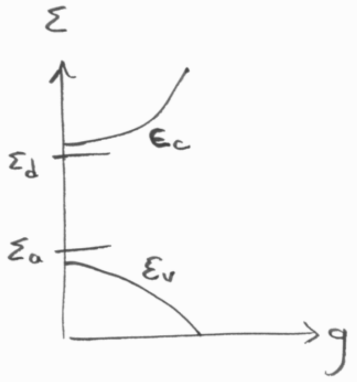
$$\mathcal{E} \simeq \frac{m^*}{m}\frac{1}{\epsilon^2} \times 13,6 \text{ eV}$$

getur verið mjög lítil

Sjálfsamkvæmt $\mathcal{E} << 13,6$ eV -> $a_0^* >> a_0$

rafeindin sér stórt svæði úr kristallinum

-> ϵ og m^* hafa þýðingu!



bindiorka $\ll E_g$

Si í Ga

$E_d \sim 5,9$ meV

$a_0 \sim 97,7$ Å

Sætni raf-gjafa og þega

Í jafnvægi gildir almennt

fjöldi einda í ástandi j

orka ástands j

$$\langle n \rangle = \frac{\sum_j N_j e^{-\beta(E_j - \mu N_j)}}{\sum_j e^{-\beta(E_j - \mu N_j)}}$$

N.B.

engin víxlverkun milli raf-gjafa og þega (ekki hár styrkur)

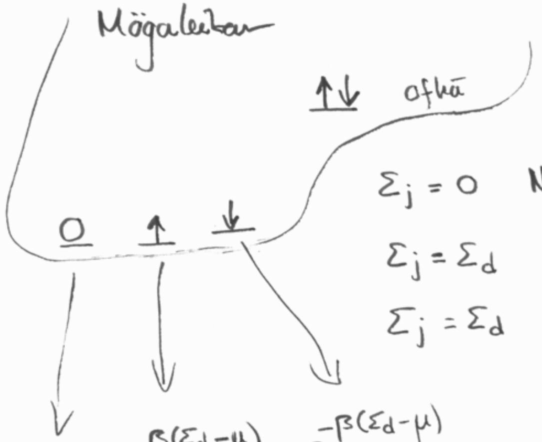
$N_a \leftarrow$ þéttni rafþega

$N_d \leftarrow$ .... rafgjafa

$n_a \leftarrow$ þéttni setinna rafþega

$n_d \leftarrow$ - - - .... gjafa

Rafgjafar



$\varepsilon_j = 0 \quad N_j = 0$

$\varepsilon_j = \varepsilon_d \quad N_j = 1$

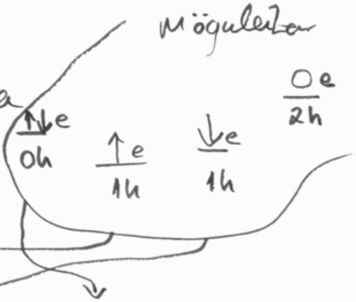
$\varepsilon_j = \varepsilon_d \quad N_j = 1$

$$\langle n\rangle = \frac{n_d}{N_d} = \frac{0 + e^{-\beta(\varepsilon_d-\mu)} + e^{-\beta(\varepsilon_d-\mu)}}{e^{-0} + e^{-\beta(\varepsilon_d-\mu)} + e^{-\beta(\varepsilon_d-\mu)}}$$

$$= \frac{2e^{-\beta(\varepsilon_d-\mu)}}{1+2e^{-\beta(\varepsilon_d-\mu)}} = \frac{1}{\frac{1}{2}e^{\beta(\varepsilon_d-\mu)}+1}$$

