Final Exam, SIF4052, Fall 2000
Solutions

Problem 1

We Fourier transform Eq. (1.1) to find

$$\omega^2 \tilde{u} = \left(\frac{c}{\rho}\right) k^2 \tilde{u} \ , \tag{s1.1}$$

leading to a long wavelength dispersion relation

$$\omega^2 = \left(\frac{c}{\rho}\right) k^2 \ . \tag{s1.2}$$

We then expand the exact dispersion relation in Eq. (1.2) to lowest order in k to get the long wavelength limit:

$$\omega^2 = \left(\frac{4K}{M}\right) \left(\frac{ka}{2}\right)^2 \ . \tag{s1.3}$$

Comparing Eqs. (s1.2) and (s1.3), we find

$$c = \frac{Ka^2}{M} \rho = \frac{K}{a} \ , \tag{s1.4}$$

where we have used that $\rho = M/a^3$.

Note that this expression is somewhat different from the one given in Elliott's book ($c = Ka$ — on page 222). The reason for this is that Elliott considers a one-dimensional system, while we are dealing with a three-dimensional crystal.

Problem 2

a) The periodic boundary conditions impose the periodicities

$$\vec{u}(\vec{r} + L\vec{e}_x) = \vec{u}(\vec{r}) \ , \tag{s2.1}$$

and

$$\vec{u}(\vec{r}+L\vec{e}_y)=\vec{u}(\vec{r}) \ , \tag{s2.2}$$

where L is linear size of system, so that $L^2=Na^2$. Looking at Fourier modes of the wave $\vec{u}(\vec{r},t)=\vec{u}(\vec{k},t)\exp(i\vec{k}\cdot\vec{r})$, Eqs. (s2.1) and (s2.2) impose

$$e^{ik_xL}=1 \ , \tag{s2.3}$$

and

$$e^{ik_yL}=1 \ . \tag{s2.4}$$

Hence, we have that

$$k_x=\frac{2\pi n_x}{L} \ , \tag{s2.5}$$

and

$$k_x=\frac{2\pi n_y}{L} \ , \tag{s2.6}$$

where n_x and n_y are integers. The spacing between allowed $\vec{k}$ values in the x direction is $2\pi(n_x+1)/L-2\pi(n_x)=2\pi/L$, and likewise for the y direction. Hence, the density is

$$\rho=\left(\frac{L}{2\pi}\right)^2=\frac{Na^2}{4\pi^2} \ . \tag{s2.7}$$

b) k_D is given by the equation

$$\rho\pi k_D^2=N \ . \tag{s2.8}$$

Combining this expression with Eq. (s2.7) gives

$$k_D=\sqrt{\frac{N}{\rho\pi}}+\sqrt{\frac{N4\pi^2}{\pi Na^2}}=\frac{2}{a}\sqrt{\pi} \ , \tag{s2.9}$$

which is the answer.

c) The density of states in $\vec{k}$ space is

$$g(k)dk=\rho 2\pi k dk \ , \tag{s2.10}$$

where ρ is given in Eq. (s2.7). The dispersion relation of the system is

$$\omega=vk \ . \tag{s2.11}$$

Hence, the density of states is given by

$$g(\omega)d\omega = g(k)\ \frac{dk}{d\omega}\ d\omega = 2\pi\rho\ \frac{\omega}{v}\ \frac{1}{v}\ d\omega\ . \qquad (s2.12)$$

where we also used Eq. (s2.11). Combining this expression with Eq. (s2.7), we find the final answer

$$g(\omega) = \left(\frac{Na^2}{2\pi v^2}\right)\ \omega\ . \qquad (s2.13)$$

d) The Debye model calls for introducing a cutoff in the density of states at a frequency ω_D. This cutoff is determined by the integral

$$\int_0^{\omega_D} g(\omega)\ d\omega = \frac{Na^2}{4\pi v^2}\ \omega_D^2 = 2N\ . \qquad (s2.14)$$

Hence,

$$\omega_D = \sqrt{8\pi}\ \frac{v}{a}\ . \qquad (s2.15)$$

The relation between ω_D and the Debye temperature Θ_D is

$$\hbar\omega_D = k_B\Theta_D\ . \qquad (s2.16)$$

Thus, we have

$$\Theta_D = \sqrt{8\pi}\ \frac{\hbar v}{k_B a}\ . \qquad (s2.16)$$

The heat capacity is given by

$$C = \frac{\partial U}{\partial T}\ , \qquad (s2.17)$$

where the energy is given by

$$U = \int_0^{\omega_D} \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}\ g(\omega)d\omega = \int_0^{\hbar\omega_D} \frac{Na^2}{4\pi\hbar^2 v^2}\ \frac{(\hbar\omega)^2 d(\hbar\omega)}{e^{\hbar\omega/k_BT}-1}\ . \qquad (s2.18)$$

