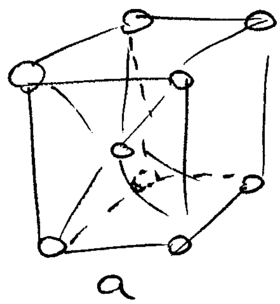
Exam 2007-06-20

Cond-mat I

① a) Wanted: Filling fraction of "hard sphere" atoms arranged in bcc and diamond structure

Solution

bcc:



2 at/cell $\left(8 \times \frac{1}{8} + 1 = 2\right)$

atoms touch along diagonal

$4r = \sqrt{3}a$

$$f = \frac{2 \cdot \frac{4}{3}\pi r^3}{a^3} = \frac{8\pi}{3}\left(\frac{r}{a}\right)^3 = \frac{8\pi}{3}\cdot\left(\frac{\sqrt{3}}{4}\right)^3 = \frac{\sqrt{3}\pi}{8} \approx \underline{\underline{0.68}}$$

diamond: as fcc + basis of 2 at along diagonal; $\bar{0}, \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)a$

$$2r = \frac{1}{4}\cdot\sqrt{3}a \Rightarrow f = \frac{8 \cdot \frac{4}{3}\pi r^3}{a^3} = \frac{\sqrt{3}\pi}{16} \approx \underline{\underline{0.34}}$$

(fcc: 4 at/cell, basis of 2 $\Rightarrow$ $2 \cdot 4 = 8$ at/cell)

b) Wanted: Coordination numbers for the atoms in bcc, diamond

Solution: ζ = # nearest neighbors

bcc: 8, diamond: 4

c) Wanted: hcp has lower or higher coordination number?

Answer: Higher, since higher number $\Leftrightarrow$ higher at. density

Closepacked $\rightarrow$ highest density

(both fcc, hcp have coordination number 12)

d) Wanted: Cell volume of smallest possible cell to generate diam. structure

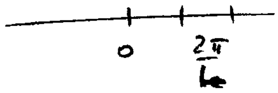
Solution: Diamond str = fcc + basis of 2 atoms

Primitive cell of fcc contains 1 atom

$\Rightarrow$ Smallest cell contains 2 atoms $\Rightarrow$ cell volume $\frac{2}{8}a^3 = \frac{a^3}{4}$

② a) Wanted : Density of states $g(\varepsilon)$ for el. in 1D, 2D, 3D

Solution : $\boxed{1D}$:



$g(k)\,dk = 2 \cdot \frac{L}{2\pi}\,dk$

pos
neg k

$$g(\varepsilon)\,d\varepsilon = g(k)\,dk$$

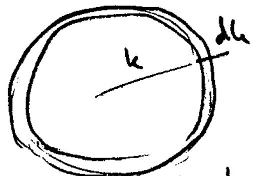
$$g(\varepsilon) = g(k)\,\frac{dk}{d\varepsilon} = \left\{ \varepsilon = \frac{\hbar^2 k^2}{2m} \right\} = 2 \cdot \frac{L}{2\pi} \cdot \frac{m}{\hbar^2 k} = \frac{L}{\pi\hbar}\frac{\sqrt{2m}}{\sqrt{\varepsilon}}$$

$$\left\{ d\varepsilon = \frac{\hbar^2 k}{m}\,dk \qquad k = \frac{\sqrt{2m\varepsilon}}{\hbar} \right\}$$

Spin ⟹ additional factor of 2

1D, 2D, 3D

$\boxed{2D}$:



$2\pi k\,dk$ = area

$$g(k)\,dk = \frac{2\pi k\,dk}{\left(\frac{2\pi}{L}\right)^2} = \frac{L^2 k\,dk}{2\pi} = \frac{L^2}{2\pi}\,\frac{m}{\hbar^2}\,d\varepsilon$$

$$\boxed{g(\varepsilon) = \frac{L^2 m}{2\pi\hbar^2}}$$

$\boxed{3D}$:

$$g(k)\,dk = \frac{4\pi k^2\,dk}{\left(\frac{2\pi}{L}\right)^3} = \frac{L^3}{2\pi^2}\,\frac{\sqrt{2m\varepsilon}}{\hbar}\,\frac{m\,d\varepsilon}{\hbar^2}$$

