

PHYSICS 525, CONDENSED MATTER

Homework 1

Due Tuesday, 26th September 2006

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Problem 1

We are asked to study the penetration of normally incident, linearly polarized—with polarization parallel to the surface—electromagnetic radiation into a conductor using the Drude model. Let the surface be located at $z = 0$, with $z > 0$ vacuum and $z \leq 0$ be a conductor. We may assume that the relaxation rate is large relative to the plasma frequency, so $\omega_p \tau \gg 1$, and that the plasma frequency is large relative to the incident radiation, $\omega \omega_p \ll 1$; we should allow $\omega \tau$ to be arbitrary.

a) Let us first consider the limit of a free electron plasma, where $1/\tau \rightarrow 0$. We are to solve for the full pattern of the electric field both within and without the conductor, calculate the skin depth, and determine quantitative skin depth in this approximation for visible light at 6×10^{14} Hz incident on copper.

We begin by reminding ourselves of some simple electrodynamics learned by rote long ago when we took Jackson: for light incident on a surface at $z = 0$, with outward normal \vec{n} , the conditions to be imposed at the boundary are that the normal components of \mathbf{B} and \mathbf{D} and the tangential components of \mathbf{E} and \mathbf{H} are continuous. If we express the fields in question as

$$\mathbf{E}_{in} = \Re \left\{ \hat{x} E_{in} e^{-i(kz + \omega t)} \right\} \quad \mathbf{E}_{ni} = \Re \left\{ \hat{x} E_{ni} e^{i(kz - \omega t)} \right\} \quad \mathbf{E}_r = \Re \left\{ \hat{x} E_r e^{-i(k'z + \omega t)} \right\}, \quad (\text{a.1})$$

where \mathbf{E}_{ni} is the reflected wave and the others are self-evident, then making use of Maxwell's equations to relate \mathbf{B}_i to \mathbf{E}_i then we find these boundary conditions—the ones for \mathbf{E} and \mathbf{H} —imply that

$$(\mathbf{E}_{in} + \mathbf{E}_{ni} - \mathbf{E}_r) \wedge \vec{n} = 0 \quad \implies \quad E_r = E_{in} + E_{ni}; \quad (\text{a.2})$$

$$(\vec{k} \wedge \mathbf{E}_{in} - \vec{k} \wedge \mathbf{E}_{ni} - \vec{k}' \wedge \mathbf{E}_r) \wedge \vec{n} = 0 \quad \implies \quad k' E_r = k (E_{in} - E_{ni}). \quad (\text{a.3})$$

Now, Maxwell's equations give us $-\nabla^2 \mathbf{E} = \frac{\omega^2}{c^2} \epsilon(\omega) \mathbf{E}$, so $k = \frac{\omega}{c}$ in the vacuum and $k' = \frac{\omega}{c} \sqrt{\epsilon}$ in the medium. This allows us to solve the boundary conditions above rather straight-forwardly in no more than a couple of lines of algebra:

$$\boxed{E_{ni} = E_{in} \frac{1 - \sqrt{\epsilon}}{1 + \sqrt{\epsilon}} \quad \text{and} \quad E_r = E_{in} \frac{2}{1 + \sqrt{\epsilon}}.} \quad (\text{a.4})$$

After the above preliminaries, we are ready to perform the more specific challenges of the problem. We can easily find the limit of the expression for $\epsilon(\omega)$ predicted by the Drude model when $1/\tau \rightarrow 0$:

$$\begin{aligned} \epsilon(\omega) &= 1 + \frac{4\pi i n e^2 \tau}{m\omega(1 - i\omega\tau)}, \\ &= 1 + \frac{4\pi i n e^2}{m\omega(1/\tau - i\omega)}, \\ &\xrightarrow{q/\tau \rightarrow 0} 1 - \frac{4\pi n e^2}{m\omega}. \end{aligned}$$

For much of the range of light frequency¹, this is a negative, real-valued dielectric constant, which means that light essentially does not penetrate the surface. To see this, recall that $k' = \sqrt{\epsilon}$, so if ϵ is real and negative k' is pure imaginary, which means that the strength of the refracted wave dies exponentially inside the surface. This exactly follows our intuition about plasmas. The skin depth is given by

$$\boxed{\delta = \frac{c}{\omega} \frac{1}{\sqrt{\frac{4\pi n e^2}{m\omega^2} - 1}}.} \quad (\text{a.5})$$

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¹The point at which k becomes real for copper (in this approximation, which is crude) is 2.6×10^{15} Hz.

Before we move on, we are to calculate the skin depth of copper in this approximation, using real numbers—a headache to most theorists. To do this we need to choose a consistent set of units. I will use the units for which

$$e^2 = 1.907 \times 10^{-72} \text{ m}^2 \quad m_e = 6.764 \times 10^{-58} \text{ m}.$$

These work out quite well and one finds that

$$\boxed{\delta_{\text{Cu}} = 19 \text{ nm.}} \tag{a.6}$$

b) We are now asked to generalize our work above to the situation where there is scattering in general. We should simplify our expressions as much as possible by keeping only leading terms in ω/ω_p and $1/(\omega_p\tau)$. We are to determine the resulting electric fields for the situation of part **a** above, calculate the absorption coefficient and plot this as a function of $\omega\tau$.

Just in case the grader is keeping a tally, please notice that our solution for the full electric field pattern in part **a** above did not depend on the assumption that there was no scattering, so the result applied exactly.

Before we begin, we should comment that we have found nothing slight of horrendous in this problem. There is little elegance, and in general, everything becomes messy very fast. Let us just clarify our starting point and our goal: we know that in the Drude model

$$\epsilon(\omega) = 1 + \frac{i\omega_p^2\tau}{\omega(1 - i\omega\tau)}, \tag{b.1}$$

and from our course in electrodynamics so many years ago² that the absorption coefficient is given by

$$T = \frac{4\Re\{\sqrt{\epsilon}\}}{|1 + \sqrt{\epsilon}|^2}. \tag{b.2}$$

Let us now begin. We will make repeated use of the fact that $\omega_p\tau \gg 1$ and $\omega_p/\omega \gg 1$. The first instance of this appears in the third line, if you're paying attention. To simplify life a lot, we will define the parameter ξ so that $\sinh \xi = \omega\tau$.

$$\begin{aligned} \epsilon &= 1 + \frac{i\omega_p^2\tau}{\omega(1 - i\omega\tau)} \frac{(1 + i\omega\tau)}{(1 + i\omega\tau)}, \\ &= 1 - \frac{\omega_p^2\tau^2}{1 + \sinh^2 \xi} \left\{ 1 - \frac{i}{\sinh \xi} \right\}, \\ &\approx -\frac{\omega_p^2\tau^2}{\cosh^2 \xi} \left\{ 1 - \frac{i}{\sinh \xi} \right\}, \\ &= \frac{\omega_p^2\tau^2}{\cosh \xi \sinh \xi} e^{i(\theta + \pi)}. \end{aligned}$$

In the last line, we used some hyperbolic trigonometric identities normalizing ϵ where we have defined the phase $\theta = \text{Arg}\{1 - i/\sinh \xi\} = \arctan(1/\omega\tau)$.

Now before we jump through the last hoops, it is useful to notice right now that $\Re\{\sqrt{\epsilon}\} \propto \omega_p\tau$, so if we are keeping things to order $1/(\omega_p\tau)$, then we need only look at terms in the denominator of the expression for T that are second order at least. Indeed, this means we can drop the $1 + 2\Re\{\sqrt{\epsilon}\}$ bit from the denominator, simplifying life enormously. Okay, so with that big approximation made clear, we see directly that

$$\begin{aligned} T &= \frac{4\Re\{\sqrt{\epsilon}\}}{|1 + \sqrt{\epsilon}|^2} \approx \frac{4\Re\{\sqrt{\epsilon}\}}{|\epsilon|}, \\ &= \frac{4\omega_p\tau}{\sqrt{\cosh \xi \sinh \xi}} \cos\left(\frac{1}{2}(\pi - \arctan(1/\omega\tau))\right) \left(\frac{\omega_p^2\tau^2}{\cosh \xi \sinh \xi}\right)^{-1}, \end{aligned}$$

²It is not really necessary to quote the result, because considering that the power is $\frac{\epsilon}{2}|\mathbf{E}|^2$, this expression is fairly obvious from our work in part **a**.

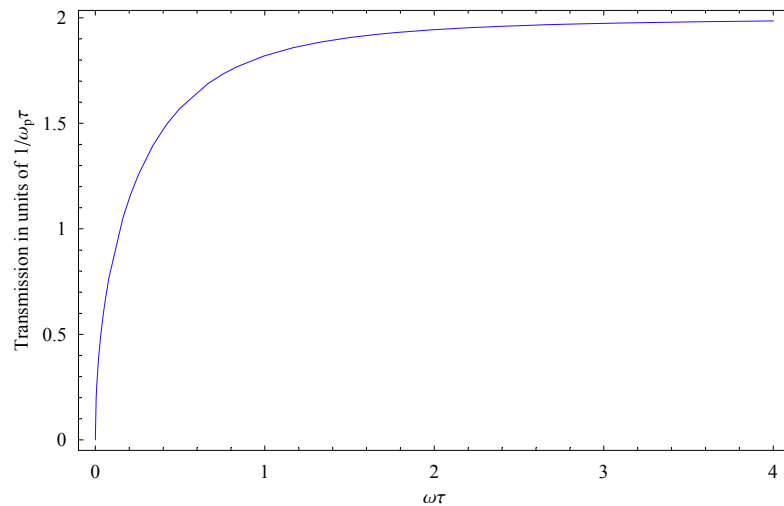


FIGURE 1. The absorption coefficient T as a function of $\omega\tau$ as estimated in problem (1.b).

$$\therefore T \simeq \frac{4}{\omega_p\tau} \sqrt{\omega\tau\sqrt{1+\omega^2\tau^2}} \cos\left(\frac{1}{2}(\pi - \arctan(1/\omega\tau))\right). \quad (\text{b.3})$$

This is shown in Figure 1.

c) We are to compute the skin depth of copper for $\tau = 2.7 \times 10^{-14}$ sec using our work above at various frequencies.

From our work above in part **b** it we can easily see that (in the approximation used there)

$$\Im\{\sqrt{\epsilon}\} = \frac{\omega_p\tau}{\sqrt{\omega\tau\sqrt{1+\omega^2\tau^2}}} \sin\left(\frac{1}{2}(\pi - \arctan(1/\omega\tau))\right), \quad (\text{c.1})$$

which allows us to write the skin depth

$$\delta = \frac{c}{\omega \Im\{\sqrt{\epsilon}\}}. \quad (\text{c.2})$$

Using Mathematica so I wouldn't make any silly mistakes, I found the following:

$$\delta_{\text{Cu}}(60 \text{ Hz}) = 8.08 \text{ mm} \quad \delta_{\text{Cu}}(10^{10} \text{ Hz}) = 0.625 \mu\text{m} \quad \delta_{\text{Cu}}(6 \times 10^{14} \text{ Hz}) = 18.2 \text{ nm}. \quad (\text{c.3})$$

Problem 2

We are to modify the Sommerfeld theory of electrical and thermal conductivity to incorporate two disparate types of scattering events: those with a relaxation time of τ_v which are elastic but thermally randomize the direction of an electron's velocity; and those with a relaxation time of τ_e which fully equilibrate the electron's energy to thermal equilibrium while leaving the speed and direction of the electron unchanged. This is perfectly valid in the limit of temperatures well below the Fermi temperature, because in that case virtually all of the 'effective' conduction electrons are on the Fermi surface and have velocity v_F .

a) We are to compute the electrical conductivity in this two-scattering generalization of the Sommerfeld model.

There are various ways we could make this a bit more rigorous, but our intuition strongly argues that the scatterings which leave the direction of motion unchanged will not contribute to resistance. Indeed, if one were to follow the same type of analysis we did in the one-scattering case, we would find the average velocity at a time dt to be given by

$$\langle \vec{v}(dt) \rangle = \left(1 - \frac{dt}{\tau_v}\right) \left(1 - \frac{dt}{\tau_e}\right) \left(\langle \vec{v}(t=0) \rangle - e\vec{E}\right) + \frac{dt}{\tau_e} \langle \vec{v}(t=0) \rangle + \mathcal{O}(dt^2), \quad (\text{a.1})$$

where the last term is added because with a probability of $\frac{dt}{\tau_e}$ during the interval dt the electrons can scatter via these inelastic pathways which do not alter the velocity. A quick glance at the equation above shows that this cancels the resistive force caused by the τ_e scattering, so there is no change to our derivation of the electrical conductivity in the original model. Therefore, we see that

$$\sigma = \frac{ne^2\tau_v}{m}. \quad (\text{a.2})$$

b) We are to compare thermal conductivity in this model with the original Sommerfeld model.

Unfortunately, we will need to work a little less rigorously than we would otherwise prefer. Most of the results we can more-or-less guess by considering the symmetries and limits that any solution must have; indeed, it is easy to see that if $1/\tau_e \rightarrow 0$ the thermal conductivity will vanish, and similarly if $\tau_v \rightarrow 0$; in the first case there are too few inelastic scatterings to transport information about temperature gradients, and in the latter case any thermally interesting transport is washed out by rapid elastic scattering.

Let us first compute the expected scattering time for the combined, independent scattering processes. This is rather straightforward: notice that the probability for an electron to survive until a time t without scattering elastically is e^{-t/τ_v} and the probability to survive until a time t without scattering 'thermally' is e^{-t/τ_e} . Because these are independent random variables, the probability to survive to a time t without any collision is simply the product, or $e^{-t\frac{\tau_e+\tau_v}{\tau_e\tau_v}}$. For this, the differential probability of not scattering is $\frac{\tau_e+\tau_v}{\tau_e\tau_v} e^{-t\frac{\tau_e+\tau_v}{\tau_e\tau_v}}$; and from here the evaluation of an elementary integral shows that the expected time between collisions is

$$\langle t \rangle = \frac{\tau_e\tau_v}{\tau_e + \tau_v}. \quad (\text{a.1})$$

This of course satisfies our intuition because when one of τ_e or τ_v is small, it will always dominate: if one process is much more rapid, the other can be effectively ignored.

Now, a correct derivation would begin by using the fact that only the inelastic scatterings will contribute to the thermal current. One would find something along the lines of

$$\begin{aligned}
 j &= \frac{n}{2} \eta \frac{v_F}{3} [\varepsilon(T(x = -v_F \tau_e)) - \varepsilon(T(x = v_F \tau_e))], \\
 &= \frac{n}{2} \eta \frac{v_F}{3} \left[\varepsilon(T(x = 0)) - v_F \tau_e \frac{\partial \varepsilon}{\partial T} \frac{\partial T}{\partial x} - \varepsilon(T(x = 0)) - v_F \tau_e \frac{\partial \varepsilon}{\partial T} \frac{\partial T}{\partial x} + \dots \right], \\
 &= -\eta \frac{v_F^2}{3} \tau_e \left(n \frac{\partial \varepsilon}{\partial T} \right) \nabla_x T, \\
 &= \eta \tau_e \frac{v_F^2}{3} c_v, \\
 &= \frac{2\varepsilon_F}{3m} \eta \tau_e \frac{\pi^2}{2} n \frac{k_B^2 T}{\varepsilon_F}, \\
 &= \frac{\pi^2}{3} \frac{\eta \tau_e k_B^2 T}{m},
 \end{aligned}$$

where we have introduced the parameter η which parameterizes our ignorance (not fundamentally, just the ignorance of the author): η represents the fraction of electrons arriving at x from a given side such that their last scattering was inelastic. A good guess for η would be³

$$\eta \stackrel{?}{=} \frac{\tau_v}{\tau_v + \tau_e}. \quad (\text{a.2})$$

At least it has the right properties and limits. If this were the case, then we would find

$$\frac{\kappa}{\sigma T} = \frac{1}{3} \frac{\pi^2 k_B^2}{e^2} \frac{\tau_e}{\tau_e + \tau_v}. \quad (\text{a.3})$$

³Note added in revision: this is the right answer.