If we now scale the integration variable in this integral, $\hbar\omega \to \hbar\omega/k_BT = x$, Eq. (s2.18) becomes

$$U = \frac{Na^2}{4\pi\hbar^2 v^2}\ (k_BT)^3\ \int_0^{\Theta_D/T} \frac{x^2 dx}{e^x-1}\ , \qquad (s2.19)$$

where we have used the definition of $\Theta_D = \hbar\omega_D/k_B$. We now take into account that we are only interested in the low-temperature limit, $T \ll \Theta_D$. As the integrand behaves as $x^2\exp(-x)$ it disappears very rapidly and the integral converges towards a constant. Hence, we may extend the upper limit of the integral to infinity without making any appreciable error. Hence, we have

$$U = \frac{Na^2}{4\pi\hbar^2 v^2}\,(k_B T)^3 \int_0^\infty \frac{x^2 dx}{e^x - 1}\ , \qquad (s2.20)$$

and combining this expression with Eq. (s2.17), we find

$$C = \frac{3Na^2 k_B^3}{4\pi\hbar^2 v^2}\,T^2 \int_0^\infty \frac{x^2 dx}{e^x - 1} \propto T^2\ . \qquad (s2.21)$$

Problem 3

a) The total potential is given by

$$V(x) = \sum_{j=-\infty}^{j=+\infty} V_j(x) = \sum_{j=-\infty}^{j=+\infty} [V_{2j}(x) + V_{2j+1}(x)]\ . \qquad (s3.1)$$

where we on the right hand side sum explicitly both over the atoms at positions ja and positions $ja + a/4$. We may relate each of the potentials around each atom to the one around the atom at the origin,

$$V(x) = \sum_{j=-\infty}^{j=+\infty} [V_0(x - aj) + V_0(x - a/4 - aj)]\ . \qquad (s3.2)$$

The Fourier components of the potential is

$$\tilde{V}_G = \frac{2\pi}{a} \sum_{j=-\infty}^{j=+\infty} \int_{-a/2}^{+a/2} [V_0(x - ja) + V_0(x - a/4 - ja)]\; e^{i(2\pi/a)kx}\ dx\ , \qquad (s3.3)$$

where $G = k(2\pi/a)$. By changing variable $x \to x - aj$, we may rewrite this integral

$$\tilde{V}_G = \frac{2\pi}{a} \sum_{j=-\infty}^{j=+\infty} \int_{-a/2-aj}^{+a/2-aj} [V_0(x) + V_0(x - a/4)]\; e^{i(2\pi/a)kx}\ dx\ . \qquad (s3.4)$$

