MIDTERM EXAM – SOLUTIONS

1) FREE ELECTRON MODELS

$$n = 0.6022 \times 10^{24} \frac{Z \rho_m}{A}$$

For copper

$\rho_m = 8.94$ g/cm^3 – mass density

$Z = 1$ – number of electrons contributing to the Fermi gas

$A = 63.5$ g – atomic mass

$$\Rightarrow \quad n = 8.5 \times 10^{22} \text{ cm}^{-3}$$

$$k_F = (3\pi^2 n)^{1/3} = 1.36 \times 10^8 \text{ cm}^{-1}$$

– Fermi speed

$$v_F = \frac{\hbar k_F}{m} = \frac{(1.05 \times 10^{-27} \text{ erg}\cdot\text{s})(1.36 \times 10^8 \text{ cm}^{-1})}{(9.11 \times 10^{-28} \text{ g})} = \boxed{1.57 \times 10^8 \text{ cm/s}}$$

– Fermi energy

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \boxed{(7.0 \text{ eV})(1.6 \times 10^{-12} \text{ erg})}$$

– The energy per electron E/N, in the ground state ($T = 0$) is (see A./M. pag. 38, formula 2.31)

$$\frac{E}{N} = \frac{3}{5}\varepsilon_F = \boxed{4.2\ eV}$$

The average kinetic energy of free particles in a classical ideal gas is $\frac{3}{2}k_BT$, which vanishes at $T=0$.

HARMONIC CRYSTAL VIBRATIONS

c) When $k_B T$ is large compared with all the phonon energies $\hbar\omega$ (i.e. when every normal mode is in a highly excited state), the specific heat reduces to the classical law of Dulong and Petit. This is the high-temperature limit (A/M. pag. 454).

At $T = 1K$ we can use the Debye model

$$c_{v,ph} \propto \left(\frac{T}{T_D}\right)^3 \frac{N}{V} k_B \qquad \text{(ep. 23.27)}$$

where N is the number of ions in the crystal.

The electronic contribution to the specific heat is given by

$$c_{v,el} \propto \left(\frac{T}{T_F}\right) \frac{N'}{V} k_B$$

where N' is the number of free electrons.

At low temperature we can assume that $N' = N$, thus

$$\left.\frac{c_{v,ph}}{c_{v,el}} \cong T^2 \frac{T_F}{T_D^3}\right|_{T=1} = \boxed{0.01}$$

b) $u_{n+1} = e^{ika} u_n$ for $ka = \pi$ $\boxed{\frac{u_{n+1}}{u_n} = -1}$

$$v_g = \frac{\partial \omega}{\partial k} = \sqrt{\frac{Ca^2}{M}} \cos\left(\frac{1}{2}ka\right)$$

Kittel, pag. 93, ep. 10
pag 94, ep. 14

$$\boxed{v_g\Big|_{ka=\pi} = 0}$$

c) For $ka \ll \pi$ (see Kittel pag. 98, eq. 23, 24), the optical branch dispersion gives

$$\omega^2 \cong 2C\left(\frac{1}{M_{Ga}} + \frac{1}{M_{As}}\right)$$

C is the force constant between nearest-neighbor planes

$$\Rightarrow C = \frac{M_{Ga} M_{As} \omega^2}{2(M_{Ga} + M_{As})} = \frac{70 \cdot 75\, m_p^2 \omega^2}{2(70+75)\, m_p} \cong 18\, m_p \omega^2$$

$$= 18 \times \frac{9.4 \times 10^8\ eV}{(3 \times 10^{10}\ cm\ s^{-1})^2} (2\pi \times 8 \times 10^{12}\ s^{-1})^2 \cong \boxed{4.7 \times 10^{16}\ eV/cm^2}$$

The acoustical branch dispersion for $ka \ll \pi$ is

$$\omega^2 \cong \left(\frac{C/2}{M_{Ga} + M_{As}}\right) k^2 a^2$$

$$v_g = \frac{\partial \omega}{\partial k} = \left(\frac{C/2}{M_{Ga} + M_{As}}\right)^{1/2} a = \left(\frac{4.7 \times 10^{16}\ eV\,cm^{-2}}{2(70+75)\ 9.4 \times 10^8\ eV}\right)^{1/2} (3 \times 10^{10}\ cm\,s^{-1})\, a$$

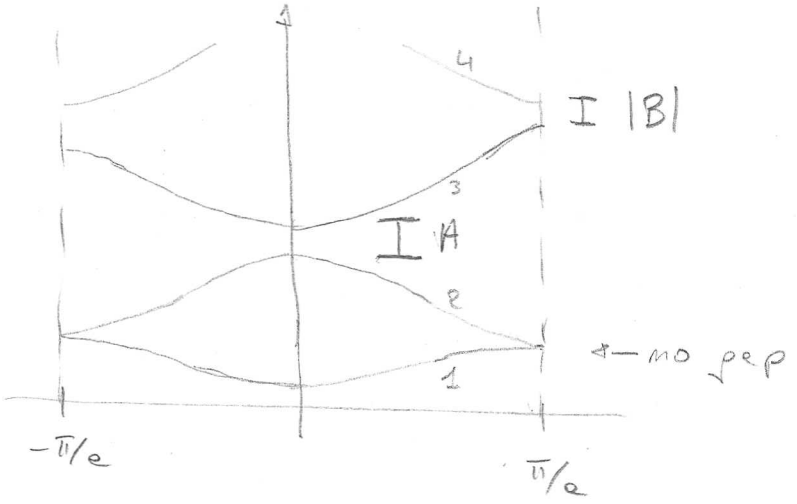
$$\cong \boxed{7 \times 10^5\ cm/s}$$

ELECTRONIC BAND STRUCTURES

a) In the nearly free-electron approximation the periodic potential is treated as a perturbation relative to the kinetic energy of the electrons. Thus the potential energy must be much smaller than the kinetic energy:

$$|V_0| \ll \frac{\hbar^2}{2m}\left(\frac{G_1}{2}\right)^2 ; \quad |A| \ll \frac{\hbar^2}{2m}\left(\frac{3}{2}G_1\right)^2 ; \quad |B| \ll \frac{\hbar^2}{2m}(2G_1)^2$$

$G_1 = \frac{2\pi}{a}$



b) The degeneracy of energies is removed by mixing the corresponding wavefunctions and the perturbation potential (A./M. pag. 160). The perturbation potential does not have Fourier component for G_1 and there is no gap at $k = \pi/a$ between $n=1$ and $n=2$

$$\frac{1}{Na}\int_0^{Na} V(x)\, e^{-ikx}\, e^{i(k-2\pi/a)x}\, dx = \langle \psi_1 | V(x) | \psi_2 \rangle = 0$$

c) The delta-Dirac potential has all Fourier components of the same value

$$\frac{1}{Na}\int_0^{Na} V(x)\, e^{-i 2\pi m x/a} = V_0$$

$Na = L$ is the total length of the system

$$\Delta E = 2V_0$$

In the nearly free-electron approximation the band gaps are all the same. If we solve the problem exactly (see Kittel pgs. 169-170), we have gaps of different values.