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Homework 2

Due Tuesday, 3rd October 2006

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Problem 1

Consider a trigonal Bravais lattice generated by the primitive vectors \vec{a}_i for $i = 1, 2, 3$ such that $\vec{a}_i \cdot \vec{a}_j = a^2 \cos \theta$ for $i \neq j$.

- a) We are to determine for what angles θ this lattice is three-dimensional.

There are many ways by which this answer can be visualized, but to be a bit more mathematically explicit (and ergo avoiding the necessity of diagrams), we will proceed differently. If the vectors \vec{a}_i are to be taken as a basis in three-dimensions, then the volume element is given by the square-root of the determinant of the corresponding metric—the metric's elements are $g_{ij} = \vec{a}_i \cdot \vec{a}_j$. That is,

$$(\text{Volume form})^2 = a^2 \begin{vmatrix} 1 & \cos \theta & \cos \theta \\ \cos \theta & 1 & \cos \theta \\ \cos \theta & \cos \theta & 1 \end{vmatrix} \propto (\cos \theta - 1)^2 (\cos \theta + \frac{1}{2}). \quad (\text{a.1})$$

From the above, it is clear that the space is three-dimensional iff the volume-form is real and non-vanishing. We therefore see that when $\cos \theta = 1, -\frac{1}{2}$ the volume vanishes—corresponding to a two-dimensional lattice. Furthermore, we see that because equation (a.1) has a positive coefficient for $\cos^3 \theta$ and it's lowest root at $\cos \theta = -\frac{1}{2}$, the expression is negative for $\cos \theta < -\frac{1}{2}$ which amounts to an imaginary volume element¹.

Therefore, a three-dimensional Bravais lattice is obtained only for $\theta \in (0, 2\pi/3)$.

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- b) Let us show that as θ varies, the trigonal lattice becomes each of the higher-symmetry cubic lattices.

There are three values of θ which give rise to enhanced symmetry. The first, and most obvious to see, is for $\theta = \pi/2$ which clearly gives rise to a simple cubic lattice. The other two cases are a bit more subtle.

Consider the plane spanned by \vec{a}_1 and \vec{a}_2 . When $\theta = \pi/3$, we see that a two-dimensional lattice of equilateral triangles is spanned. Now, because \vec{a}_3 lies out of the plane at an equal angle, the four points $\vec{0}, \vec{a}_1, \vec{a}_2, \vec{a}_3$ form the corners of a regular tetrahedron, which obviously gives rise to enhanced symmetry. We know that this structure—an equilateral triangle of points with a point on the next layer directly in the center—gives rise to the close-packing of spheres in three-dimensions, so our lattice must either be face-centred-cubic (fcc) or hexagonal-close-packed (hcp). It is not hard to see that our Bravais lattice gives only fcc: if a corner of the 'canonical' fcc cube is taken as the origin, then the vectors \vec{a}_i correspond to the points at the centres of the three faces which are coincident at the corner in question.

The last case of enhanced symmetry arises when $\{\vec{a}_1, \vec{a}_2, \vec{a}_3, -(\vec{a}_1 + \vec{a}_2 + \vec{a}_3)\}$ form a regular tetrahedron. For those of us who loved high-school chemistry, we know that the internal angle of a regular tetrahedron—which is the angle between two hydrogen atoms in CH_4 —is $\arccos(-1/3) \approx 109.5^\circ$. And so our answer is: when $\theta = \arccos(-1/3)$ the trigonal Bravais lattice is the body-centred-cubic (bcc) lattice. Just to motivate the answer for bcc a little better, recall from the textbook that the bcc Bravais lattice can given as follows: let a corner of the 'canonical' bcc cube be placed at the origin with the three edges meeting at the corner coincident with the x, y and z -axes. Then the bcc Bravais lattice can be spanned by \vec{a}_i which point toward the

¹There are really clear ways of visualizing the unacceptability of $\cos \theta < -1/2$. For example, consider the case where $\cos \theta$ is very near -1 : here, we see that this means that \vec{a}_2 and \vec{a}_3 are both to be nearly anti-coincident with \vec{a}_1 , which means that they cannot be mutually so.

centres of the cubes in, e.g., the $(+++)$, $(-+-)$, and $(-+-)$ quadrants. And the centre of the cube in the $(+--)$ quadrant is given by $-\sum_i \vec{a}_i$. Now, there are a lot of fancy tricks to determine the internal angle of a tetrahedron; but we shall be brief, dry and boring and simply compute it directly. In our coordinates, in units of the lattice spacing a , the vectors $\vec{a}_1 = \frac{1}{\sqrt{3}}(1, 1, 1)$ and $\vec{a}_2 = \frac{1}{\sqrt{3}}(-1, -1, 1)$. Being unit vectors, $\vec{a}_1 \cdot \vec{a}_2 = \frac{1}{3}(1 - 2) = -1/3 = \cos \theta$. Therefore, the angle θ is given by $\arccos(-1/3)$.

c) We are to find the reciprocal lattice of the trigonal lattice and verify the special cases found above.

We can use the canonical expressions for the reciprocal lattice vectors:

$$\vec{b}_i \equiv \pi \frac{\epsilon^{ijk}(\vec{a}_j \times \vec{a}_k)}{\vec{a}_i \cdot (\vec{a}_2 \times \vec{a}_3)}, \quad (\text{c.1})$$

where Einstein summation convention is employed². At any rate, we find easily that $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = a^3 \sin^2 \theta$ and that this implies $|\vec{b}_i| = \frac{2\pi}{a \sin \theta}$. Using the usual identities about the inner product of two pairs of cross-products, we see that

$$\vec{b}_i \cdot \vec{b}_j = \frac{4\pi^2}{a^6 \sin^4 \theta} (a^4 \cos^2 \theta - a^4 \cos \theta) \quad \text{for } i \neq j. \quad (\text{c.2})$$

Therefore, the angles between the reciprocal basis vector \vec{b}_i are all equal, and given by φ where

$$\begin{aligned} \cos \varphi &= \frac{\vec{b}_1 \cdot \vec{b}_2}{|\vec{b}_1|^2}, \\ &= \left(\frac{a^2 \sin^2 \theta}{4\pi^2} \right) \left(\frac{4\pi^2}{a^2 \sin^4 \theta} \right) (\cos^2 \theta - \cos \theta), \\ &= \frac{\cos^2 \theta - \cos \theta}{1 - \cos^2 \theta}, \\ &\boxed{\therefore \cos \varphi = \frac{-\cos \theta}{1 + \cos \theta}} \end{aligned} \quad (\text{c.3})$$

For the special values of θ which correspond to the three cubic lattices, we see

- fcc: $\theta = \pi/3 \implies \cos \varphi = \frac{-1/2}{1+1/2} = -1/3$. This is the angle which was found to generate the bcc lattice.
- simple cubic: $\theta = \pi/2 \implies \cos \varphi = 0$ which corresponds to another simple cubic lattice.
- bcc: $\cos \theta = -1/3 \implies \cos \varphi = \frac{1/3}{1-1/3} = 1/2$; so $\varphi = \pi/3$, which corresponds to a fcc lattice.

These results match our understanding of reciprocal these reciprocal lattices.

²The factor of π in the expression is correct: it accounts for the fact that when summing over jk there will be two contributions.

Problem 2

Consider an ideal, two-dimensional honeycomb lattice of atoms—this could be, for example, graphene. For specificity, take the honeycomb lattice to be aligned in the xy -plane with the y -axis parallel to one of the nearest-neighbour atomic spacings. Call the distance between nearest-neighbours d .

a) We are to specify and sketch the reciprocal lattice and state the magnitude of the smallest reciprocal lattice vector for graphene, where $d \cong 1.4 \text{ \AA}$.

The honeycomb lattice can be considered a (2-dimensional) trigonal Bravais lattice with a basis containing two atoms. For specificity, a little trigonometry tells us that if d is the spacing between two atoms, then in our chosen orientation of the plane, our Bravais lattice is generated by

$$\vec{a}_1 \equiv d\sqrt{3}(1,0) \quad \text{and} \quad \vec{a}_2 \equiv d\sqrt{3}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right). \quad (\text{a.1})$$

The Bravais lattice with basis generated by these vectors is illustrated in Figure 1.

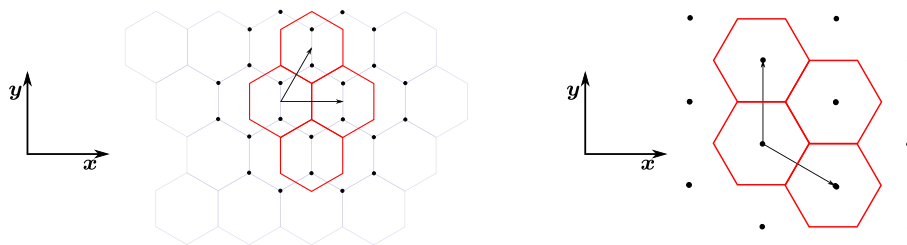


FIGURE 1. This figure shows the original honeycomb lattice, as viewed as a Bravais lattice of hexagonal cells each containing two atoms, and also the reciprocal lattice of the Bravais lattice (not to scale, but aligned properly).

To find the corresponding reciprocal lattice, we must satisfy the defining equations $\vec{b}_1 \cdot \vec{a}_1 = 2\pi$ and $\vec{b}_1 \cdot \vec{a}_2 = 0$, and a similar system for \vec{b}_2 . These are easily found by hand, and it is seen at once that the required reciprocal lattice is generated by

$$\vec{b}_1 \equiv \frac{4\pi}{3d}\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \quad \text{and} \quad \vec{b}_2 \equiv \frac{4\pi}{3d}(0,1). \quad (\text{a.2})$$

This clearly generates the same lattice as \vec{a}_1 and \vec{a}_2 , but rotated by $\pi/2$. This is illustrated also in Figure 1.

Using our expression in equation (a.2) above, we see that if $d \cong 14 \text{ nm}$, then the smallest reciprocal lattice vector has magnitude $\frac{4\pi}{3d} \cong 2.46 \text{ \AA}^{-1}$.

b) Treating the atoms as identical scatterers, we are to determine the intensity of all the Bragg peaks, normalized so that the strongest peak has unit intensity.

If we let $\vec{r}_0 = (0, d/2)$, then the density function $\rho(\vec{r})$ over one cell is given by

$$\rho(\vec{r}) = \delta(\vec{r} - \vec{r}_0) + \delta(\vec{r} + \vec{r}_0), \quad (\text{b.1})$$

which gives a form factor of

$$\{e^{i\vec{q}\cdot\vec{r}_0} + e^{-i\vec{q}\cdot\vec{r}_0}\} \propto \cos(\vec{q}\cdot\vec{r}_0). \quad (\text{b.2})$$

We know that the wave function in \vec{q} space can be expressed as this form factor times a piece from the Bravais lattice; the Bravais lattice piece gives a multiplicative factor of N (the number of lattice cells) and enforces that \vec{q} is in the reciprocal lattice—that is, the wave function identically vanishes for \vec{q} not in the reciprocal lattice.

Now, an arbitrary \vec{q} in the reciprocal lattice is given by $\vec{q} = n_1\vec{b}_1 + n_2\vec{b}_2$, where $n_1, n_2 \in \mathbb{Z}$ and \vec{b}_1, \vec{b}_2 are given in equation (a.2). This shows us immediately that for \vec{q} in the reciprocal lattice,

$$\vec{q} \cdot \vec{r}_0 = \frac{\pi}{3} (2n_2 - n_1). \quad (\text{b.3})$$

Combining this with our work above, we see that

$$I \propto |\psi_s|^2 \propto \cos^2 \left(\frac{\pi}{3} (2n_2 - n_1) \right), \quad (\text{b.4})$$

and furthermore, the expression has the desired feature of intensity—that the strongest peak has unit intensity—so that we find the normalized intensity to be given by

$$I(n_1, n_2) = \cos^2 \left(\frac{\pi}{3} (2n_2 - n_1) \right). \quad (\text{b.5})$$

This is shown in Figure 2.

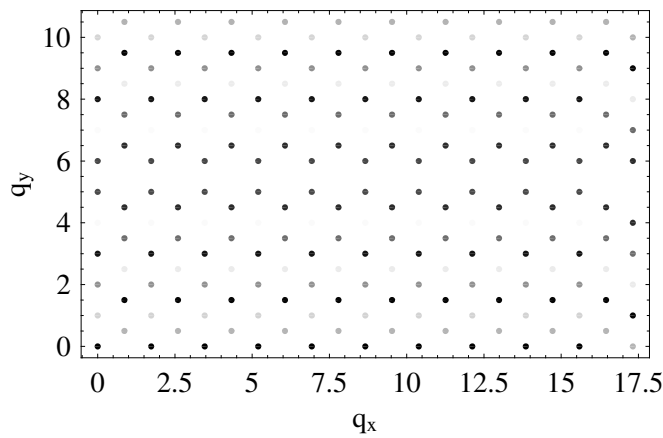


FIGURE 2. This is a plot of the intensity as a function of \vec{q} (in units where the smallest reciprocal vector is of unit length). Only at discrete values of \vec{q} is there any scattering, and the intensity is given by the expression (b.5).

c) Consider the cases where the two atoms in the unit cell are distinct, call them A and B , each with different scattering amplitudes f_A and f_B . We may assume that they are both real. What condition on the relative scattering amplitudes will cause the intensities of some of the Bragg peaks to vanish?

Because both f_A and f_B are real, we may without loss of generality suppose that $f_B = \beta f_A$. Just to be exceedingly explicit, we will say that the A atoms are located at $\vec{R} + \vec{r}_0$ and the B atoms are located at $\vec{R} - \vec{r}_0$ where \vec{R} is the Bravais lattice and $\vec{r}_0 = (0, d/2)$ as above. With separate scattering sites, we see that the wave function for scattering goes like³

$$\begin{aligned} \psi_s &\sim f_A \sum_{\vec{R}} e^{i\vec{q} \cdot (\vec{R} + \vec{r}_0)} + f_B \sum_{\vec{R}} e^{i\vec{q} \cdot (\vec{R} - \vec{r}_0)}, \\ &\propto f_A (e^{i\vec{q} \cdot \vec{r}_0} + \beta e^{-i\vec{q} \cdot \vec{r}_0}). \end{aligned}$$

Therefore, we find that the intensity evolves like

$$\begin{aligned} I \propto |\psi_s|^2 &\propto (1 + \beta e^{2i\vec{q} \cdot \vec{r}_0} + \beta e^{-2i\vec{q} \cdot \vec{r}_0} + \beta^2), \\ &= 1 + 2\beta \cos(2\vec{q} \cdot \vec{r}_0) + \beta^2, \\ &= 4\beta \cos^2(\vec{q} \cdot \vec{r}_0) + (1 - \beta)^2. \end{aligned}$$

³In the second line we make use of the fact that the amplitude is non-vanishing only for \vec{q} in the reciprocal lattice.

Now, to see if there is any β which will cause some of the Bragg peaks to vanish, we merely need to see if there are any roots to the equation above. It is a simple quadratic and it is easily reduced to $I = 0$ iff

$$\beta = 1 - 2 \cos^2(\vec{q} \cdot \vec{r}_0) \pm 2 \cos(\vec{q} \cdot \vec{r}_0) \sqrt{\cos^2(\vec{q} \cdot \vec{r}_0) - 1}. \quad (\text{c.1})$$

Because we have assumed that both amplitudes are real, $\beta \in \mathbb{R}$; and because $\cos^2(\theta) \leq 1$, we see that there is a solution iff $\cos^2(\vec{q} \cdot \vec{r}_0) = 1$, for which we see that $\beta = -1$.

Therefore, if $\beta = -1$ there is interference causing all the Bragg peaks for which $\cos^2(\vec{a} \cdot \vec{r}_0) = 0$; this is satisfied if $2n_2 - n_1 = 3m$ for some $m \in \mathbb{Z}$, which correspond to the momentum transfers $\vec{q} = \frac{4\pi}{3d} \left(n_2\sqrt{3} + 3m\frac{\sqrt{3}}{2}, 3m \right)$.