$$\boxed{g(\varepsilon) = \frac{L^3}{4\pi^2\hbar^3}(2m)^{3/2}\sqrt{\varepsilon}}$$

b) Wanted : ε_F in 2D, 3D

Solution :

$$N = \int_0^{\varepsilon_F} g(\varepsilon)\,d\varepsilon$$

$$2D:\; N = \frac{L^2 m}{\pi\hbar^2}\int_0^{\varepsilon_F} d\varepsilon = \frac{L^2 m}{\pi\hbar^2}\,\varepsilon_F \implies \boxed{\varepsilon_F^{2D} = \frac{\pi\hbar^2}{m}\cdot\frac{N}{L^2}}$$

$$3D:\; N = \frac{L^3}{2\pi^2\hbar^3}(2m)^{3/2}\int_0^{\varepsilon_F}\sqrt{\varepsilon}\,d\varepsilon = \frac{L^3}{2\pi^2\hbar^3}(2m)^{3/2}\,\frac{\varepsilon_F^{3/2}}{3/2}$$

$$\implies \boxed{\varepsilon_F = \hbar^2\left(\frac{3\pi^2 n}{2m}\right)^{3/2}} \quad \text{where } n = \frac{N}{L^3}$$

2c) Show: $d(hkl) = \dfrac{2\pi}{|\bar{G}(hkl)|}$

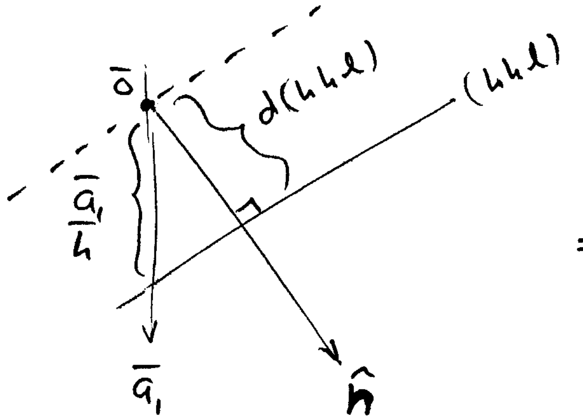
Solution:

One lattice plane goes through origin

Construct unit vector normal to (hkl):

$$\hat{n} = \frac{\bar{G}(hkl)}{|\bar{G}(hkl)|}$$

Make projection of intercept $\dfrac{\bar{a}_1}{h}$:



$$d(hkl) = \frac{\bar{a}_1}{h} \cdot \hat{n} =$$

$$= \frac{\bar{a}_1}{h} \cdot \frac{h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3}{|\bar{G}(hkl)|} =$$

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

$$= \frac{2\pi h}{h} \cdot \frac{1}{|\bar{G}(hkl)|} = \frac{2\pi}{|\bar{G}(hkl)|}$$

3 a) Describe: difference between ε_F and μ

Solution: ε_F is a zero temp. property, μ at non-zero temp.

b) Show: $\mu - \varepsilon_F \propto T^2$ in free-el model.

Solution: $D(\varepsilon)\,d\varepsilon = 2 \cdot \frac{V}{8\pi^3} 4\pi k^2 dk$ $\qquad \varepsilon = \frac{\hbar^2 k^2}{2m}$ free el model

Sommerfeld: $$\int_0^\infty A(\varepsilon) f(\varepsilon)\, d\varepsilon = \int_0^\mu A(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 A'(\mu)$$

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1}$$

$$N = \int_0^\infty D(\varepsilon) f(\varepsilon)\, d\varepsilon = \{\text{Sommerfeld}\} = \int_0^\mu D(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 \underbrace{D'(\mu)}_{\approx D'(\varepsilon_F)}$$

but $N = \int_0^{\varepsilon_F} D(\varepsilon)\, d\varepsilon$ and $\int_0^\mu D(\varepsilon)\, d\varepsilon \approx \int_0^{\varepsilon_F} D(\varepsilon)\, d\varepsilon + D(\varepsilon_F)(\mu - \varepsilon_F)$

$$\Rightarrow \quad D(\varepsilon_F)(\mu - \varepsilon_F) = -\frac{\pi^2}{6}(k_B T)^2 D'(\varepsilon_F)$$

$$\mu - \varepsilon_F = -\frac{\pi^2}{6}(k_B T)^2 \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} \quad \propto T^2$$

$$\left.\begin{aligned} D(\varepsilon) &\sim \sqrt{\varepsilon} \\ D'(\varepsilon) &= \frac{1}{2\varepsilon} D(\varepsilon) \end{aligned}\right\} \quad \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} = \frac{1}{2\varepsilon_F} \quad \Rightarrow \quad \mu - \varepsilon_F = -\frac{1}{3\varepsilon_F}\left(\frac{\pi k_B T}{2}\right)^2$$

3c) Describe: Concept of thermopower + typical temp. dep.