Rafþegar

Ein föst $\ominus$ hleðsla



$$\langle n\rangle = \frac{e^{-\beta(\varepsilon_a-\mu)} + e^{-\beta(\varepsilon_a-\mu)} + 2e^{-\beta(2\varepsilon_a-2\mu)}}{e^{-\beta(\varepsilon_a-\mu)} + e^{-\beta(\varepsilon_a-\mu)} + e^{-\beta(2\varepsilon_a-2\mu)}}$$

talið eftir rafeinda ástöndum

$$\langle n\rangle = \frac{2e^{\beta\mu} + 2e^{-\beta(\varepsilon_a-2\mu)}}{2e^{\beta\mu} + e^{-\beta(\varepsilon_a-2\mu)}} = \frac{e^{\beta(\mu-\varepsilon_a)}+1}{\frac{1}{2}e^{\beta(\mu-\varepsilon_a)}+1}$$

$$\langle p\rangle = 2 - \langle n\rangle, \quad \langle p\rangle = \frac{p_a}{N_a}$$

↑ mesti fjöldi rafeinda

$$\rightarrow \boxed{p = \frac{N_a}{\frac{1}{2}e^{\beta(\mu-\varepsilon_a)}+1}}$$

Sami orkustiga
íbotts hálfl.
í jafnvægi

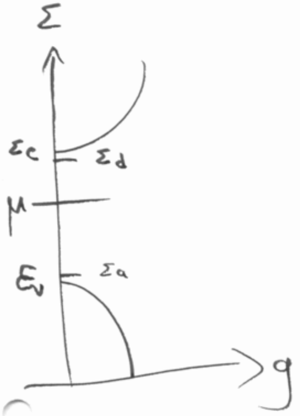
N_a : rafþegar

N_d : rafgjafar

$T = 0 \qquad N_d \geqslant N_a$

$$n_c + n_d - p_v - p_a = N_d - N_a$$

Gerum ráð fyrir



$$\Sigma_d - \mu >> k_B T \qquad E_g >> k_B T$$

$$\mu - \Sigma_a >> k_B T$$

$$\Downarrow$$

$$\left.\begin{matrix} n_d << N_d \\ p_a << N_a \end{matrix}\right\}$$

jónaðir
ratgjafar
+
þegar

$$\Delta n = n_c - p_v \simeq N_d - N_a$$

$$\rightarrow \quad \begin{Bmatrix} n_c \\ p_v \end{Bmatrix} = \frac{1}{2}\left[(N_d - N_a)^2 + 4n_i^2\right]^{1/2} \pm \frac{1}{2}\left[N_d - N_a\right]$$

$$\frac{N_d - N_a}{n_i} = 2 \sinh \beta(\mu - \mu_i)$$

$E_g >> k_B T$ og $|N_d - N_a|$ er ekki mörgum stærðargráðum minni en n_i

$$\rightarrow \mu \sim \mu_i$$

---

lág íbót

$$n_i >> |N_d - N_a|$$

$$\begin{Bmatrix} n_c \\ p_v \end{Bmatrix} = n_i\left[\frac{(N_d - N_a)^2}{4n_i^2} + 1\right]^{1/2} \pm \frac{1}{2}\left[N_d - N_a\right]$$

$$\simeq n_i \pm \frac{1}{2}\left[N_d - N_a\right]$$

mikil íbót

$n_i << |N_d - N_a|$, en $\quad \Sigma_d - \mu >> k_B T$

$\mu - \Sigma_a >> k_B T$

$$n_c \simeq N_d - N_a$$

$$p_v \simeq \frac{1}{2}\left((N_d - N_a)^2 + 4n_i^2\right)^{1/2}$$

$$- \frac{1}{2}(N_d - N_a)$$

$N_d > N_a$

n-efni

$$\simeq \frac{1}{2}(N_d - N_a)\left(1 + \frac{4n_i^2}{(N_d - N_a)^2}\right)^{1/2} - \frac{1}{2}(N_d - N_a)$$

$$\simeq \frac{1}{2}(N_d - N_a)\left(1 + \frac{2n_i^2}{(N_d - N_a)^2} \cdots\right) - \frac{1}{2}(N_d - N_a) \simeq \frac{n_i^2}{N_d - N_a}$$