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d) Now let us assume that the atoms A and B are placed randomly on the honeycomb lattice with an even probability distribution. For this random crystal, we are to determine what fraction of the total scattering intensity is in the Bragg peaks (i.e. not diffuse scattering).

Let us define a map $\sigma : \vec{R} \rightarrow \{-1, 1\}$, a function whose value is either $+1$ or -1 for each point of the Bravais lattice \vec{R} . It must have the property that $|\sigma^{-1}(-1)| = |\sigma^{-1}(1)|$, which means that its average value over the lattice is zero. We will take $\sigma(\vec{R})$ to signify the direction of the A atom relative to the center of the cell at the Bravais lattice point \vec{R} . With this in mind, the atom density functions for A and B are given by

$$\rho_A(\vec{r}) = \sum_{\vec{R}} \delta(\vec{r} - \vec{R} - \sigma(\vec{R})\vec{r}_0) \quad \text{and} \quad \rho_B(\vec{r}) = \sum_{\vec{R}} \delta(\vec{r} - \vec{R} + \sigma(\vec{R})\vec{r}_0), \quad (\text{d.1})$$

where we again use the definition $\vec{r}_0 = (0, d/2)$.

Let us again say that $f_B = \beta f_A$. We now find that the scattering amplitude goes like⁴—*This is where the equation goes wrong: because of the assumption stated in the footnote, we are effectively only calculating the Bragg contribution.*

$$\begin{aligned} \psi_s &\sim f_A \left\{ \sum_{\vec{R}} e^{i\vec{q} \cdot (\vec{R} + \sigma(\vec{R})\vec{r}_0)} + \beta \sum_{\vec{R}} e^{i\vec{q} \cdot (\vec{R} - \sigma(\vec{R})\vec{r}_0)} \right\}, \\ &\propto \left\{ \sum_{\vec{R}} e^{i\sigma(\vec{R})\vec{q} \cdot \vec{r}_0} + \beta \sum_{\vec{R}} e^{-i\sigma(\vec{R})\vec{q} \cdot \vec{r}_0} \right\}. \end{aligned}$$

Now, when we expand out the two sums we find that because $\sigma(\vec{R}) = +1$ for half of the sites and $\sigma(\vec{R}) = -1$ for the other half, each sum has an equal number of terms with positive exponents and negative exponents. Recall that $\exp\{+i\theta\} + \exp\{-i\theta\} = 2 \cos(\theta)$. Therefore, up to a constant of proportionality, we have

$$\psi_s \propto \{ \cos(\vec{q} \cdot \vec{r}_0) + \beta \cos(\vec{q} \cdot \vec{r}_0) \}. \quad (\text{d.2})$$

This is not right.

⁴In the second line we again make use of the fact that the amplitude will in general vanish unless \vec{q} is in the reciprocal lattice, i.e. $\vec{q} \cdot \vec{R} = 2\pi$ for all \vec{R} in the Bravais lattice.

e) Let us consider fully three-dimensional graphite which has a simple hexagonal Bravais lattice. We are to show that the reciprocal lattice of a simple hexagonal Bravais lattice is also a simple hexagonal lattice. For graphite, we are to show that the internal symmetries of the basis gives rise to the vanishing of certain Bragg scattering directions and list which reciprocal lattice vectors show this complete interference.

First, let us state the vectors which generate the Bravais lattice of graphite. It is not hard to extend our two-dimensional analysis to three-dimensions:

$$\vec{a}_1 \equiv (d\sqrt{3}, 0, 0) \quad \vec{a}_2 \equiv \left(d\frac{\sqrt{3}}{2}, d\frac{3}{2}, 0\right) \quad \vec{a}_3 \equiv (0, 0, \lambda), \quad (\text{e.1})$$

where λ is the height between the graphite layers.

Using our general expression for the reciprocal lattice vectors, equation (1.c.2), we can quite directly compute

$$\vec{b}_1 \equiv \frac{2\pi}{3d} (\sqrt{3}, -1, 0) \quad \vec{b}_2 \equiv \frac{4\pi}{3d} (0, 1, 0) \quad \vec{b}_3 \equiv \frac{2\pi}{\lambda} (0, 0, 1). \quad (\text{e.2})$$

To see that these generate a simple hexagonal lattice, notice that the angle between \vec{b}_1 and \vec{b}_2 , called θ_{12} is given by

$$\cos \theta_{12} = -\frac{1}{2}, \quad (\text{e.3})$$

which obviously generates a hexagonal lattice in the xy -plane; and because \vec{b}_3 is in the z -direction, we see that the set \vec{b}_i generate a simple hexagonal lattice.

If we consider scattering off a perfect graphite lattice, we know that there will be a Bragg condition forcing the momentum transfers \vec{q} to be elements of the reciprocal lattice:

$$\vec{q} = n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3. \quad (\text{e.4})$$

Recall that, for a perfect crystal

$$\psi_s(\vec{q} \in \vec{G}) \propto \int_{\text{one cell}} d\vec{r} \rho(\vec{r}) e^{i\vec{q} \cdot \vec{r}}, \quad (\text{e.5})$$

and ψ_s vanishes for $\vec{q} \notin \vec{G}$, where \vec{G} denotes the reciprocal lattice. Now, in the basis cell, there are four atoms located at

$$\vec{r}_1 = (0, 0, 0) \quad \vec{r}_2 = (0, d, 0) \quad \vec{r}_3 = (0, d, \lambda/2) \quad \vec{r}_4 = (\sqrt{3}d/2, d/2, \lambda/2). \quad (\text{e.6})$$

These give delta-functions in the density, which turn the integral into a discrete sum:

$$\psi_s \propto \left\{ \sum_{i=1}^4 e^{i\vec{q} \cdot \vec{r}_i} \right\}. \quad (\text{e.7})$$

Notice that $\vec{r}_3 = \vec{r}_2 + \vec{r}_4 - \vec{a}_2$. Therefore, we see that

$$\psi_2 \propto (1 + e^{i\vec{q} \cdot \vec{r}_2}) (1 + e^{i\vec{q} \cdot \vec{r}_4}) = \left(1 + e^{i\frac{2\pi}{3}(2n_1 - n_2)}\right) \left(1 + e^{i\pi n_3} e^{-i\frac{\pi}{3}(n_1 + n_2)}\right). \quad (\text{e.8})$$

Now, the exponential in the first parenthesis cannot be -1 because there are no integer solutions to the equation $2n_2 - n_1 = \frac{3}{2}$. Therefore, the only way for the intensity to vanish is if the second term in parenthesis vanishes, which requires that simultaneously,

$$(n_1 + n_2) = 0 \pmod{3} \quad \text{and} \quad n_3 \in (2\mathbb{Z} + 1). \quad (\text{e.9})$$

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PHYSICS 525, CONDENSED MATTER

Homework 3

Due Tuesday, 16th October 2006

JACOB LEWIS BOURJAILY

Problem 1: Electron in a Weak Sinusoidal Potential¹

Consider an electron moving in a one-dimensional periodic potential $U(r) = V \cos(2\pi r/a)$. We are to obtain the eigenenergies $\epsilon_n(q)$ and corresponding wavefunctions $\psi_{n,q}(r)$ of the lowest two bands, treating the potential perturbatively.

a) Away from the edge of the Brillouin zone, there are no degeneracies in the lowest energy band. Using this fact, we are to compute $\epsilon_1(q)$ to order V^2 and the corresponding wavefunctions to order V .

We begin by doing what amounts to Fourier transforming $\psi(r)$ into momentum space, making use of Bloch's theorem to write

$$\psi_q(r) = \sum_G c_{q-G} e^{i(q-G)r}, \quad (1.a.1)$$

where G represents the reciprocal lattice, which is in this one-dimensional problem generated simply by $b \equiv \frac{2\pi}{a}$. Following Ashcroft and Mermin, we will study the Schrödinger equation in momentum space:

$$\left[\frac{\hbar^2}{2m}(q-G) - \epsilon \right] c_{q-G} + \sum_{G'} U_{G'-G} c_{q-G} = 0, \quad (1.a.2)$$

where U_k are Fourier modes of the potential. In our case, this is extremely easy to extract: every kindergartener should be able to take the Fourier transform of a cosine; we find:

$$U_{+1} = U_{-1} = \frac{V}{2} \quad \text{and} \quad U_{i \neq \pm 1} = 0. \quad (1.a.3)$$

We are going to be interested in a wave function concentrated well within the first Brillouin zone, in the limit where there are no nearly degenerate bands. Writing $\epsilon_q^0 = \frac{\hbar^2}{2m}q^2$ and inserting our potential U_k into the Schrödinger equation, we see

$$(\epsilon - \epsilon_q^0) c_q = \frac{V}{2} (c_{q+b} + c_{q-b}) \quad \implies \quad c_q = \frac{V}{2(\epsilon - \epsilon_q^0)} (c_{q+b} + c_{q-b}). \quad (1.a.4)$$

This expression does not reflect our interest in the first Brillouin zone: it is valid for all q . Indeed, we see that we can iteratively unfold the equation to obtain an expansion in terms of $\frac{V}{2(\epsilon - \epsilon_{q'}^0)}$:

$$c_q = \frac{V}{2(\epsilon - \epsilon_q^0)} (c_{q+b} + c_{q-b}), \quad (1.a.5)$$

$$= \frac{V}{2(\epsilon - \epsilon_q^0)} \left\{ \frac{V}{2(\epsilon - \epsilon_{q+b}^0)} (c_q + c_{q+2b}) + \frac{V}{2(\epsilon - \epsilon_{q-b}^0)} (c_q + c_{q-2b}) \right\}, \quad (1.a.6)$$

$$= \frac{V^2 c_q}{4(\epsilon - \epsilon_q^0)} \left\{ \frac{1}{(\epsilon - \epsilon_{q+b}^0)} + \frac{1}{(\epsilon - \epsilon_{q-b}^0)} \right\} + \left[\frac{V^3}{8(\epsilon - \epsilon_q^0)(\epsilon - \epsilon_{q+b}^0)(\epsilon - \epsilon_{q+2b}^0)} (c_{q+b} + c_{q+3b}) + (b \leftrightarrow -b) \right]; \quad (1.a.7)$$

&tc. Now, because we are expanding in $\frac{V}{2(\epsilon - \epsilon_q^0)}$, we may safely drop the $\mathcal{O}(V^3)$ terms. Also, notice that in the curly brackets that we have the expressions $\epsilon - \epsilon_{q \pm b}^0$. Now, because the bands are non-degenerate and we know the band energies are only affected by terms leading in V^2 , we can be allowed to take $(\epsilon - \epsilon_{q \pm b}^0) \mapsto (\epsilon_q^0 - \epsilon_{q \pm b}^0)$ to this order of approximation. With that in mind, we may divide both sides of the expression above by $c_q/(\epsilon - \epsilon_q^0)$ obtaining

$$(\epsilon - \epsilon_q^0) = \frac{V^2}{4} \left\{ \frac{1}{(\epsilon_q^0 - \epsilon_{q+b}^0)} + \frac{1}{(\epsilon_q^0 - \epsilon_{q-b}^0)} \right\} + \mathcal{O}(V^3). \quad (1.a.8)$$

¹Note added in revision: the solution presented follows Ashcroft and Mermin—which is absolutely horrendous. The entire first problem can be done in a couple of lines if you read the first few pages of Griffith's *Quantum Mechanics* chapter on (time independent) perturbation theory first! Honestly, believe me; learn non-degenerate perturbation theory first (and see how to apply it in the degenerate case) and the problem will be MUCH easier.

It is not altogether delightful, but this expression can of course be quite dramatically simplified.

$$\begin{aligned}
\epsilon &= \epsilon_q^0 + \frac{V^2 2m}{4\hbar^2 b} \left\{ \frac{2q + b - 2q + b}{(4q^2 - b^2)} \right\} + \mathcal{O}(V^3), \\
&= \epsilon_q^0 + \frac{V^2 m}{\hbar^2} \left\{ \frac{1}{(4q^2 - \frac{4\pi^2}{a^2})} \right\} + \mathcal{O}(V^3), \\
\therefore \epsilon &= \frac{\hbar^2}{2m} q^2 + \frac{V^2 m}{4\hbar^2 (q^2 - \frac{\pi^2}{a^2})} + \mathcal{O}(V^3).
\end{aligned} \tag{1.a.9}$$

$\dot{\psi}\pi\epsilon\rho \dot{\epsilon}\delta\epsilon\iota \pi\omega\eta\sigma\alpha\iota$

Now we are asked to determine the corrected wave function to leading order in V . To do this, we start by combining the right hand sides of equations (1.a.5) and (1.a.7):

$$\begin{aligned}
\frac{V}{2(\epsilon - \epsilon_q^0)} (c_{q+b} + c_{q-b}) &= \frac{V^2 c_q}{4(\epsilon - \epsilon_q^0)} \left\{ \frac{1}{(\epsilon_q^0 - \epsilon_{q+b}^0)} + \frac{1}{(\epsilon_q^0 - \epsilon_{q-b}^0)} \right\} + \mathcal{O}(V^3), \\
\implies (c_{q+b} + c_{q-b}) &= c_q \frac{V}{2} \left\{ \frac{1}{(\epsilon_q^0 - \epsilon_{q+b}^0)} + \frac{1}{(\epsilon_q^0 - \epsilon_{q-b}^0)} \right\} + \mathcal{O}(V^2), \\
&= c_q \frac{Vm}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} + \mathcal{O}(V^2).
\end{aligned} \tag{1.a.10}$$

Now, remember that equation (1.a.4) allows to write c_{q-b} in terms of c_q and c_{q-2b} , for example. Using this to rearrange equation (1.a.10), we see

$$\begin{aligned}
c_{q+b} &= -c_{q-b} + c_q \frac{Vm}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} + \mathcal{O}(V^2), \\
&= -\frac{V}{2(\epsilon_q^0 - \epsilon_{q-b}^0)} (c_q + c_{q-2b}) + c_q \frac{Vm}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} + \mathcal{O}(V^2), \\
&= c_q \left\{ \frac{Vm}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} - \frac{V}{2(\epsilon_q^0 - \epsilon_{q-b}^0)} \right\} + \mathcal{O}(V^2), \\
&= c_q \frac{Vm}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left\{ 1 - \frac{1}{2\pi} (aq + \pi) \right\} + \mathcal{O}(V^2); \\
\therefore c_{q+b} &= c_q \frac{Vm}{4\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left(1 - \frac{aq}{\pi} \right) + \mathcal{O}(V^2).
\end{aligned} \tag{1.a.11}$$

We don't need to reproduce the above steps for c_{q-b} : it comes for free once we have c_{q+b} :

$$\begin{aligned}
c_{q-b} &= -c_{q+b} + c_q \frac{Vm}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} + \mathcal{O}(V^2), \\
&= c_q \frac{Vm}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left(1 - \frac{1}{2} \left(1 - \frac{qa}{\pi} \right) \right) + \mathcal{O}(V^2); \\
\therefore c_{q-b} &= c_q \frac{Vm}{4\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left(1 + \frac{qa}{\pi} \right) + \mathcal{O}(V^2).
\end{aligned} \tag{1.a.12}$$

Inserting this in the expansion for $\psi_q(r)$, we find directly,

$$\begin{aligned}
\psi_q(r) &= c_q e^{iqr} + c_{q+b} e^{iqr} e^{ibr} + c_{q-b} e^{iqr} e^{-ibr} + \mathcal{O}(V^2), \\
&= c_q e^{iqr} \left\{ 1 + \frac{Vm}{4\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left[\left(1 - \frac{aq}{\pi} \right) e^{irb} + \left(1 + \frac{qa}{\pi} \right) e^{-irb} \right] \right\} + \mathcal{O}(V^2); \\
\therefore \psi_q(r) &= c_q e^{iqr} \left\{ 1 + \frac{Vm}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left(\cos\left(\frac{2\pi r}{a}\right) - \frac{iqu}{\pi} \sin\left(\frac{2\pi r}{a}\right) \right) \right\}.
\end{aligned} \tag{1.a.13}$$

$\dot{\psi}\pi\epsilon\rho \dot{\epsilon}\delta\epsilon\iota \pi\omega\eta\sigma\alpha\iota$

b) At the edge of the Brillouin zone there are degeneracies for small V . We are to work perturbatively near the zone edge to diagonalize the single electron Hamiltonian within the two-state Hilbert space of the two nearly-degenerate lowest-energy free-electron momentum eigenstates of the same crystal momentum. Then, we are to add the effects of the higher bands perturbatively. We are to obtain the eigenenergies of the lowest two energy bands to order V^2 and the wave functions to order V as before. We are to verify that for small V these results match our work for part (a) when one moves far enough away from the edge of the Brillouin zone. We are to sketch the dispersions $\epsilon_n(q)$ and determine how small V must be for this perturbation analysis to be reliable.