Answer: Electrical field caused by temp. gradient

$\bar{E} = Q \nabla T$ $\qquad$ or $\qquad U = S \cdot \Delta T$, $\quad S \sim T$ Seebeck coeff.

$Q = -\frac{C_v}{3ne}$ $\qquad C_v \propto T$ (el)

$\left(U = \int \bar{E}\, d\bar{l}\right)$

4a) <u>Show</u> that the thermal expansion of a lattice with harmonic interactions is zero.

<u>Solution</u>:

Harmonic interactions:

Potential $U \sim (r-r_0)^2$ where r_0 = eq. distance
r = distance

Set $x = r - r_0$

Assume classical model - Bolzmann statistics

We should show that $\langle x \rangle = 0$ (or indep. of T.)

average

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x \cdot e^{-U(x)/k_BT} dx}{\int_{-\infty}^{\infty} e^{-U(x)/k_BT} dx} = \frac{\int_{-\infty}^{\infty} x \cdot e^{-C \cdot x^2/k_BT} dx}{\int_{-\infty}^{\infty} e^{-Cx^2/k_BT} dx}$$

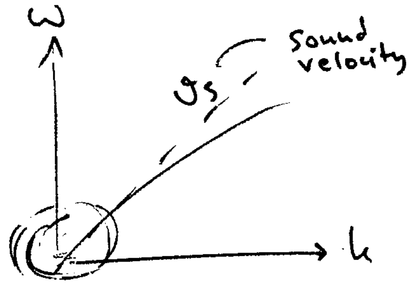
But $\int_{-\infty}^{\infty} x \cdot e^{-Cx^2/k_BT} dx$ is integral over odd×even funct.

$$\Longrightarrow \int = 0 \Rightarrow \langle x \rangle = 0$$

4b) Describe the difference between sound propagation and heat conductivity in el. isolators

Solution

Active phonons for sound propagation have small ω and k :



$$v_s = \lim_{k \to 0} \frac{\partial \omega}{\partial k}$$

Such phonons undergo elastic scatterings with each other, n-processes, where $\sum k$ and $\sum \omega$ are preserved

In heat conductivity, phonons with all ω and k may participate. Many U-processes will occur. (otherwise there would be no way to get thermal equilibrium)

Comment

$k = \frac{2\pi}{\lambda}$ long wavelengths $\Longleftrightarrow$ small k

Sound: $v_s \sim 10^3\, m/s$ freq $\sim$ 500 Hz

$$\lambda \sim \frac{v_s}{f} \sim 2m$$

$$\Rightarrow k \sim 1\, m^{-1} \ll k_{max} \sim \frac{2\pi}{a} = 10^{10}\, m^{-1}$$

5a) Describe the tightbinding model

Overlap of atomic wave functions weak — Use when

$\Rightarrow$ Start out a description of electrons in the material by using atomic wave functions

$$\Rightarrow \left[\hat{H}_{at} + \Delta U\right] \Psi = \varepsilon \Psi$$

original atomic Hamiltonian

additional potential from lattice

Energy eigenvalues of $\hat{H}_{at}$ will form bands not too far away from the atomic energy levels.