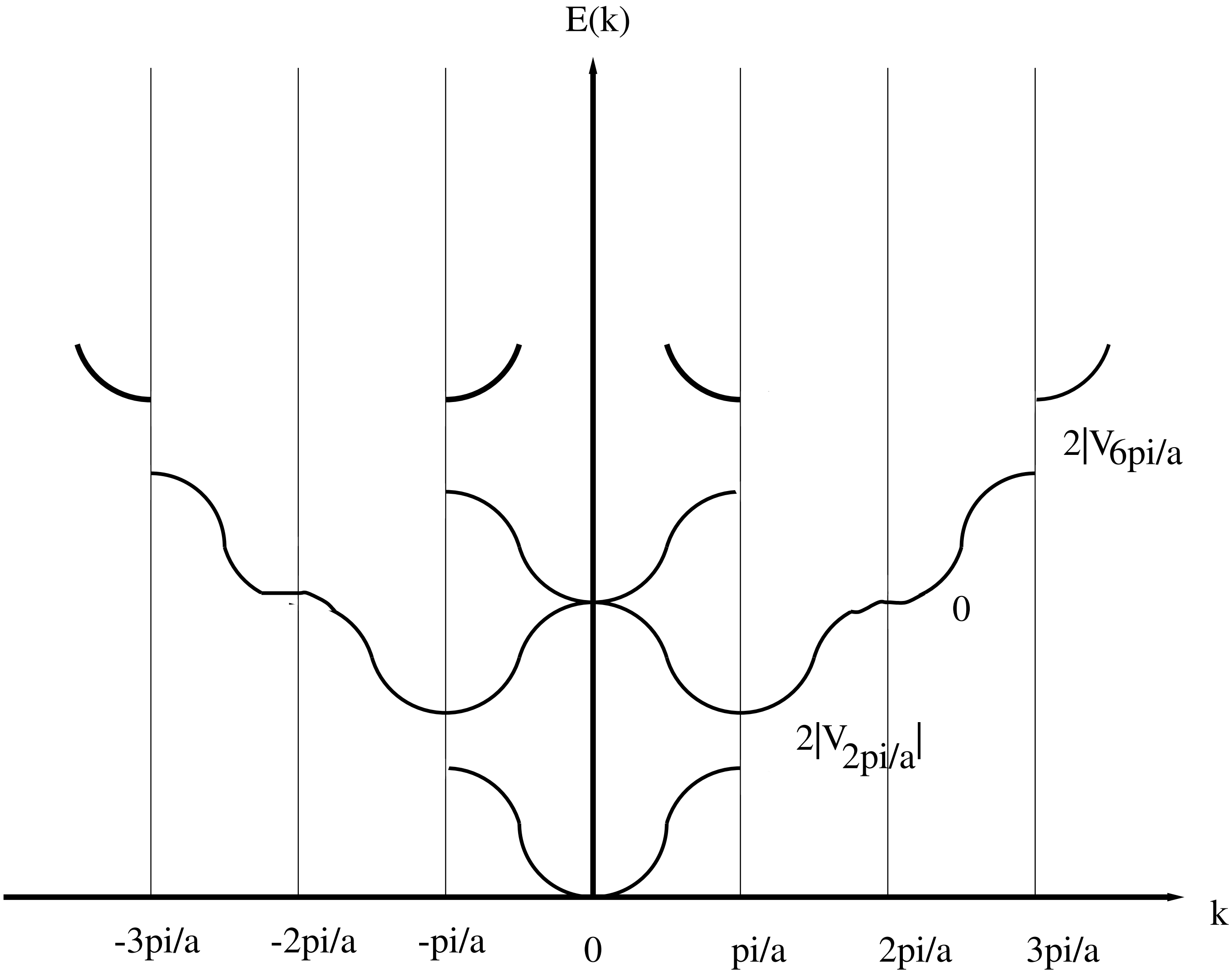

Figure 1: Sketch of band structure.

We now note that

$$\sum_{j=-\infty}^{j=+\infty} \int_{-a/2-aj}^{+a/2-aj} dx = \int_{-\infty}^{+\infty} dx \ . \qquad (s3.5)$$

Hence, Eq. (s3.4) becomes

$$\tilde{V}_G = \frac{2\pi}{a} \int_{-\infty}^{+\infty} [V_0(x) + V_0(x - a/4)] \ e^{i(2\pi/a)kx} \ dx \ . \qquad (s3.6)$$

In the second factor in the integral, we make the change of variable $x \to x + a/4$, and as a result, Eq. (s3.6) becomes

$$\tilde{V}_G = \frac{2\pi}{a} \int_{-\infty}^{+\infty} V_0(x)[e^{i(2\pi/a)kx} + e^{i(2\pi/a)kx+i(2\pi/a)k(a/4)}] \ . \qquad (s3.7)$$

This equation may be further simplified to

$$\tilde{V}_G = \frac{2\pi}{a} \int_{-\infty}^{+\infty} V_0(x)e^{i(2\pi/a)kx}[1 + e^{ik\pi/2}] \ , \qquad (s.3.8)$$

which is the Fourier component in its final form. We see that for $k = 2$, $\exp(ik\pi/2) = \exp(i\pi) = -1$, and Eq. (s3.8) is zero.

b) To lowest order, gap number k is proportional to $2|V_G|$ where $G = k(2\pi/a)$ — see Eq. (5.79) and Fig. 5.17 in Elliott. In our case, the second gap is zero, othwerwise the figure asked for in the present problem is identical to Figs. 5.17a and b in Elliott. The result is shown in Fig. 1.