We are going to proceed along lines similar to those encountered in part (a). Specifically, let us start by again by equating the right hand sides of equations (1.a.5) and (1.a.7)—only this time, we will not use the assumption that all the eigenenergies are non-degenerate.

$$(\epsilon - \epsilon_q^0) = \frac{V^2}{4} \left\{ \frac{1}{(\epsilon - \epsilon_{q+b}^0)} + \frac{1}{(\epsilon - \epsilon_{q-b}^0)} \right\} + \mathcal{O}(V^3). \quad (1.b.14)$$

Now, we are going to consider perturbing the system near the Bragg plane at $q = \frac{\pi}{a}$; this will mean that we can consider the term $\epsilon - \epsilon_{q+b}^0 \equiv \zeta$ where $1/\zeta$ is at most linear in V —we will justify this and give an explicit expression for ζ later.

Manipulating equation (1.b.14), we see that

$$\begin{aligned} (\epsilon - \epsilon_q^0)(\epsilon - \epsilon_{q-b}^0) &= \frac{V^2}{4} \left(1 + \frac{\epsilon - \epsilon_{q-b}^0}{\zeta} \right) + \mathcal{O}(V^3), \\ \implies \epsilon^2 - \epsilon \left(\epsilon_q^0 + \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \right) + \epsilon_q^0 \epsilon_{q-b}^0 - \frac{V^2}{4} \left(1 - \frac{\epsilon_{q-b}^0}{\zeta} \right) &= 0. \end{aligned}$$

This quadratic is easily solved by calling upon kindergarten identities:

$$\begin{aligned} \epsilon &= \frac{1}{2} \left(\epsilon_q^0 + \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \right) \pm \frac{1}{2} \left\{ \left(\epsilon_q^0 + \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \right)^2 - 4\epsilon_q^0 \epsilon_{q-b}^0 + V^2 \left(1 - \frac{\epsilon_{q-b}^0}{\zeta} \right) \right\}^{1/2}; \\ \therefore \epsilon &= \frac{1}{2} \left(\epsilon_q^0 + \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \right) \pm \frac{1}{2} \left\{ \left(\epsilon_q^0 - \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \right)^2 + V^2 \right\}^{1/2}. \end{aligned} \quad (1.b.15)$$

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To evaluate the expression, one can simply insert the equation itself iteratively into $\zeta = \epsilon - \epsilon_{q+b}^0$ —and observe that that it always gives a well-defined expression up to terms of order $\mathcal{O}(V^3)^2$. This band structure is shown in Figure 1.

We should check that this result makes sense—and verify that it agrees with our previous work once we are far enough away from the Bragg plane. First, notice that at the Bragg plane, where $q = b - q = \pi/a$, we have

$$\begin{aligned} \epsilon \left(q = \frac{\pi}{a} \right) &= \epsilon_{\pi/2}^0 + \frac{V^2}{8\zeta} \pm \frac{V}{2} \left\{ 1 + \frac{V^2}{16\zeta^2} \right\}^{1/2}, \\ &= \frac{\hbar^2 \pi^2}{2m a^2} \pm \frac{V}{2} + \frac{V^2}{8\zeta} + \mathcal{O}(V^3). \end{aligned}$$

Inserting this into definition of ζ as prescribed, we obtain

$$\therefore \epsilon \left(q = \frac{\pi}{a} \right) = \frac{\hbar^2 \pi^2}{2m a^2} \pm \frac{V}{2} - \frac{V^2 m a^2}{32 \pi^2 \hbar^2} + \mathcal{O}(V^3). \quad (1.b.16)$$

²The reason for being implicit here is that the two cases we are interested—near and far from the Bragg plane—give different results; but the implicit expression is always correct.

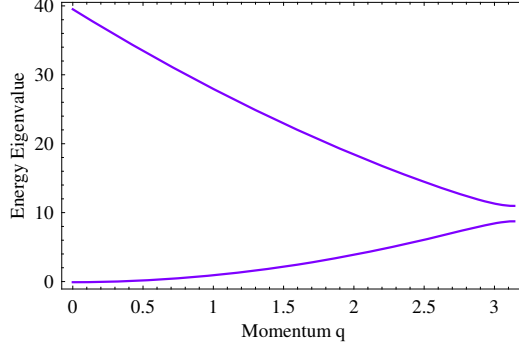


FIGURE 1. The second-order band structure for a one-dimensional system in a weak sinusoidal potential.

Similarly, we can check that equation (1.b.15) gives the right answer when we are far enough away from the Bragg plane. When we are far from the Bragg plane, then $\epsilon_q^0 - \epsilon_{q-b}^0 \gg V^2$ so that we may expand

$$\begin{aligned}
\epsilon &= \frac{1}{2} \left(\epsilon_q^0 + \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \right) \pm \frac{1}{2} \left\{ \left(\epsilon_q^0 - \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \right)^2 + V^2 \right\}^{1/2}, \\
&= \frac{1}{2} \left(\epsilon_q^0 + \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \pm (\epsilon_q^0 - \epsilon_{q-b}^0) \left\{ \frac{V^2}{(\epsilon_q^0 - \epsilon_{q-b}^0)^2} + \left(1 + \frac{V^2}{4\zeta(\epsilon_q^0 - \epsilon_{q-b}^0)} \right)^2 \right\}^{1/2} \right), \\
&= \frac{1}{2} \left(\epsilon_q^0 + \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \pm (\epsilon_q^0 - \epsilon_{q-b}^0) \left\{ 1 + \frac{V^2}{(\epsilon_q^0 - \epsilon_{q-b}^0)^2} + \frac{V^2}{2\zeta(\epsilon_q^0 - \epsilon_{q-b}^0)} + \mathcal{O}(V^4) \right\}^{1/2} \right), \\
&= \frac{1}{2} \left(\epsilon_q^0 + \epsilon_{q-b}^0 + \frac{V^2}{4\zeta} \pm \left((\epsilon_q^0 - \epsilon_{q-b}^0) + \frac{V^2}{2(\epsilon_q^0 - \epsilon_{q-b}^0)} + \frac{V^2}{4\zeta} + \mathcal{O}(V^4) \right) \right).
\end{aligned}$$

Taking the solution corresponding to the lower band³,

$$\begin{aligned}
\epsilon_1(q) &= \epsilon_q^0 + \frac{V^2}{4} \left\{ \frac{1}{2\zeta} + \frac{1}{\epsilon_q^0 - \epsilon_{q-b}^0} + \frac{1}{2\zeta} \right\} + \mathcal{O}(V^3), \\
&= \epsilon_q^0 + \frac{V^2}{4} \left\{ \frac{1}{\epsilon_q^0 - \epsilon_{q+b}^0} + \frac{1}{\epsilon_q^0 - \epsilon_{q-b}^0} \right\} + \mathcal{O}(V^3),
\end{aligned}$$

and this we recognize as equation (1.a.8), which implies that this formula (1.b.15) does indeed agree with our results from part (a).

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Our last task is to determine the wave function for electrons at the Bragg plane to first order in V . We will follow similar lines of thought to those travelled in part (a). Using the same logic as there—only this time being careful not to ignore degeneracies—we can begin our work with the equations

$$c_{q+b} + c_{q-b} = c_q \frac{V}{2} \left\{ \frac{1}{(\epsilon - \epsilon_{q+b}^0)} + \frac{1}{(\epsilon - \epsilon_{q-b}^0)} \right\} + \mathcal{O}(V^2) \quad \text{and} \quad c_q = \frac{V}{2(\epsilon - \epsilon_q^0)} (c_{q+b} + c_{q-b}). \quad (1.b.17)$$

³The solutions corresponding to the respective ‘ \pm ’ sign the equation (1.b.15) have now switched—this is simply because when we extracted $(\epsilon_q^0 - \epsilon_{q-b}^0)$ from the square root, the signs one again become arbitrarily assigned.

This system yields exactly our result in part (a) for the case of c_{q+b} :

$$\begin{aligned}
c_{q+b} &= c_q \frac{V}{2} \left\{ \frac{1}{(\epsilon - \epsilon_{q+b}^0)} + \frac{1}{(\epsilon - \epsilon_{q-b}^0)} \right\} - c_{b-q} + \mathcal{O}(V^2), \\
c_{q+b} &= c_q \frac{V}{2} \left\{ \frac{1}{(\epsilon - \epsilon_{q+b}^0)} + \frac{1}{(\epsilon - \epsilon_{q-b}^0)} - \frac{1}{(\epsilon - \epsilon_{q-b}^0)} \right\} + \mathcal{O}(V^2), \\
c_{q+b} &= c_q \frac{V}{2(\epsilon - \epsilon_{q+b}^0)} + \mathcal{O}(V^2), \\
c_{q+b} &= c_q \frac{V}{2(\epsilon_q^0 - \epsilon_{q+b}^0)} + \mathcal{O}(V^2), \\
&= -c_q \frac{V^2 m a}{4\pi \hbar^2 (q + \frac{\pi}{a})} + \mathcal{O}(V^2); \\
\therefore c_{q+b} &= c_q \frac{V^2}{4\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left(1 - \frac{q a}{\pi} \right) + \mathcal{O}(V^2). \tag{1.b.18}
\end{aligned}$$

The story changes, however, for c_{q-b} . It is not hard to jump a bit in the calculation and see

$$c_{q-b} = c_q \frac{V}{2(\epsilon - \epsilon_{q-b}^0)} + \mathcal{O}(V^2). \tag{1.b.19}$$

Now, from our calculation of the eigenenergies at the Bragg plane we know that

$$\epsilon_{\pi/a} - \epsilon_{\pi/a-b}^0 = \pm \frac{V}{2} - \frac{V^2 m a}{16\pi \hbar^2 (q + \frac{\pi}{a})} + \mathcal{O}(V^3), \tag{1.b.20}$$

so we see

$$\begin{aligned}
c_{q-b} &= c_q \frac{V}{2 \left(\pm \frac{V}{2} - \frac{V^2 m a}{16\pi \hbar^2 (q + \frac{\pi}{a})} \right)} + \mathcal{O}(V^2), \\
&= c_q \frac{1}{\pm \left(1 \mp \frac{V^2 m a}{8\pi \hbar^2 (q + \frac{\pi}{a})} \right)} + \mathcal{O}(V^2), \\
\therefore c_{q-b} &= \pm c_q \left(1 + \frac{V m}{8\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left(\frac{q a}{\pi} - 1 \right) \right) + \mathcal{O}(V^2). \tag{1.b.21}
\end{aligned}$$

Putting all this together, we see

$$\psi_{q=\frac{\pi}{a}}^{\pm}(r) = c_q e^{iqr} \left\{ 1 \pm e^{-ibr} + \frac{V m}{4\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left(1 - \frac{aq}{\pi} \right) \left(e^{ibr} \mp \frac{e^{-ibr}}{2} \right) \right\},$$

so that

$$\psi^+(r) \propto c_q e^{iqr} \left\{ 2e^{-i\frac{br}{2}} \cos\left(\frac{\pi r}{a}\right) + i \frac{V m}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left(1 - \frac{aq}{\pi} \right) \left[\sin\left(\frac{2\pi r}{a}\right) - i \frac{e^{-ibr}}{4} \right] \right\}; \tag{1.b.22}$$

and

$$\psi^-(r) \propto c_q e^{iqr} \left\{ 2ie^{-i\frac{br}{2}} \sin\left(\frac{\pi r}{a}\right) + \frac{V m}{2\hbar^2 (q^2 - \frac{\pi^2}{a^2})} \left(1 - \frac{aq}{\pi} \right) \left[\cos\left(\frac{2\pi r}{a}\right) - \frac{e^{-ibr}}{4} \right] \right\}. \tag{1.b.23}$$

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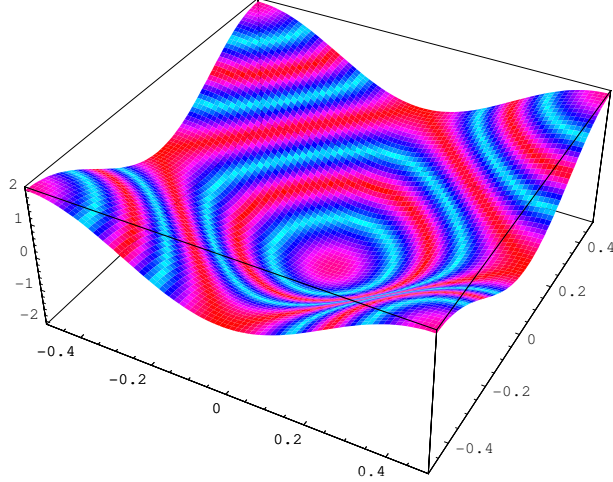


FIGURE 2. The first Brillouin zone dispersion for a tight-binding model on a two-dimensional square lattice.

Problem 2: Tight-Binding Model on a Square Lattice

Consider a tight-binding model on a square, two-dimensional square lattice (lattice spacing a) with on-site energy ϵ^0 and nearest-neighbour hopping matrix element t :

$$H = \sum_{\mathbf{r}} \left\{ \epsilon^0 |\mathbf{r}\rangle \langle \mathbf{r}| + t \left[|\mathbf{r}\rangle \langle \mathbf{r} + a\hat{x}| + |\mathbf{r}\rangle \langle \mathbf{r} - a\hat{x}| + |\mathbf{r}\rangle \langle \mathbf{r} + a\hat{y}| + |\mathbf{r}\rangle \langle \mathbf{r} - a\hat{y}| \right] \right\}.$$

a) We are to obtain the dispersion relation for this model.

Just for the sake of clearing up notation, our Bravais lattice here will be generated by $\vec{a}_1 = a(1, 0)$ and $\vec{a}_2 = a(0, 1)$ which has the associated reciprocal lattice generated by $\vec{b}_1 = \frac{2\pi}{a}(1, 0)$ and $\vec{b}_2 = \frac{2\pi}{a}(0, 1)$. We will write all momenta in terms of the reciprocal lattice, so $\vec{q} = q_1\vec{b}_1 + q_2\vec{b}_2$. Using Bloch's theorem it is quite easy to see that the Hamiltonian of this system is given by

$$H\psi = \left\{ \epsilon^0 + t \left(e^{i\vec{q}\cdot\vec{a}_1} + e^{-i\vec{q}\cdot\vec{a}_1} + e^{i\vec{q}\cdot\vec{a}_2} + e^{-i\vec{q}\cdot\vec{a}_2} \right) \right\} \psi, \quad (2.a.1)$$

$$= \left\{ \epsilon^0 + t \left(e^{i2\pi q_1} + e^{-i2\pi q_1} + e^{i2\pi q_2} + e^{-i2\pi q_2} \right) \right\} \psi, \quad (2.a.2)$$

$$= \left\{ \epsilon^0 + 2t \left(\cos(2\pi q_1) + \cos(2\pi q_2) \right) \right\} \psi; \quad (2.a.3)$$

$$\therefore \epsilon(\vec{q}) = \epsilon^0 + 2t \left\{ \cos(2\pi q_1) + \cos(2\pi q_2) \right\}. \quad (2.a.4)$$

This dispersion relation is shown in the first Brillouin zone in Figure 2.

b-d) Let us sketch the Fermi surface in the first Brillouin zone when the band is less than and more than half-full, assuming a particle-like band ($t < 0$). And we are to make an accurate drawing of the Fermi surface for the case of a precisely half-filled band.