Small overlap of atomic wave functions

$\Updownarrow$

narrow bands

model describes band width

5b) Describe nearly free electron model

Use when effective potential is weak (due to Pauli principle, screening)

Model describes band gap

Start out with a free electron model and add a weak periodic potential

5c) Given:
$$\varepsilon = \frac{1}{2}\left(\varepsilon^{\circ}_{\bar{k}-\bar{G}} + \varepsilon^{\circ}_{\bar{k}}\right) \pm \sqrt{\frac{1}{4}\left(\varepsilon^{\circ}_{\bar{k}-\bar{G}} - \varepsilon^{\circ}_{\bar{k}}\right)^2 + U^2}$$

Explain: $\varepsilon^{\circ}_{\bar{k}} = \dfrac{\hbar^2 k^2}{2m}$

U = potential coefficient $\left(U(r) = \sum_{\bar{G}} U_{\bar{G}}\, e^{i\bar{G}\cdot\bar{r}} \right)$

$$U_{\bar{G}} = \begin{cases} U & \bar{G} = \pm 2\bar{k} \\ 0 & \text{otherwise} \end{cases}$$

$\bar{G}$ = reciprocal lattice vector

Show: that group velocity vanishes when $\bar{k} \to \dfrac{\bar{G}}{2}$

Solution:
$$v_g = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial k} = \frac{1}{\hbar}\frac{\partial}{\partial k}\left[\frac{1}{2}\left(\varepsilon^{\circ}_{\bar{k}-\bar{G}} + \varepsilon^{\circ}_{\bar{k}}\right) \pm \sqrt{\frac{1}{4}\left(\varepsilon^{\circ}_{\bar{k}-\bar{G}} - \varepsilon^{\circ}_{\bar{k}}\right)^2 + U^2}\right]$$

$$= \frac{1}{\hbar}\cdot\frac{1}{2}\cdot\frac{\hbar^2}{2m}\left(2(k-G) + 2k\right) \pm \frac{\frac{1}{4}\cdot 2\left(\varepsilon^{\circ}_{\bar{k}-\bar{G}} - \varepsilon^{\circ}_{\bar{k}}\right)\cdot\frac{\hbar^2}{2m}\left(2(k-\bar{G}) - 2k\right)}{2\sqrt{\ \cdots}}$$

$$k \to \frac{G}{2} \Rightarrow v_g = \frac{\hbar}{2m}\underbrace{\left(\left(\frac{G}{2} - G\right) + \frac{G}{2}\right)}_{=0} \pm \frac{0}{\sqrt{U^2}} = 0$$

$$\varepsilon^{\circ}_{\bar{k}-\bar{G}} = \varepsilon^{\circ}_{\bar{k}}$$

5d) Given: $\varepsilon(k) = \dfrac{\hbar^2}{ma^2}\left(\dfrac{7}{8} - \cos ka + \dfrac{1}{8}\cos 2ka\right)$

Wanted: Effective mass at bottom of band

Solution:
$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k^2} = \frac{1}{ma^2}\left(a^2\cdot\cos ka - \frac{(2a)^2}{8}\cos 2ka\right)$$

Bottom of band: $k = 0$

$$k \to 0 \Rightarrow \cos ka \approx 1 \Rightarrow \frac{1}{m^*} = \frac{1}{m}\left(1 - \frac{1}{2}\right) = \frac{1}{2m}$$

$$\boxed{m^* = 2m}$$

6a) Use Hund's rules to write spectroscopic notation ($^{2S+1}L_J$)
for ground states of the ions Cu^+ and Eu^{3+}

Solution

Cu^+ : [ ] $3d^{10}$ $\longrightarrow$ full d-shell

Hund's rules:
① Maximize S — $S=0$
② Maximize L — $L=0$
③ take $J=|L-S|$ or $L+S$ — $J=0$
(less than half filled or more than half filled)

$\Rightarrow \boxed{^1S_0}$

Eu^{3+} : [ ] $4f^6$

4f :