→ $n_c >> p_v$

þegar $N_a > N_d$

$$n_c \simeq \frac{n_i^2}{N_a - N_d}$$

→ $p_v >> n_c$

$$p_v \simeq N_a - N_d$$

p - efni

---

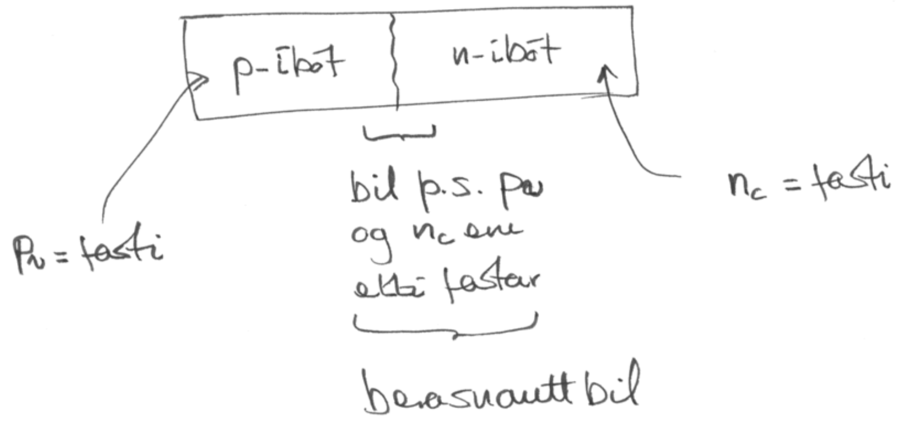
p-n samskeyti í jafnvægi

Hálfleiðaratækni byggðist mest á p-n samsk. sem dregin eru upp úr bráð.

Síðan bætast við

MBE samskeyti, íbót δ-íbót
LPE yfirgrindur, smámótun
⋮ ⋮

en p-n-samskeyti gefa innsýn í einföldustu hlutina



Veljum líkan skarpra skila

$$N_d(x) = \begin{cases} N_d & x > 0 \\ 0 & x < 0 \end{cases}$$

$$N_a(x) = \begin{cases} 0 & x > 0 \\ N_a & x < 0 \end{cases}$$

<u>Hálfsígilt líkan</u> $\qquad e\Delta\phi a \ll E_g$

$$n_c(x) = N_c(T)\exp\left\{-\frac{(\Sigma_c - e\phi(x) - \mu)}{k_BT}\right\}$$

$$p_v(x) = P_v(T)\exp\left\{-\frac{(\mu - \Sigma_v + e\phi(x))}{k_BT}\right\}$$

<u>Jaðarskilyrði</u> $\qquad$ <u>hleðsluberar hlýgas</u>

$$n_c(\infty) = N_c(T)\exp\left\{-\frac{(\Sigma_c - e\phi(\infty) - \mu)}{k_BT}\right\} = N_d$$

$$p_v(-\infty) = P_v(T)\exp\left\{-\frac{(\mu - \Sigma_v + e\phi(-\infty))}{k_BT}\right\} = N_a$$

<u>Jafnvægi</u> $\longrightarrow$ <u>μ: fasti</u>

$\rightarrow$

$$N_aN_d = N_c(T)P_v(T)\exp\left\{-\frac{(\Sigma_c - \Sigma_v + e\phi(-\infty) - e\phi(\infty))}{k_BT}\right\}$$

$$\ln\left\{\frac{N_aN_d}{N_cP_v}\right\} = -\frac{(\Sigma_c - \Sigma_v + e\phi(-\infty) - e\phi(\infty))}{k_BT}$$

$$\rightarrow \quad e\phi(\infty) - e\phi(-\infty) = \Sigma_c - \Sigma_v + k_BT\ln\left\{\frac{N_aN_d}{N_cP_v}\right\}$$

$$\rightarrow \quad \boxed{e\Delta\phi = E_g + k_BT\ln\left\{\frac{N_dN_a}{N_cP_v}\right\}}$$