When the Fermi surface is very near the bottom of the band energy, then it is approximately a circle: for $q_i \ll 1$, we can expand the $\cos(2\pi q_i)$'s to see that $\epsilon(q) \sim \epsilon^0 + 2t - 2\pi t \vec{q}^2 + \mathcal{O}(\vec{q}^3)$, the solution to which is precisely a circle.

As the energy increases, the Fermi surface flattens out along the diagonal directions, becoming a square when the band is half-filled. When the band is more than half-filled, the square breaks into four disjoint components which encircle the corners of the Brillouin zone. Expanding $\cos(2\pi q_i)$ about $q_i \sim \frac{1}{2}$ shows that when the band is nearly filled, the Fermi surface components do in fact become circles.

These are shown in detail in Figure 3.

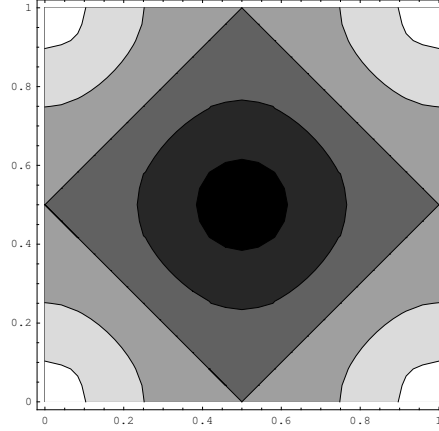


FIGURE 3. Several Fermi surfaces observed for a tight-binding square lattice model. Dark colouring indicates lower energy—Fermi surfaces are included for the band both more than and less than half filled. The half-filled Fermi surface is the clearly visible square in the plot.

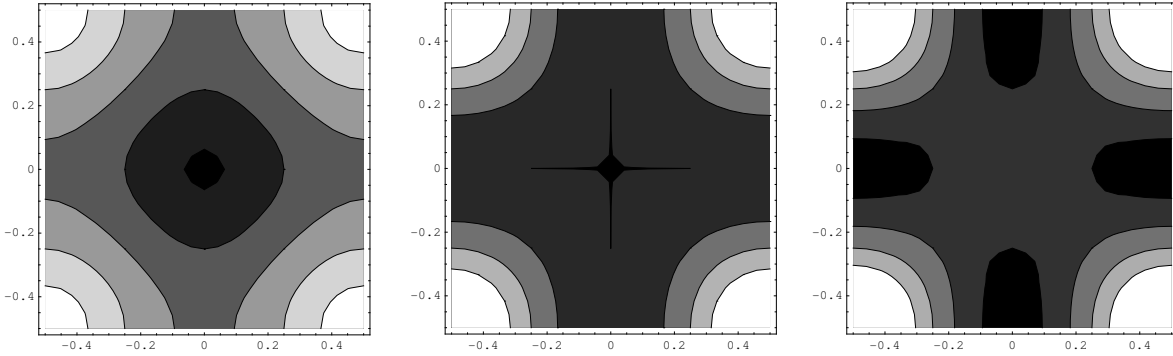


FIGURE 4. Fermi surfaces in the tight-binding square-lattice model with $t' > 0$ next-to-nearest-neighbour couplings for various values of $t'/|t|$. From left to right: $t'/|t| = 1/10$, $t'/|t| = 1/2$, and $t'/|t| = 7/10$. Notice the sharp transition at $t'/|t| = 1/2$.

e-f) We are to add a matrix element t' for hopping between next-to-nearest-neighbour sites and sketch how the Fermi surface of the half-filled band changes for $t' > 0$ and $t' < 0$.

It is simple enough to write down the new dispersion relation coming from the the Hamiltonian similar to part (a) above. Following that analysis, we find

$$\begin{aligned}
 H\psi &= \left\{ \epsilon^0 + 2t \left(\cos(2\pi q_1) + \cos(2\pi q_2) \right) + t' \left(e^{i\vec{q} \cdot (\vec{a}_1 + \vec{a}_2)} + e^{i\vec{q} \cdot (\vec{a}_1 - \vec{a}_2)} + e^{i\vec{q} \cdot (\vec{a}_2 - \vec{a}_1)} + e^{-i\vec{q} \cdot (\vec{a}_1 + \vec{a}_2)} \right) \right\} \psi, \\
 &= \left\{ \epsilon^0 + 2t \left(\cos(2\pi q_1) + \cos(2\pi q_2) \right) + t' \left(e^{i2\pi(q_1 + q_2)} + e^{-i2\pi(q_1 + q_2)} + e^{i2\pi(q_1 - q_2)} + e^{-i2\pi(q_1 - q_2)} \right) \right\} \psi, \\
 &= \left\{ \epsilon^0 + 2t \left(\cos(2\pi q_1) + \cos(2\pi q_2) \right) + 2t' \left(\cos(2\pi(q_1 + q_2)) + \cos(2\pi(q_1 - q_2)) \right) \right\} \psi; \\
 \therefore \epsilon(\vec{q}) &= \epsilon^0 + 2t \left(\cos(2\pi q_1) + \cos(2\pi q_2) \right) + 2t' \left(\cos(2\pi(q_1 + q_2)) + \cos(2\pi(q_1 - q_2)) \right). \quad (2.f.5)
 \end{aligned}$$

This modification can have a rather drastic effect on the Fermi surface—especially if $t'/|t|$ can be as large as around $\pm \frac{1}{2}$. Using equation (2.f.5) we have little difficulty plotting Fermi surfaces for various values of t'/t . In Figure 4 we show three qualitatively different Fermi surfaces for $t' > 0$ for different values of $t'/|t|$ and in Figure 5 we show these for $t' < 0$.

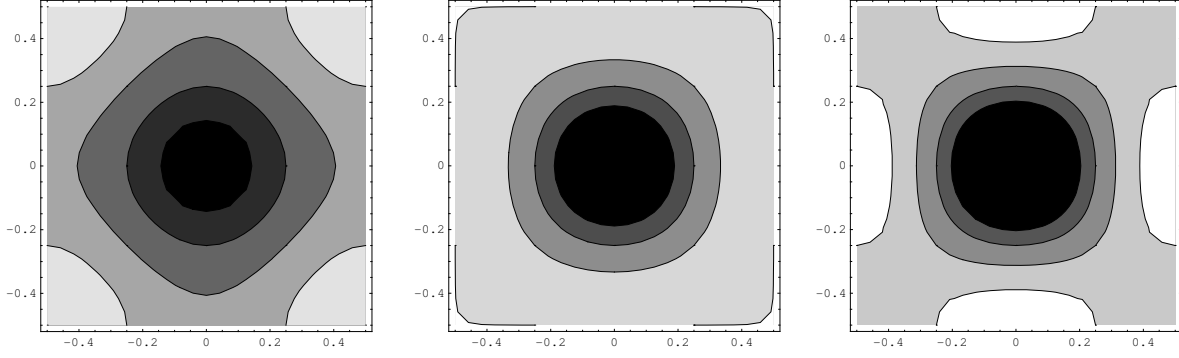


FIGURE 5. Fermi surfaces in the tight-binding square-lattice model with $t' < 0$ next-to-nearest-neighbour couplings for various values of $t'/|t|$. From left to right: $t'/|t| = -1/10$, $t'/|t| = -1/2$, and $t'/|t| = -9/10$. Notice the sharp transition at $t'/|t| = -1/2$.

Problem 3: Band Structure of Graphene and Nanotubes

Recall the honeycomb lattice used to describe graphene in homework 2. We are to consider a tight-binding model with a single level per site on a two-dimensional honeycomb lattice with only nearest-neighbour hopping with on-site energy ϵ^0 and nearest neighbour hopping matrix element t .

a-b) We are to find the energy bands of this model and determine at what momenta the two bands are degenerate.

Just to get our bearings, let us recall the Bravais and reciprocal lattices of the honeycomb lattice:

$$\vec{R} = \langle \vec{a}_1, \vec{a}_2 \rangle \quad \text{with} \quad \vec{a}_1 = a\sqrt{3}(1, 0) \quad \text{and} \quad \vec{a}_2 = a\sqrt{3}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \quad (3.a.1)$$

$$\vec{Q} = \langle \vec{b}_1, \vec{b}_2 \rangle \quad \text{with} \quad \vec{b}_1 = \frac{4\pi}{3a}\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \quad \text{and} \quad \vec{b}_2 = \frac{4\pi}{3a}(0, 1). \quad (3.a.2)$$

In this model, the wave function on each Bravais cell contains two linearly independent parts, coming from the two atoms in each cell; let's call them atoms A and B . The Hamiltonian of the system can be described by a 2×2 matrix, the diagonal parts coming from the on-site energy ϵ^0 and the off-diagonal parts describing the hopping matrix elements. The two off-diagonal entries are Hermitian conjugates of each other: one describe hopping from $A \rightarrow B$ and the other describes hopping from $B \rightarrow A$. Because the two processes are conjugate, it is sufficient to describe one.

Let $\vec{q} = q_1\vec{b}_1 + q_2\vec{b}_2$ —where q_1 and q_2 are not required to be integers. Although it will be very quickly brushed away, let us say that the vector \vec{v}_{AB} connects the atom at site A to that at site B . The hopping, or off-diagonal, part of the Hamiltonian is given by⁴

$$H_{A \rightarrow B} = te^{i\vec{q} \cdot \vec{v}_{AB}} \left\{ 1 + e^{i\vec{q} \cdot \vec{a}_2} + e^{i\vec{q} \cdot (\vec{a}_2 - \vec{a}_1)} \right\}, \quad (3.a.3)$$

$$\propto t \left\{ 1 + e^{i2\pi q_2} + e^{i2\pi(q_2 - q_1)} \right\}, \quad (3.a.4)$$

$$= t \left\{ 1 + 2e^{i\pi(2q_2 - q_1)} \cos(\pi q_1) \right\}. \quad (3.a.5)$$

Let us briefly observe that if H_{AB} were represented as $re^{i\theta}$, then the solution to the eigenvalue equation is

$$\begin{vmatrix} \epsilon^0 - \epsilon & re^{i\theta} \\ re^{-i\theta} & \epsilon^0 - \epsilon \end{vmatrix} = 0 \quad \implies \quad \epsilon = \epsilon_0 \pm r. \quad (3.a.6)$$

Using this and the work above, we can directly write down the dispersion relation:

$$\epsilon(\vec{q}) = \epsilon^0 \pm t\sqrt{1 + 4\cos(\pi(2q_2 - q_1))\cos(\pi q_1) + 4\cos^2(\pi q_1)}. \quad (3.a.7)$$

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⁴The proportionality is used to ignore a phase factor, which will not affect our analysis of energy eigenvalues.

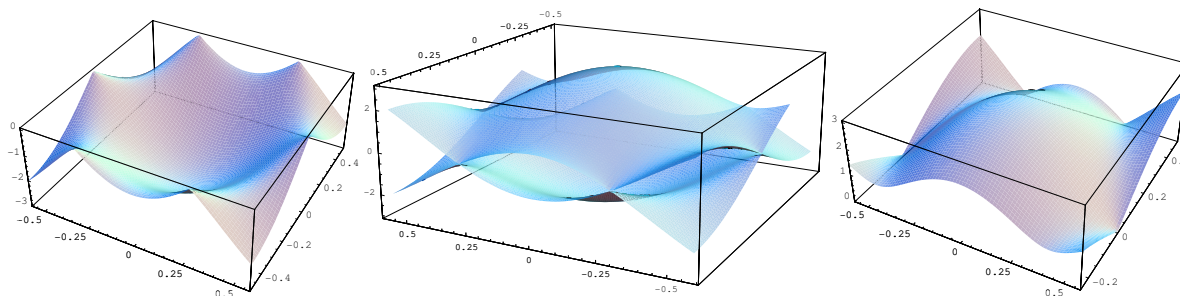


FIGURE 6. Energy bands calculated for graphene: the bands are shown separately on the right and left, and shown together in the middle. Notice there are precisely six degeneracies located in the first Brillouin zone.

We see that degeneracy implies that the above discriminant vanishes. This will be the case if

$$e^{i\pi(2q_2 - q_1)} \cos(\pi q_1) = -\frac{1}{2}. \quad (3.a.8)$$

At first glance, there are two possibilities we may try: first, we know that $e^{i\pi(2q_2 - q_1)} \in \mathbb{R}$, so it must be ± 1 . If $e^{i\pi(2q_2 - q_1)} = 1$ then $2q_2 - q_1 = 2n$ for $n \in \mathbb{Z}$; the equation above requires $\cos(\pi q_1) = -\frac{1}{2}$, which means that $q_1 = \frac{2}{3}$ or $\frac{4}{3}$. This gives us an infinite class of degenerate solutions, and by adding and subtracting reciprocal lattice vectors, we find six, essentially equivalent degeneracies at the corners of the first Brillouin zone:

$$\left(\frac{1}{3}, -\frac{1}{3}\right) \quad \left(-\frac{1}{3}, \frac{1}{3}\right) \quad \left(\frac{1}{3}, \frac{2}{3}\right) \quad \left(\frac{2}{3}, \frac{1}{3}\right) \quad \left(-\frac{2}{3}, -\frac{1}{3}\right) \quad \left(-\frac{1}{3}, -\frac{2}{3}\right), \quad (3.a.9)$$

where the components refer to the values of q_1, q_2 in $\vec{q} = q_1 \vec{b}_1 + q_2 \vec{b}_2$. Now, because adding and subtracting lattice vectors brought us into the other condition for degeneracy—with $2q_2 - q_1$ an odd integer—we know that all of the degeneracies have been accounted for.

The energy bands are plotted in Figure 6, where the six degenerate points are clearly visible.

c-d) Describe and sketch the topology for various Fermi surfaces that can occur as the filling of bands is varied. We should also describe the Fermi surface when the lower band is completely filled.

For very low ϵ_F , the fermi surface is a circle inscribed within the bowl seen in Figure 6.

As the energy increases, the Fermi surface appears more and more hexagonal until finally it breaks into six arcs—one about each of the corners of the first Brillouin zone. These six regions shrink as $\epsilon_F \rightarrow \epsilon^0$, when they vanish. This is shown in Figure 7.

As ϵ_F grows above ϵ^0 , the Fermi surface lies on the upper band and progresses in reverse of the lower-band: for low energies above ϵ^0 , the Fermi surface is composed of six distinct circular components which grow until they become nearly hexagonal; at high energies, the Fermi surface again approaches a single circular section. This progression is also shown in Figure 7.

In the case when the lower band is completely full, the Fermi ‘surface’ is the union of the six distinct Dirac points (of course, only two of them are inequivalent).

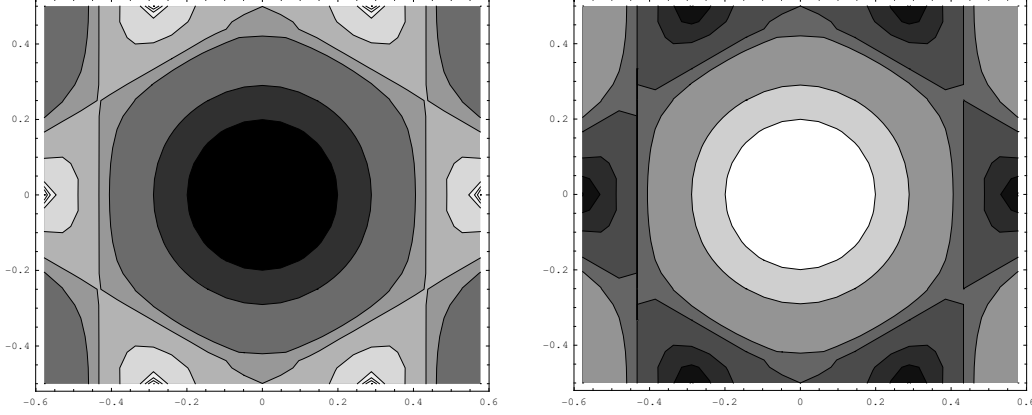


FIGURE 7. Contours indicating the Fermi surfaces for various ϵ_F in the lower (left) and upper (right) bands for the graphene tight-binding model. In both plots the energy is lower in the darker region—regions in white on the left plot match to the regions in black on the right plot.

e) If we were to compactify a sheet of graphene in one direction, the result would be a carbon nanotube. Depending on which Bravais lattice vector is taken as the compactifying direction, there may or may not be a band gap—if there is a gap, then the nanotube is an insulator; if the two bands are degenerate, then the tube is metallic. We are to determine which types of carbon nanotubes will be metallic and which would be insulating.