↑	↑	↑	↑	↑	↑	
3	2	1	0	-1	-2	-3

$S = \sum s = 3$

$L = \sum \ell = 3$

$J = |L-S| = 0$

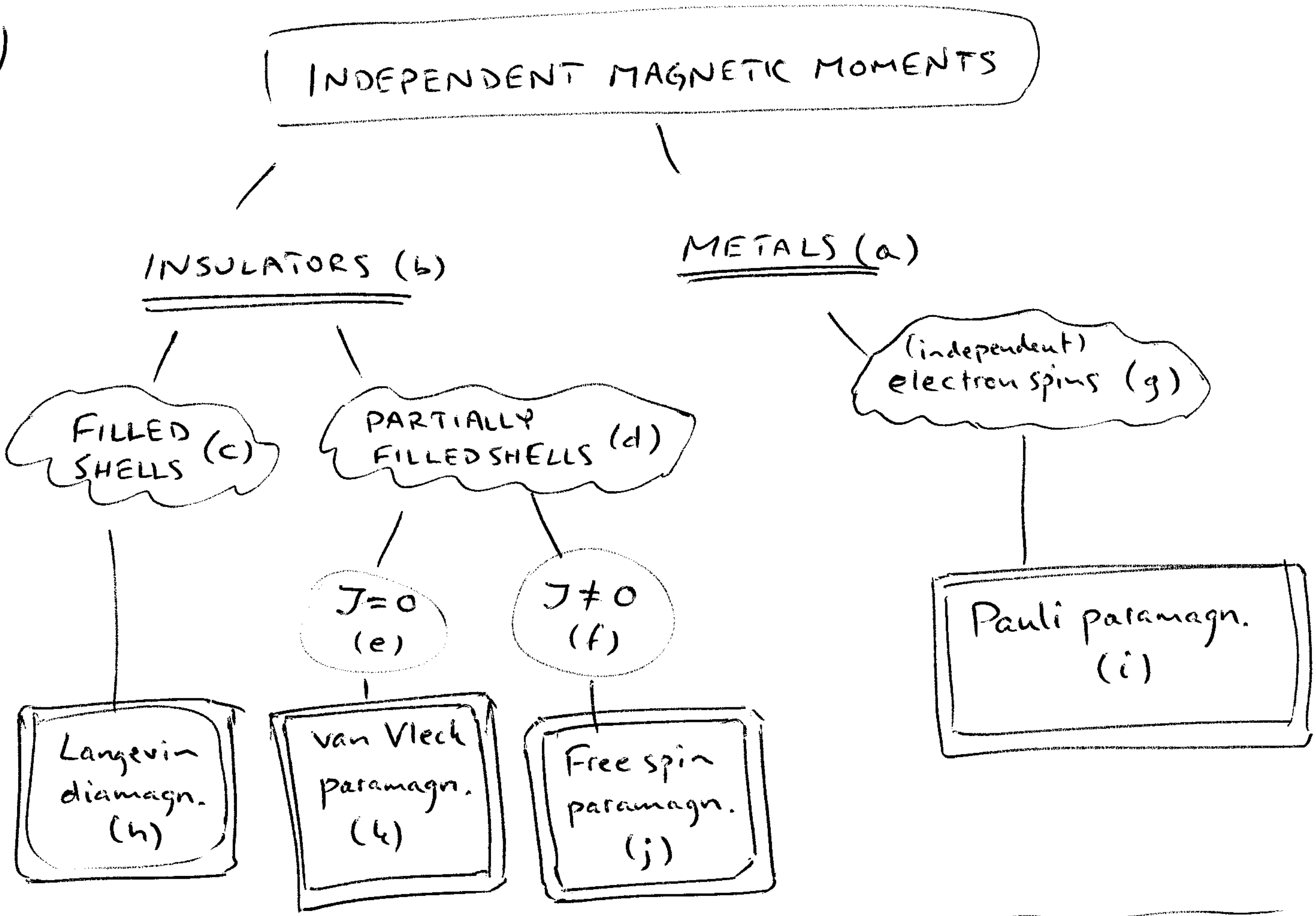
↳ less than half-filled shell

$2S+1 = 7$

$L=3$ is written as F $\left(\begin{array}{ccccc} S & P & D & F & G \\ 0 & 1 & 2 & 3 & 4 \end{array}\right)$

$\boxed{^7F_0}$

6b)



6c) Superconducting gap: Gap in the normal state density of states around ε_F

Cooper pairs: Pair of coupled electrons forming a boson

Tunneling: Passing a barrier (insulator) either as a single particle (Giaever) or as a Cooper pair (Josephson)

Isotope effect: T_c varies with isotope mass: $T_c \sim \frac{1}{\sqrt{M}}$

Condensation energy: The energy gained by the system when electrons pair up and condense into a common boson ground state

Vortices: "Tubes" where superconductivity is locally depressed. Each tube carries one magnetic flux quantum, $\phi_0 = \frac{h}{2e}$

The vortices form a 2D lattice