mættis breyting v.þ.a. μ = fasti

Eins mætti skilgreina <u>rafefnamætti</u>

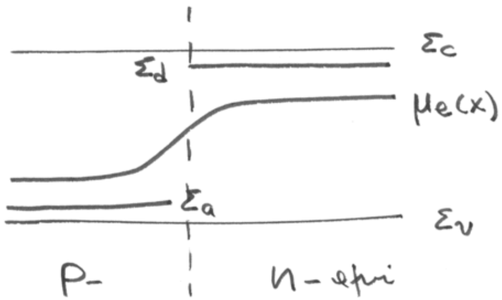
$$\mu_e(x) = \mu + e\phi(x)$$

með samsvarandi umskrift fyrir p_v og n_c

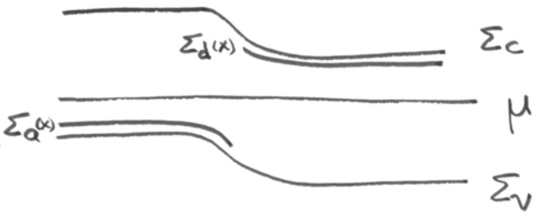
$$\rightarrow \quad e\Delta\phi = \mu_e(\infty) - \mu_e(-\infty)$$

Tvær myndir sama fyrirbæris

$\mu_e(x)$:



μ :



háð x því Σ_a miðast við Σ_v

Notum jöfnu Poissons til að reikna rafstöðumættið ϕ út frá hleðsludreifingu $\rho(x)$

↳ Borðabeyging við samskeyti

$$-\nabla^2\phi = \frac{4\pi}{\epsilon}\rho(x)$$

með

$$\rho(x) = e\left\{N_d(x) - N_a(x) - n_c(x) + p_v(x)\right\}$$

$n_c(x)$ og $p_v(x)$ eru háð $\phi(x)$

-> ólínuleg jafna $\phi(x)$ sem venjulega er leyst tölulega

Til þess að skilja samskeyti nánar eftirfarandi einfalt líkan skoðað

$$\boxed{e\Delta\phi \sim E_g >> k_BT}$$ notum

höfum $$n_c(x) = N_c(T)\exp\left\{-(\Sigma_c - e\phi(x) - \mu)\beta\right\} \quad ①$$

$$N_d = N_c(T)\exp\left\{-(\Sigma_c - e\phi(\infty) - \mu)\beta\right\} \quad ②$$

② -> $$N_c(T) = N_d\exp\left\{(\Sigma_c - e\phi(\infty) - \mu)\beta\right\}$$

notum í ①

$$n_c(x) = N_d \exp\left\{-(e\phi(\infty) - e\phi(x))\beta\right\}$$

eins fæst

$$p_v(x) = N_a \exp\left\{-(e\phi(x) - \phi(-\infty))\beta\right\}$$

$\phi'(x) \neq 0$ fyrir $-d_p \leq x \leq d_n$ ← gerum ráð fyrir

→ $n_c = N_d$ ef $x > d_n$

$p_v = N_a$ ef $x < -d_p$

vel innan bilsins gildir $n_c \ll N_d$, $p_v \ll N_a$

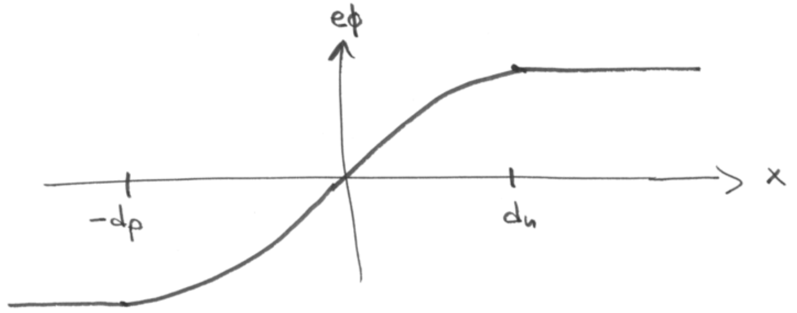
þar gildir $\rho(x) = e\left(N_d(x) - N_a(x)\right)$

Þá verður Poisson jafnan

$$\phi''(x) = \begin{cases} 0 & \text{ef} \quad x > d_n \\ -\frac{4\pi e}{\epsilon} N_d & \text{ef} \quad d_n > x > 0 \\ \frac{4\pi e}{\epsilon} N_a & \text{ef} \quad 0 > x > -d_p \\ 0 & \text{ef} \quad -d_p > x \end{cases}$$