The ‘compactification’ of graphene into a carbon nanotube can be described as taking a quotient of the Bravais lattice by one of the lattice vectors, written \vec{R}/\vec{r} where $\vec{r} = r_1\vec{a}_1 + r_2\vec{a}_2$ where in this case $r_1, r_2 \in \mathbb{Z}$. That is to say, travelling in the direction \vec{r} brings you around the nanotube and back to where you started: the atoms at sites related by $\vec{R} + \vec{r}$ are not merely *related* to those at \vec{R} , but are actually the same atoms. This means that there is no ‘phase factor’ for travelling any multiple of times along \vec{r} .

Precisely, this requires that

$$e^{i\vec{q}\cdot\vec{r}} = 1 \quad \forall \vec{q}. \quad (3.e.10)$$

This places a strong constraint on the allowed \vec{q} ’s—indeed, it breaks our continuous band of allowed values to a discrete set. Whether or not the nanotube will be a metal or an insulator is completely determined by whether or not this discrete subset of allowed momenta include the Dirac points explored above.

The condition $e^{i\vec{q}\cdot\vec{r}} = e^{i2\pi(q_1r_1 + q_2r_2)} = 1$ is that

$$q_1r_1 + q_2r_2 \in \mathbb{Z}. \quad (3.e.11)$$

Recall that the six Dirac points were located at \vec{q} with components (with respect to \vec{b}_1, \vec{b}_2 basis) given in equation (3.a.9). There are two ‘types’ of points to check: the first two Dirac points listed in equation (3.a.9) will be present in the nanotube iff

$$\frac{r_1}{3} - \frac{r_2}{3} \in \mathbb{Z} \quad \implies \quad (r_1 - r_2) \in 3\mathbb{Z}; \quad (3.e.12)$$

the second type of point will be present in the nanotube iff

$$\frac{r_1}{3} + \frac{2r_2}{3} \in \mathbb{Z} \quad \implies \quad (r_1 + 2r_2) \in 3\mathbb{Z}. \quad (3.e.13)$$

It is not hard to show that these two conditions are in fact equivalent⁵. Therefore, a carbon nanotube will be a metal in this model only if

$$r_1 - r_2 = 3\ell \quad \text{for some } \ell \in \mathbb{Z}. \quad (3.e.14)$$

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⁵Say $r_1 - r_2 = 3\ell$, then $r_1 + 2r_2 = 3\ell + r_2 + 2r_2 = 3(\ell + r_2) \in 3\mathbb{Z}$; and conversely, say $r_1 + 2r_2 = 3m$, then $r_1 - r_2 = 3m - 2r_2 - r_2 = 3(m - r_2) \in 3\mathbb{Z}$. QED

Problem 4: Thermodynamics Near a Dirac Point

Let us return our attention to the tight-binding model of graphene from problem 3. We may for the sake of convenience take $\epsilon^0 = 0$.

a) The points where two bands become degenerate are called ‘Dirac points.’ We are to determine the low-temperature behaviour of the specific heat and magnetic spin susceptibility near the Dirac point for graphene.

The first step in our analysis will be to expand the dispersion relation (3.a.7) found in problem 3 above near the Dirac points. Now, because the six Dirac points are obviously translationally related, it is sufficient to consider just one for the moment.

Let us expand equation (3.a.7) about the Dirac point $(1/3, -1/3)$ ⁶:

$$\begin{aligned}
\epsilon &= \pm t \left\{ 1 + 4 \cos \left(\pi + \frac{3\pi\delta q}{\sqrt{2}} \right) \cos \left(\frac{\pi}{3} + \frac{\pi\delta q}{3\sqrt{2}} \right) + 4 \cos^2 \left(\frac{\pi}{3} + \frac{\pi\delta q}{3\sqrt{2}} \right) \right\}^{1/2}, \\
&= \pm t \left\{ 1 + 4 \left(-1 + \frac{9\pi^2\delta q^2}{4} + \dots \right) \left(\frac{1}{2} - \frac{1}{2}\sqrt{\frac{3}{2}}\pi\delta q - \frac{\pi^2\delta q^2}{8} + \dots \right) + 4 \left(\frac{1}{2} - \frac{1}{2}\sqrt{\frac{3}{2}}\pi\delta q - \frac{\pi^2\delta q^2}{8} + \dots \right)^2 \right\}^{1/2}, \\
&= \pm t \left\{ 1 + 2 \left(-1 + \frac{9\pi^2\delta q^2}{4} + \dots \right) \left(1 - \sqrt{\frac{3}{2}}\pi\delta q - \frac{\pi^2\delta q^2}{4} + \dots \right) + \left(1 - \sqrt{\frac{3}{2}}\pi\delta q - \frac{\pi^2\delta q^2}{4} + \dots \right)^2 \right\}^{1/2}, \\
&= \pm t \left\{ 1 + 2 \left(-1 + \frac{9\pi^2\delta q^2}{4} + \dots \right) \left(1 - \sqrt{\frac{3}{2}}\pi\delta q - \frac{\pi^2\delta q^2}{4} + \dots \right) + 1 - 2\sqrt{\frac{3}{2}}\pi\delta q - \frac{\pi^2\delta q^2}{2} + \frac{3\pi^2\delta q^2}{2} + \dots \right\}^{1/2}, \\
&= \pm t \left\{ 1 + 2 \left(-1 + \sqrt{\frac{3}{2}}\pi\delta q + \frac{\pi^2\delta q^2}{4} + \frac{9\pi^2\delta q^2}{4} + \dots \right) + 1 - 2\sqrt{\frac{3}{2}}\pi\delta q - \frac{\pi^2\delta q^2}{2} + \frac{3\pi^2\delta q^2}{2} + \dots \right\}^{1/2}, \\
&= \pm t \{ 6\pi^2\delta q^2 + \dots \}^{1/2}; \\
&\quad \therefore \epsilon \simeq \pm t\pi\sqrt{6}\delta q. \tag{4.a.1}
\end{aligned}$$

This allows us to compute the density of states about a *single* Dirac point is given by

$$\begin{aligned}
g(\epsilon) &= 2 \int_{d\epsilon} \frac{d^2q}{(2\pi)^2} \delta^{(2)}(0 \leq \pi\sqrt{6}\delta q \leq d\epsilon), \\
&= \frac{\delta q d\epsilon}{t\pi^2\sqrt{6}};
\end{aligned}$$

$$\therefore g_{\text{one Dirac point}}(\epsilon) = \frac{\epsilon}{6t^2\pi^3} \quad \implies \quad g_{\text{tot}}(\epsilon) = \frac{\epsilon}{t^2\pi^3}. \tag{4.a.2}$$

With the density of states, we may compute the total energy⁷,

$$\begin{aligned}
u &= u_0 + \int_0^\infty d\epsilon g(\epsilon) f(\epsilon) \epsilon, \\
&= u_0 + \frac{1}{t^2\pi^3} \int_0^\infty \frac{\epsilon^2 d\epsilon}{e^{\epsilon/(k_B T)} + 1}, \\
&= u_0 + \frac{3\zeta(3)}{2t^2\pi^3} k_B^3 T^3 + \mathcal{O}(T^4),
\end{aligned}$$

where $\zeta(n)$ is the Riemann zeta function. Therefore, we see that

$$c_v = \frac{9\zeta(3)k_B^3}{2t^2\pi^3} T^2 + \mathcal{O}(T^3). \tag{4.a.3}$$

⁶We will expand in $\frac{\delta q}{\sqrt{2}}$ so that $|\delta\vec{q}| = \delta q$.

⁷Using *Mathematica* for the integrals.

To find the magnetic susceptibility we will begin by referring to the textbook or class notes wherein it is found that the total magnetization (in the Pauli model) is given by

$$M = \mu^2 H \int d\epsilon g'(\epsilon) f(\epsilon). \quad (4.a.4)$$

Evaluating this integral directly, we see

$$\chi = \frac{\partial M}{\partial H} = \mu^2 \frac{k_B T \log(2)}{t^2 \pi^3} + \mathcal{O}(T^2). \quad (4.a.5)$$

b) Consider doping graphene so that ϵ_F is just above the Dirac point, but by an amount much less than that of T ; we are to again describe the low-temperature approximations of the specific heat and magnetic spin susceptibility.

I am pretty sure that the picture we are supposed to envision is that we are some ϵ_F separated from the Dirac point, yet close enough to it that $g(\epsilon)$ can be still viewed as a linear function of ϵ . If this is the appropriate, then we can take

$$g(\epsilon) = \frac{\epsilon - \epsilon_F}{t^2 \pi^3} \quad \text{and} \quad f(\epsilon) = \frac{1}{e^{(\epsilon - \epsilon_F)/(k_B T)} + 1},$$

and integrate above the Fermi surface⁸. Using a computer algebra package, we find

$$\begin{aligned} u &= u_0 + \frac{1}{t^2 \pi^3} \int_{\epsilon_F}^{\infty} \frac{\epsilon(\epsilon - \epsilon_F) d\epsilon}{e^{(\epsilon - \epsilon_F)/(k_B T)} + 1}, \\ &= \frac{\epsilon_F k_B^2}{12 t^2 \pi} T^2 + \frac{3\zeta(3) k_B^3}{2 t^2 \pi^3} T^3 + \mathcal{O}(T^4). \end{aligned}$$

(It is comforting that this reproduces our earlier result for vanishing ϵ_F .) This allows us to directly conclude that

$$\therefore c_v = \frac{\epsilon_F k_B^2}{6 t^2 \pi} T + \frac{9\zeta(3) k_B^3}{2 t^2 \pi^3} T^2 + \mathcal{O}(T^3). \quad (4.b.1)$$

Now, to find the magnetic susceptibility, we perform the same steps as before and see

$$M = \mu^2 H \int d\epsilon g(\epsilon) f(\epsilon) = \mu^2 H \frac{1}{t^2 \pi^3} \left(k_B T \log(2) + \frac{\epsilon_F}{2} \right), \quad (4.b.2)$$

and so

$$\therefore \chi = \mu^2 \frac{1}{t^2 \pi^3} \left(k_B T \log(2) + \frac{\epsilon_F}{2} \right). \quad (4.b.3)$$

⁸There are alternative ways of looking at this.

PHYSICS 525, CONDENSED MATTER

Homework 4

Due Tuesday, 24th October 2006

JACOB LEWIS BOURJAILY

Problem 1: Electron in a Two-Dimensional, Weak Sinusoidal Potential

Consider electrons moving in a two-dimensional, weak periodic potential given by

$$V(x, y) = U \left[\cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{a}\right) \right],$$

where $U > 0$.

a. We are asked to find the two lowest-eigenenergies and eigenstates to first order in U at the edge of the Brillouin zone, but away from the corners.

To write the Schrödinger equation in momentum space we will need the Fourier modes of the potential function; the non-vanishing modes are $U_{\pm b_x} = U_{\pm b_y} = U/2$, where $b_x = b\hat{q}_x$ and $b_y = b\hat{q}_y$ where $b = \frac{2\pi}{a}$ and a is the lattice spacing.

There are four ‘edges’ of the Brillouin zone, and the essential result will be identical for all four of them. Without loss of generality, let us consider the Schrödinger equation for the wave function with momentum on the Bragg plane $q = (\pi/a, 0)$. Letting $\varepsilon_q^0 = \frac{\hbar^2}{2m}q^2$, we see that $\varepsilon_q^0 = \varepsilon_{q-b_x}^0$ on this plane; because this is the only ‘degeneracy’—before considering the effects of the weak potential—we know that to leading order in U the Schrödinger equation gives rise to the following system of equations¹

$$\begin{aligned} (\varepsilon - \varepsilon_q^0) c_q &= \frac{U}{2} c_{q-b_x}; \\ (\varepsilon - \varepsilon_{q-b_x}^0) c_{q-b_x} &= \frac{U}{2} c_q. \end{aligned} \tag{1.a.1}$$

This system is obviously solved by

$$\therefore \varepsilon_\pi(q) = \frac{1}{2} (\varepsilon_q^0 + \varepsilon_{q-b_x}^0) \pm \frac{1}{2} \left\{ (\varepsilon_q^0 - \varepsilon_{q-b_x}^0)^2 + U^2 \right\}^{1/2}. \tag{1.a.2}$$

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On the Bragg plane, the two lowest eigenenergies are therefore

$$\varepsilon_\pm = \frac{\hbar^2 \pi^2}{2m a^2} \pm \frac{U}{2}. \tag{1.a.3}$$

The wave functions are found by considering again equations (1.a.1). On the Bragg plane, we see that these imply

$$c_q = \pm c_{q-b_x}, \tag{1.a.4}$$

where ‘ \pm ’ refers to equation (1.a.2). Up to normalization, this implies that the wave functions are

$$\psi_+ \sim c_q e^{iq \cdot r} (1 + e^{-ibx}) \propto \cos\left(\frac{\pi x}{a}\right); \tag{1.a.5}$$

$$\psi_- \sim c_q e^{iq \cdot r} (1 - e^{-ibx}) \propto \sin\left(\frac{\pi x}{a}\right). \tag{1.a.6}$$

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¹Here we are using notation which should be common by now: the wave function $\psi_q(r) = \sum_{b \in G} c_{q-G} e^{i(q-G) \cdot r}$.

b. We are to determine the *four* lowest-energy single-electron eigenstates at the corner of the Brillouin zone to first order in U and give the corresponding wave functions.

We see at least two equivalent ways of proceeding; because they are of sufficiently different philosophy, we will present both, if briefly. The first, and quickest solution makes important use of our result in part (a) above. Each two adjacent Bragg planes have a pair of parabolic energy bands, separated by a gap U . At the corners, pairs of bands from adjacent planes would meet. From our analysis above and elsewhere, we know that when this happens in a weak potential U , the apparently degenerate bands will hybridize. That is, for example, the two ' $\varepsilon = \varepsilon_q^0 - \frac{U}{2}$ ' bands from adjacent edges will hybridize, giving the two lowest states at $\varepsilon_1 = \varepsilon_q^0 - U$ and $\varepsilon_2 = \varepsilon_q^0$. The two 'upper' bands will hybridize giving rise to $\varepsilon_3 = \varepsilon_q^0$ and $\varepsilon_4 = \varepsilon_q^0 + U$. Here, $q = (\pi/a, \pi/a)$.