Problem 4

a) See attached sketch, Fig 2. The crucial point here is that the Fermi surface approaches the zone boundaries at right angles.

b) The group velocity is given by

$$\vec{v}_g = \frac{\partial \omega}{\partial \vec{k}} = \frac{1}{\hbar} \ \vec{\nabla}_{\vec{k}} E \ . \qquad (s4.1)$$

Near the zone boundary, the gradient $\vec{\nabla}_{\vec{k}} E$ must be parallel to the zone boundary, and hence, so is the direction of the group velocity.

c) See Fig. 2. The 3BZ is the area in which "P" is inscribed, and those obtained by repeated 60° rotations.

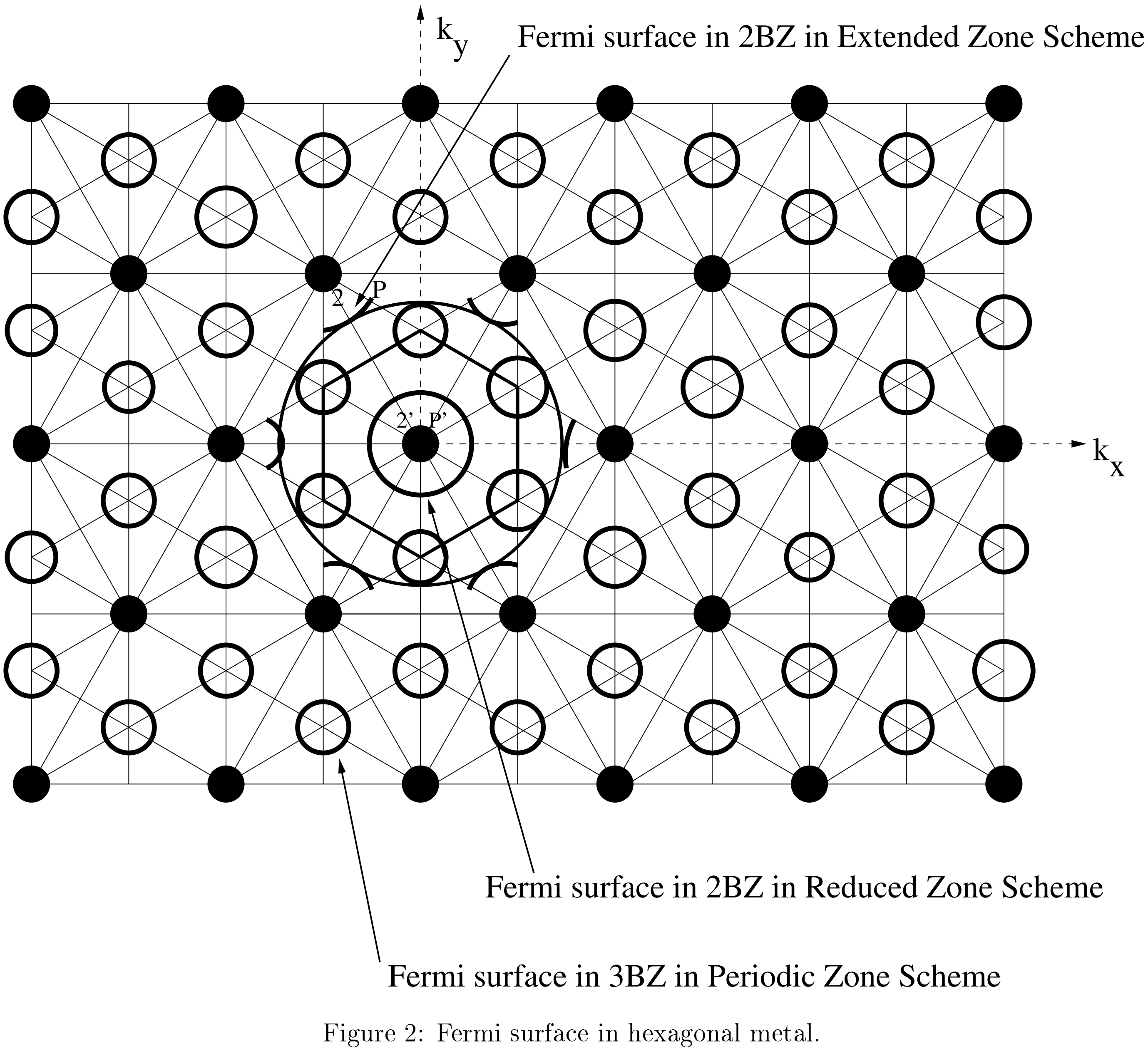

Figure 2: Fermi surface in hexagonal metal.