Sem má heilda

$$\phi(x) = \begin{cases} \phi(\infty) \\ \phi(\infty) - \left(\frac{2\pi e N_d}{\epsilon}\right)(x - d_n)^2 \\ \phi(-\infty) + \left(\frac{2\pi e N_d}{\epsilon}\right)(x + d_p)^2 \\ \phi(-\infty) \end{cases}$$



⑧

Jaðarsk. + samfella + samfella ϕ'
er uppfyllt í $x = -d_p$ og d_n

samfella ϕ' í $x=0$
gefur $N_d d_n = N_a d_p$

samfella ϕ í $x=0$
gefur $\left(\frac{2\pi e}{\epsilon}\right)(N_d d_n^2 + N_a d_p^2) = \Delta\phi$

saman jöfnur fyrir d_n og d_p

$$d_{n,p} = \left\{ \frac{\left(\frac{N_a}{N_d}\right)^{\pm 1} \epsilon \Delta\phi}{(N_d + N_a)\, 2\pi e} \right\}^{1/2}$$

muna $\Delta\phi \sim E_g$

---

①

Afriðun p-n-samsteypa

ytri spenna V lögð á samsteypuna

mest spennufall þ.s. viðnám er
mest ⟺ berasnauða bilinu

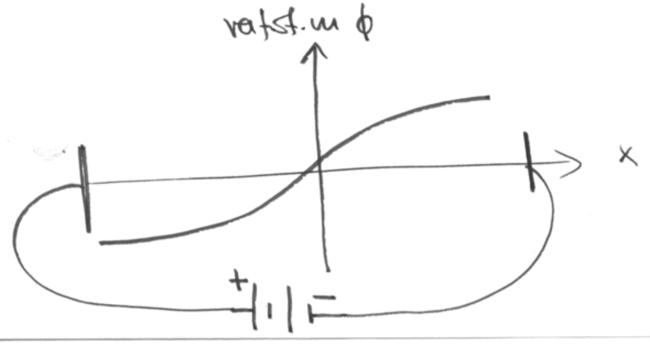
Gerum ráð fyrir að allt spennufallið
sé þar

fyrir $V=0$ var áður reiknað $\Delta\phi$
sem við köllum nú $(\Delta\phi)_0$

fyrir $V \neq 0$ er breyting rafstöðumættisins
yfir berasnauða bilið

$$\Delta\phi = (\Delta\phi)_0 - V$$

Ef V er lagt þ.a. rafstöðumætti
p-endans er hækkað m.v. n-endann



fyrir V=0 fékkst stærð berasnauða bilsins

$$d_{n,p} = \left\{ f(N_a,N_d)\,\Delta\phi \right\}^{1/2}$$

Því fæst fyrir V≠0

$$d_{n,p}(V) = d_{n,p}(0)\left\{ 1 - \frac{V}{(\Delta\phi)_0} \right\}^{1/2}$$

Athugum nú rafstraum $j = qJ$ þ.s. J er þéttleiki eindastraums, fjöldi einda sem streyma í gegnum flöt á tíma einingu

$$j_e = -eJ_e\,, \qquad j_h = eJ_h$$

$\uparrow$ rafeindastraums-þéttleiki

$\uparrow$ holustraums þéttleiki

V > 0

Berasnauðabilið minnkar

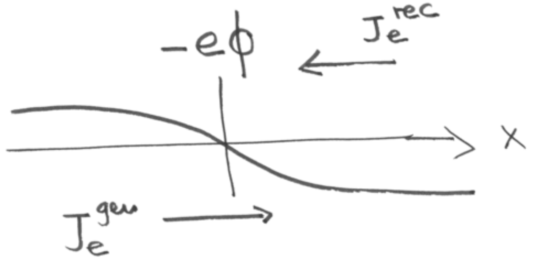
Viðnám bilsins minnkar

V < 0

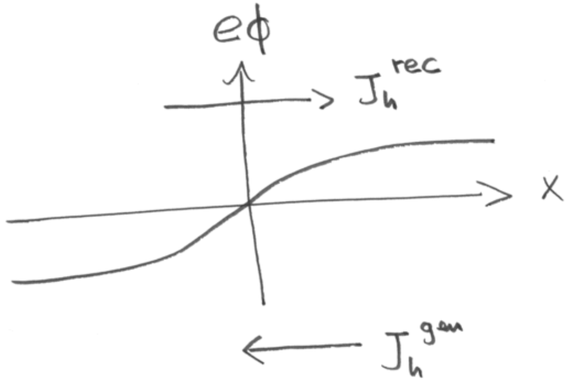
Berasnauða bilið stækkar og viðnám þess eykst