To be a bit more explicit—allowing us to determine not just the energies at the corners, but also nearby—we could have begun with the four 'nearly degenerate' states at the corners. The Schrödinger equation near the corners, to first order in U , gives rise to the system of equations

$$\begin{aligned} (\varepsilon - \varepsilon_q^0) c_q &= \frac{U}{2} (c_{q-b_x} + c_{q-b_y}); & (\varepsilon - \varepsilon_{q-b_x}^0) c_{q-b_x} &= \frac{U}{2} (c_q + c_{q-b_x-b_y}); \\ (\varepsilon - \varepsilon_{q-b_y}^0) c_{q-b_y} &= \frac{U}{2} (c_q + c_{q-b_x-b_y}); & (\varepsilon - \varepsilon_{q-b_x-b_y}^0) c_{q-b_x-b_y} &= \frac{U}{2} (c_{q-b_x} + c_{q-b_y}). \end{aligned} \quad (1.b.7)$$

This system is straight-forwardly inverted. In units where $\frac{\hbar^2}{2m} = 1$, the eigenenergies near to the corner are

$$\begin{aligned} \varepsilon_1 &= q_x^2 + q_y^2 - 2\pi(q_x + q_y) + 4\pi^2 + \frac{1}{2} \left\{ 4U^2 + 32\pi^2 (q_x^2 + q_y^2 - 2\pi(q_x + q_y) + 2\pi^2) + 4\sqrt{(U^2 + 16\pi^2(\pi - q_x)^2)(U^2 + 16\pi^2(\pi - q_y)^2)} \right\}^{1/2}; \\ \varepsilon_2 &= q_x^2 + q_y^2 - 2\pi(q_x + q_y) + 4\pi^2 - \frac{1}{2} \left\{ 4U^2 + 32\pi^2 (q_x^2 + q_y^2 - 2\pi(q_x + q_y) + 2\pi^2) + 4\sqrt{(U^2 + 16\pi^2(\pi - q_x)^2)(U^2 + 16\pi^2(\pi - q_y)^2)} \right\}^{1/2}; \\ \varepsilon_3 &= q_x^2 + q_y^2 - 2\pi(q_x + q_y) + 4\pi^2 + \frac{1}{2} \left\{ 4U^2 + 32\pi^2 (q_x^2 + q_y^2 - 2\pi(q_x + q_y) + 2\pi^2) - 4\sqrt{(U^2 + 16\pi^2(\pi - q_x)^2)(U^2 + 16\pi^2(\pi - q_y)^2)} \right\}^{1/2}; \\ \varepsilon_4 &= q_x^2 + q_y^2 - 2\pi(q_x + q_y) + 4\pi^2 - \frac{1}{2} \left\{ 4U^2 + 32\pi^2 (q_x^2 + q_y^2 - 2\pi(q_x + q_y) + 2\pi^2) - 4\sqrt{(U^2 + 16\pi^2(\pi - q_x)^2)(U^2 + 16\pi^2(\pi - q_y)^2)} \right\}^{1/2}. \end{aligned}$$

We of course did not need to do the above expansion to note that this analysis agrees with our previous one for the four energies *at the corner*:

$$\varepsilon_1 = \frac{\hbar^2 \pi^2}{m a^2} - U, \quad \varepsilon_2 = \varepsilon_3 = \frac{\hbar^2 \pi^2}{m a^2}, \quad \varepsilon_4 = \frac{\hbar^2 \pi^2}{m a^2} + U. \quad (1.b.8)$$

Making use of the Schrödinger equation (1.b.7) at the corner, we see that for $\varepsilon = \varepsilon_q^0 \pm U$ the solutions are

$$c_q = c_{q-b_x-b_y} = \pm c_{q-b_x} \quad \text{and} \quad c_{q-b_x} = c_{q-b_y}. \quad (1.b.9)$$

The two degenerate wave functions do not uniquely solve the Schrödinger equation (1.b.7)—as we should expect. For these two bands, the wave functions satisfy

$$c_q = -c_{q-b_x-b_y} \quad \text{and} \quad c_{q-b_x} = -c_{q-b_y}, \quad (1.b.10)$$

and any wave function can be build out of the two linearly independent relative pairings $c_q = \pm c_{q-b_y}$. In all, the wave functions (in order of increasing energy) at the corner are²

$$\psi_1 \sim c_q e^{iq \cdot r} \left\{ 1 - e^{-ibx} - e^{-iby} - e^{-ib(x+y)} \right\} \propto \left\{ \cos(\pi(x+y)) - \cos(\pi(x-y)) \right\}; \quad (1.b.11)$$

$$\psi_2 \sim c_q e^{iq \cdot r} \left\{ 1 - e^{-ibx} + e^{-iby} - e^{-ib(x+y)} \right\} \propto \left\{ \sin(\pi(x+y)) + \sin(\pi(x-y)) \right\}; \quad (1.b.12)$$

$$\psi_3 \sim c_q e^{iq \cdot r} \left\{ 1 + e^{-ibx} - e^{-iby} - e^{-ib(x+y)} \right\} \propto \left\{ \sin(\pi(x+y)) - \sin(\pi(x-y)) \right\}; \quad (1.b.13)$$

$$\psi_4 \sim c_q e^{iq \cdot r} \left\{ 1 + e^{-ibx} - e^{-iby} + e^{-ib(x+y)} \right\} \propto \left\{ \cos(\pi(x+y)) + \cos(\pi(x-y)) \right\}. \quad (1.b.14)$$

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²Just to reiterate: the solutions ψ_2 and ψ_3 could generically be any linear combination of what we have written.

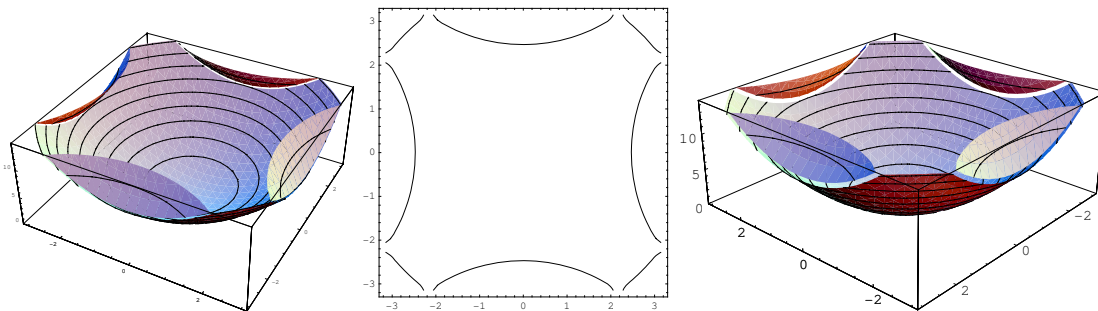


FIGURE 1. Three different views of the Fermi surfaces for the (metallic) system described in Problem 1. The figures on the left and right-hand sides show many equal-energy contours up to the Fermi energy. The middle plot shows just the Fermi surfaces. (Note that the corners of the figure are on the lower band, $n = 1$, and the edges are on the second band.)

c. Assuming that there are two electrons per unit cell, we are to find the lowest value of U for which the system is a band insulator, and below which it is a metal. We should make a qualitatively correct representation of the Fermi surface of the system when it is metallic. changes from being a band insulator to a metal. For a value of U for which the system describes a metal, we are to make a qualitatively correct sketch of the locations of the Fermi surfaces in the first Brillouin zone.

Unless we are mistaken, the only point of ‘including the electron’s spin’ is that we know there are states sufficient to fill the entire lowest energy band: when the system is a band insulator the entire first band will be filled; when the system is a metal some of the electrons will pour into the second band.

The system will be a metal only if the minimum energy of the second band is lower than the highest energy of the first band. This is particularly easy because we know from part (a) that the global minimum of the second energy is at the midpoint of one of the first Bragg planes:

$$\min(\varepsilon_2) = \frac{\hbar^2 \pi^2}{2m a^2} + \frac{U}{2}. \quad (1.c.15)$$

Similarly, we know that the global maximum of the lowest energy band occurs at the corner of the Brillouin zone (because it increases away from the centre of the Bragg plane), giving

$$\max(\varepsilon_1) = \frac{\hbar^2 \pi^2}{m a} - U. \quad (1.c.16)$$

Therefore, the system will be a band insulator if

$$\min(\varepsilon_2) - \max(\varepsilon_1) > 0 \quad \implies \quad U > \frac{\hbar^2 \pi^2}{3ma^2}. \quad (1.c.17)$$

The Fermi surfaces for the system when it is a metal are shown in Figure 1.

d. We are to make a qualitatively correct representation of how the zero-temperature spin contribution to the system’s magnetic susceptibility χ varies with U as U passes through the transition between insulator and conductor. Near-to, but on the *insulating* side of the transition, we are to describe the lowest-energy electronic excitations above the ground state at and give possible total crystal momentum for these excitations.

The last part can be done presently. Near the transition, the lowest energy excitations will bring electrons at the corners of the Brillouin zone to the centres of the Bragg planes in the second energy band. These are excitations with momentum transfer of $\Delta q = (-\frac{\pi}{2a}, 0)$, $(0, -\frac{\pi}{2a})$, $(-\frac{\pi}{a}, -\frac{\pi}{2a})$, or $(-\frac{\pi}{2a}, -\frac{\pi}{a})$. The crystal momentum will then be on the center of the Bragg plane, so $q = (\frac{\pi}{a}, 0)$, $(0, \frac{\pi}{a})$, $(-\frac{\pi}{a}, 0)$, or $(0, -\frac{\pi}{a})$.

Problem 2: A Narrow-Gap Semiconductor

Consider two bands of states which overlap but interact only weakly. Let one of them be particle-like and the other be hole-like. We may assume that they become degenerate and/or hybridize near zero momentum. The Hamiltonian conserves crystal momentum and has the following matrix elements

$$\langle 1, \mathbf{k} | H | 1, \mathbf{k} \rangle = \frac{\hbar^2 \mathbf{k}^2}{2m_e} \equiv k^2, \quad \langle 2, \mathbf{k} | H | 2, \mathbf{k} \rangle = \Delta - \frac{\hbar^2 \mathbf{k}^2}{2m_h} \equiv \Delta - \lambda k^2, \quad \langle 1, \mathbf{k} | H | 2, \mathbf{k} \rangle = \delta, \quad (2.a.1)$$

where we have introduced the constant $\lambda \equiv \frac{m_e}{m_h}$ and have chosen appropriate ‘units’ for the crystal momentum k . In (2.a.1), Δ , m_e , and m_h are all positive and δ is real.

a. We are to calculate and describe the dispersions of the resulting band structure after hybridization for each qualitatively different case which can arise.

We have done these problems enough to know that

$$\begin{vmatrix} \alpha - \varepsilon & \delta \\ \delta & \beta - \varepsilon \end{vmatrix} = 0 \quad \Longrightarrow \quad \varepsilon = \frac{1}{2}(\alpha + \beta) \pm \left\{ \left(\frac{\alpha - \beta}{2} \right)^2 + \delta^2 \right\}^{1/2}, \quad (2.a.2)$$

where in our case $\alpha = k^2$ and $\beta = \Delta - \lambda k^2$ so that the dispersion is

$$\varepsilon_{\pm} = \frac{1}{2}(k^2(1 - \lambda) + \Delta) \pm \left\{ \left(\frac{k^2(1 + \lambda) - \Delta}{2} \right)^2 + \delta^2 \right\}^{1/2}. \quad (2.a.3)$$

Notice that equation (2.a.3) implies that as long as $\delta \neq 0$, no matter how small, the two bands will not intersect.

It is at least intuitively obvious to the author that any generic set of parameters will give rise to situations where both bands have three stationary points. We can test this intuition and discover some interesting results by calculating exactly where these stationary points are for each band. Of course we can do these two cases simultaneously as follows. ε_{\pm} will have an extremum if

$$\frac{\partial \varepsilon_{\pm}}{\partial k} = 0 = k(1 - \lambda) \pm \frac{(k^2(1 + \lambda) - \Delta) k(1 + \lambda)}{\zeta} \quad \text{where} \quad \zeta = \left\{ \left(\frac{k^2(1 + \lambda) - \Delta}{2} \right)^2 + \delta^2 \right\}^{1/2}. \quad (2.a.4)$$

As long as $\delta \neq 0$ and the other parameters are real, $\zeta > 0$ —which is all we need for the moment. The first, obvious extremum is at $k = 0$, which is uninteresting for the moment. The other stationary points are then seen to satisfy

$$0 = \pm k^2 \frac{(1 + \lambda)^2}{\zeta} \mp \frac{(1 + \lambda)\Delta}{\zeta} + (1 - \lambda), \quad (2.a.5)$$

$$= \pm k^2 \mp \frac{\Delta}{1 + \lambda} + \zeta \frac{1 - \lambda}{(1 + \lambda)^2}; \quad (2.a.6)$$

$$\Longrightarrow \pm k^2 = \frac{1}{1 + \lambda} \left\{ \zeta \left(\frac{\lambda - 1}{\lambda + 1} \right) \pm \Delta \right\}. \quad (2.a.7)$$

Indeed, we see that ε_+ (ε_-) will generically have an absolute minimum (maximum) at $k^2 \neq 0$. However, there can be a conspiracy where the term in curly brackets on the right vanishes, giving rise to either ε_- or ε_+ —*but not both*—having a third-order global maximum or minimum at $k = 0$, respectively.

Let us quickly find the cases when ε_+ or ε_- does not have three distinct extrema. For ε_+ , the upper band, $\Delta, \zeta > 0$ implies that $\lambda - 1 < 0$ or that $m_e < m_h$ for (2.a.7) to vanish. Bearing in mind that $\zeta(k^2 = 0) = \sqrt{\Delta^2/4 + \delta^2}$, we have

$$\Delta(1 + \lambda) = (1 - \lambda)\zeta, \quad (2.a.8)$$

$$\Longrightarrow \Delta^2(1 + \lambda)^2 = (1 - \lambda)^2 \left(\frac{\Delta^2}{4} + \delta^2 \right); \quad (2.a.9)$$

$$\Longrightarrow \delta^2 = \frac{\Delta^2}{(1 - \lambda)^2} \left((1 + \lambda)^2 - \frac{(1 - \lambda)^2}{4} \right). \quad (2.a.10)$$

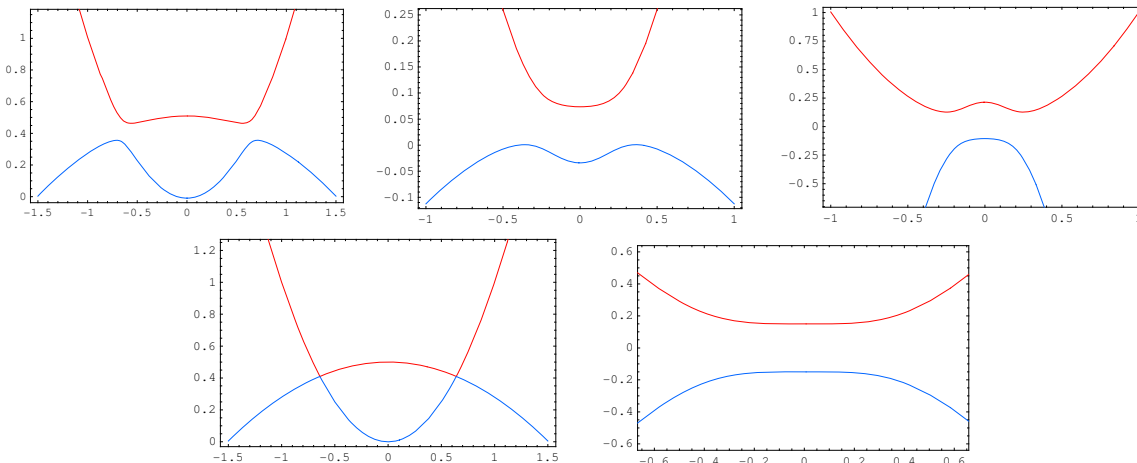


FIGURE 2. The qualitatively different possible hybridizations between particle- and hole-like bands. The possibilities are shown in the order discussed.

Similar algebra in the case of the ε_- band shows that we can have a fourth-order global maximum only when $1 - \lambda < 0$, i.e. that $m_h < m_e$. Then we have

$$\Delta(\lambda + 1) = (\lambda - 1)\zeta, \quad (2.a.11)$$

$$\implies \Delta^2(\lambda + 1)^2 = (\lambda - 1)^2 \left(\frac{\Delta^2}{4} + \delta^2 \right), \quad (2.a.12)$$

$$\implies \delta^2 = \frac{\Delta^2}{(1 - \lambda)^2} \left((1 + \lambda)^2 - \frac{(1 - \lambda)^2}{4} \right), \quad (2.a.13)$$

exactly as before (only this time we have $\lambda > 1$). Indeed, both cases are rather contrived.