Hvernig lítur mættið (stöðuorka) eindanna út

Rafeindir



Holur



J^{rec} : Sameiningar streymur (eyðir)

J^{gen} : Framleiðslu streymur (skapar)

Skoðum fyrir holur

J_h^{gen} byrjar harsum fáar holur eru en þeim er ýtt í gegnum berasnauða bilið et þar komast uomi því,
Ekki mjög háður støddini og spennufalli á bilinu

$J_h^{gen} \sim e^{-e(\Delta\phi_0)_0}$

$\uparrow$

tilburðar-líkur

J_h^{rec} Rafsviðið á bilinum vinnur á móti streyminum.
eindirnar komast yfir þröskuldin við hitaorku

$$\rightarrow J_h^{rec} \sim e^{-e((\Delta\phi_0)-V)\beta}$$

J_h^{rec} er mjög háður V andstøtt J_h^{gen}

því at $\underline{V=0}$

$$\rightarrow J_h^{rec}(V=0) = J_h^{gen}$$

og því

$$J_h^{rec}(V) = J_h^{gen} e^{eV\beta}$$

heildar holu streymsþettleikin er

$$\underline{J_h = J_h^{rec} - J_h^{gen}}$$

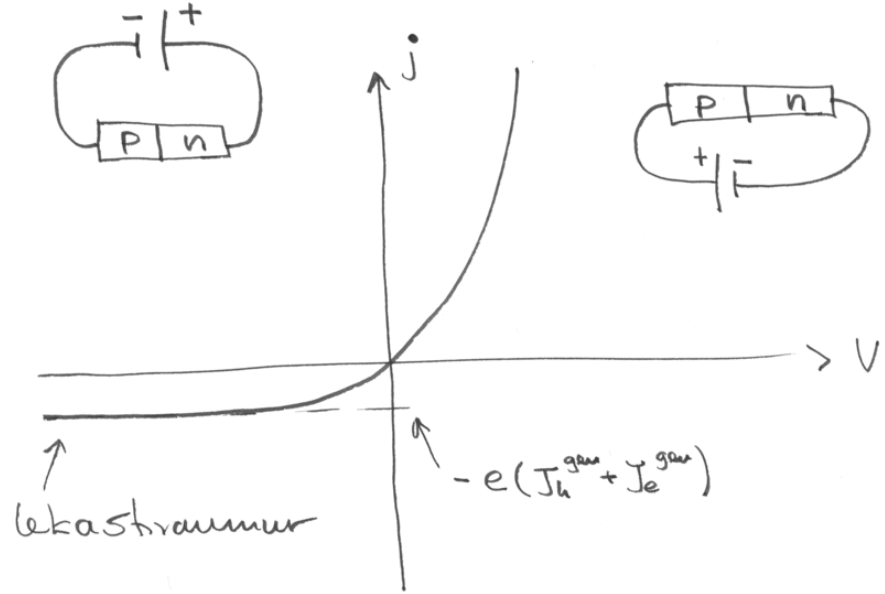
$\uparrow$

Stefnan ræðst av hlutfallinum

$$\rightarrow J_h = J_h^{rec} - J_h^{gen} = J_h^{gen}\left(e^{eV\beta} - 1\right)$$

Svipað má leiða út fyrir rafeinda streymsþettleika því fæst

$$j = e\underbrace{\left(J_h^{gen} + J_e^{gen}\right)}_{\sim \text{fasti}}\left(e^{eV\beta} - 1\right)$$



afriðlun möguleg

p-n: samskeyti -> tvistur (díóða)

margfaldari $V = (V_1 + V_2)$

$$j(V_1+V_2) \sim j(V_1)\cdot j(V_2) \quad \text{ef } eV_1, V_2 >> k_BT$$