We have therefore classified the general structure of all possible hybridizations, as illustrated in Figure 2.

- (1) Generic situation: when there is no conspiracy in any of the parameters, then both bands will feature three extrema—and global minima of ε_+ will not lie over the global maxima of ε_- .
- (2) When the upper band, ε_+ , has a fourth-order global minimum. Recall that this only occurs if $m_e < m_h$ and equation (2.a.10) is satisfied. Notice that this gives rise to two particle-like bands.
- (3) When the lower band, ε_- , has a fourth-order global maximum. Recall that this only occurs if $m_h < m_e$ and equation (2.a.13) is satisfied. Notice that this gives rise to two hole-like bands.
- (4) No interaction term: $\delta = 0$. Here the bands only ‘hybridize’ in the sense that we are perfectly free to choose our eigenenergies to be the ‘upper’ and ‘lower’ bands.
- (5) When $\lambda = 1$ and $\Delta = 0$, the two overlapping bands will separate similar to as along a Bragg plane. Here both bands stay quadratic.

b. We are to obtain the density of states for $\delta = 0$ and determine the energies and powers of the Van Hove singularities.

When $\delta = 0$, the band energies are simply given by their free-values. Because of this, it is not difficult to explicitly determine the density of states. Indeed, we find for ε_1 ³ that

$$g_1(\varepsilon) = \frac{2}{(2\pi)^3} 4\pi \frac{k(\varepsilon)^2}{\frac{\hbar^2 k(\varepsilon)}{m_e}} = \frac{k(\varepsilon)m_e}{\pi^2 \hbar^2}, \quad (2.b.14)$$

and because

$$k(\varepsilon) = \frac{\sqrt{2m_e\varepsilon}}{\hbar},$$

this implies

$$\therefore g_1(\varepsilon) = \sqrt{\varepsilon} \frac{(2m_e)^{3/2}}{2\pi^2 \hbar^3}. \quad (2.b.15)$$

Similarly, we see that

$$g_2(\varepsilon) = \frac{2}{(2\pi)^3} 4\pi \frac{k(\varepsilon)^2}{\frac{\hbar^2 k(\varepsilon)}{m_h}} = \frac{k(\varepsilon)m_h}{\pi^2 \hbar^2}, \quad (2.b.16)$$

and because in this case

$$k(\varepsilon) = \frac{\sqrt{2m_h(\Delta - \varepsilon)}}{\hbar},$$

we see

$$\therefore g_2(\varepsilon) = \sqrt{\Delta - \varepsilon} \frac{(2m_h)^{3/2}}{2\pi^2 \hbar^3}. \quad (2.b.17)$$

The Van Hove singularities are located at $\varepsilon = 0$, $\varepsilon = \Delta$ which are both $\sim \sqrt{\varepsilon}$.

c. We are to sketch the density of states for each of the qualitative cases studied in problem (a). For each one, we should comment on the Van Hove singularities and their strengths.

The density of states for each of the five cases discussed in problem (a) are shown in Figure 3. The Van Hove singularities are obvious by inspection for most of the plots—apparently the only exception is the left leg of the third plot, which should show a divergence (the right hand leg does not diverge).

Although it would have been preferable to have labeled the plots explicitly indicating the singularities and their strengths, we will need to make due with a mere discussion. Importantly, there are at most four Van Hove singularities which correspond to the at most four crystal momenta giving extrema of ε_{\pm} . Because there is always a local extrema at zero crystal momentum, two potential Van Hove singularities are at

$$\varepsilon_+(0) \quad \text{and} \quad \varepsilon_-(0). \quad (2.c.18)$$

The other two possible places where Van Hove singularities can arise are the global extrema of ε_{\pm} . In problem (a) we calculated the values of k for which ε_{\pm} would have an extrema. A bit of algebra allows one to see that the other two possible Van Hove singularity locations are

$$\varepsilon_- \left(\left(\frac{\lambda - 1}{(\lambda + 1)^2} \sqrt{\frac{\delta^2}{1 - \frac{(1-\lambda)^2}{4(\lambda+1)^2}}} + \frac{\Delta}{\lambda + 1} \right)^{1/2} \right) \quad \text{and} \quad \varepsilon_+ \left(\left(\frac{1 - \lambda}{(\lambda + 1)^2} \sqrt{\frac{\delta^2}{1 - \frac{(1-\lambda)^2}{4(\lambda+1)^2}}} + \frac{\Delta}{\lambda + 1} \right)^{1/2} \right). \quad (2.c.19)$$

A quick glance at the plots in Figure 3 shows that the ‘generic case’ has Van Hove singularities at all four of the possible locations. Plots two and three, when one of the bands has a fourth-order extrema at the origin show only three of the four possible singularities (see footnote earlier). The fourth case, where there is no coupling between the bands has only two of the singularities; the last plot, corresponding to the

³Here ε_1 refers to the particle-like band.

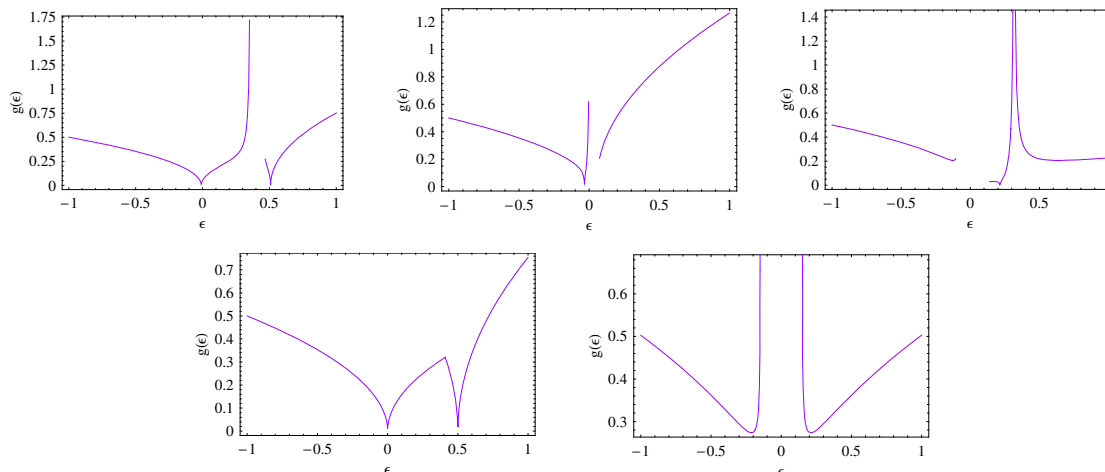


FIGURE 3. The densities of states for the band structures illustrated in Figure 2.

case where the two bands split while maintaining quadratic dependence on k gives rise to only the two singularities which are seen approaching the gap.

We can actually ‘read off’ the strength of the singularities with a little background information. Recall in part (a) above we showed that $\nabla(\varepsilon)$ was at most a cubic polynomial in k . Because $g(\varepsilon) \sim \frac{k^2}{\nabla\varepsilon}$ on general and dimensional grounds, we see that the ‘worst’ type of singularity could therefore be $1/k \sim 1/\sqrt{\varepsilon}$ which is seen as the vertical spikes in plots 1,2,3⁴ and 4 in Figure 3. All the other Van Hove singularities come about the usual way, from $g(\varepsilon) \sim k^2/k \sim \sqrt{\varepsilon}$.

d. We are to find the gap energy when $m_e = m_h$, ($\lambda = 1$).

We have done enough two-state degeneracy problems to know that the band gap energy will be 2δ . To see this, consider zooming in near where the two bands cross; locally, this is to order δ simply a two degenerate state problem that we are now so good at. Simple diagonalization gives the result we are now able to guess without diagonalizing anything.

If it were truly necessary to prove our intuition is correct, recall equation (2.c.19) which tells us where the global minimum (maximum) of ε_+ (ε_-) is to be found. Using our assumption that $\lambda = 1$, the expression greatly simplifies and we find

$$k^2 = \pm \frac{\Delta}{2}.$$

Putting this in the dispersion relation calculated in equation (2.a.3) immediately shows that

$$\therefore \varepsilon_{\text{gap}} = 2\delta. \quad (2.d.20)$$

e. In the above analyses, we considered spherically symmetric electron potentials. In any real crystal, there would be dispersion modifications giving rise to e.g. angular dependencies on the order of k^4 . We are to describe how including these effects could affect our analysis.

There are two cases when crystal structure could possibly lead to (even dramatic) alterations of our analysis above:

- (1) If m_e, m_h are too large: this would soften their intersection (making it more sensitive to higher-order effects) and also raise the size of k for which become

⁴We mentioned earlier that although the spike is not seen on the printed plot, it is nevertheless present.

nearly degenerate. In contrast, if m_e, m_h are very small compared to the reciprocal lattice, then their unperturbed intersection will be ‘steep’—ergo most sensitive to leading effects in k —and likely to be closer to small values of k , where the effects of the zone edges are small.

- (2) If Δ is too large: if the two bands are widely separated in energy, then our analysis above would simply have assumed that the two bands hybridize farther out in k -space. This is only reasonable if the region where the two bands hybridize is well within the Brillouin zone.

Baring these two caveats, many of our results above will carry over to this case with only small refinement. Specifically, the general classification of the types of hybridized bands will still be valid. If one or both of the situations described above apply, however, there will be much more variety in the types of hybridized band structures that can arise.

One possibly important change to our analysis would involve our discussion of the density of levels: k^4 terms will almost certainly add to the number of Van Hove singularities, for example. When the periodic potential is weak⁵, for example, $\nabla\varepsilon(k)$ vanishes along Bragg planes—which will certainly give rise to new Van Hove singularities in the density of levels (although perhaps not in the energy ranges we are interested in).

Problem 3: Shubnikov-de Haas-van Alphen Oscillations

The low-temperature specific heat of a piece of metal at high magnetic fields is found to be periodic in inverse field, with period 2×10^{-9} Gauss⁻¹. We are asked to interpret this observation using a one-band free-electron model for the conduction electrons and thereby determine the number density of electrons and their energy in eV. At low-fields, the oscillations are not visible because of scattering effects—the resistivity at low temperature is measure to be $0.1\mu\Omega - \text{cm}$. We are to use this to estimate the mean free path of conduction electrons in this materials within the Sommerfeld model of conduction and use this to estimate the minimum field strength necessary to observe oscillations of the specific heat.

Using Onsager’s result, we know that

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e}{\hbar} \frac{1}{A_e},$$

where in our case $\Delta(H^{-1}) = 2 \times 10^{-5}$ T⁻¹. A_e is the cross-sectional area of the Fermi surface in a plane normal to the magnetic field axis. If we take the free electron approximation, then all extremal cross sections through the Fermi surface have area πk_F^2 —a fact which is readily visualized. Inverting this and using real numbers, we see that the oscillation period observed implies a Fermi momentum of

$$k_F = 1.23 \times 10^{10} \text{ m}^{-1}. \quad (3.b.1)$$

Using all our favourite results for free electrons, we see that this implies that the density of conduction electrons is given by

$$n = \frac{k_F^3}{3\pi^2} = 6.33 \times 10^{28} \text{ m}^{-3}. \quad (3.b.2)$$

And the Fermi energy is then

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m_e} = 5.83 \text{ eV}. \quad (3.b.3)$$

Using some book work in Ashcroft and Mermin, we know how the resistivity is related to the mean free path and the scattering time. Specifically, we have the mean free path ℓ is given by

$$\ell = \frac{50.1 \text{ eV}}{\varepsilon_F \rho_\mu} \times 92 \times 10^{-8} \text{ cm} \quad (3.b.4)$$

⁵Ashcroft and Mermin point out that this is also often true when the potential is not weak: because Bragg planes are regions of high-symmetry it should not come as a surprise that energy bands are often forced to meet Bragg planes symmetrically—i.e. smooth crossing in the extended zone scheme.

where ρ_μ is the resistivity in $\mu\Omega - \text{cm}$. We have

$$\ell = 8.00 \times 10^{-7} \text{ m} \quad (3.b.5)$$

Even at zero temperature, the oscillations will be broadened because of scattering, effectively washing out the signal. To see the effect—as discussed in class—it the field H must be such that

$$\frac{eH}{mc}\tau \gg 1 \quad \implies \quad H \gg \frac{\hbar k_F}{e\ell} \simeq 10 \text{ Tesla}. \quad (3.b.6)$$

Problem 4: Tight-Binding Resonant Conduction

Consider the one-dimensional tight-binding model with Hamiltonian

$$H = \varepsilon_0|0\rangle\langle 0| + \sum_n t_n \left(|n\rangle\langle n+1| + |n+1\rangle\langle n| \right), \quad (4.a.1)$$

where $t_{-1} = t_-$, $t_0 = t_+$ and all other $t_n = t$. There is an impurity at site $n = 0$. We are to obtain the probability of transmission across the impurity for an incident electron with zero energy. We are to examine the case when ε_0 , t_- , and t_+ are all much less than t , showing its resonant form.

In the zero-temperature limit with the Fermi level at zero energy, we are to obtain the current resulting from a linear potential difference across the impurity. We should estimate the size of the voltage for which this limit is valid.

Consider the test wave function

$$|\psi\rangle = |0\rangle + \sum_{m>0} \left\{ (Ae^{iqm} + Re^{-iqm}) |m\rangle + Se^{-iqm} |-m\rangle \right\}. \quad (4.a.2)$$

Although the notation is a bit compact, this is nothing but an incoming wave with momentum $-q$ ⁶ toward the origin. The wave function is of course not normalized. The part of $|\psi\rangle$ proportional to S is nothing more than the transmitted wave, and the part proportional to R is the reflected wave.

We are seeking a zero-energy eigenstate $|\psi\rangle$. Acting with the Hamiltonian on our test function, we see

$$\begin{aligned} H|\psi\rangle = & (\varepsilon_0 + t_+ (Ae^{iq} + Re^{-iq}) + t_- Se^{-iq}) |0\rangle + (t_+ + t (Ae^{i2q} + Re^{-i2q})) |1\rangle + (t_- + tSe^{-i2q}) |-1\rangle \\ & + \sum_{m\geq 2} t \left\{ (Ae^{iq(m+1)} + Re^{-iq(m+1)} + Ae^{iq(m-1)} + Re^{-iq(m-1)}) |m\rangle + S (e^{-iq(m+1)} + e^{-iq(m-1)}) |-m\rangle \right\}. \end{aligned} \quad (4.a.3)$$

If $|\psi\rangle$ is an eigenvector of H with eigenvalue 0, then the coefficient of every basis ket $|\ell\rangle$ must vanish in the expression above. This gives us a large system of constraints. The constraint coming from the coefficient of $|-m\rangle$ in equation (4.a.3)—the pieces proportional to S shows that

$$(e^{-iq(m+1)} + e^{-iq(m-1)}) = 0 \quad \forall m \quad \implies \quad (e^{-iq} + e^{iq}) \propto \cos(q) = 0. \quad (4.a.4)$$

Therefore we see that $q = \pm \frac{\pi}{2}$ ⁷. To match our sign conventions, this implies that $q = -\frac{\pi}{2}$. We will save some time analyzing the other constraint equations by automatically inserting $e^{iq} = e^{-i\pi/2} = -e^{i\pi/2} = -i$ as it is encountered. The other constraint equations then are then

$$t_+ - t(A + R) = 0, \quad (4.a.5)$$

$$t_- - tS = 0, \quad (4.a.6)$$

$$\varepsilon_0 + it_+(R - A) + it_-S = 0. \quad (4.a.7)$$

⁶The signs are consistent if annoying—the author did not find time to clean up less-than pedagogical trivialities.

⁷We can take q to be in the first Brillouin zone without loss of generality.

These three equations are linearly independent and allow us to completely solve for A , R and S in terms of t_{\pm} , t and ε_0 . Indeed, we have

$$S = \frac{t_-}{t} \quad \text{and} \quad A = \frac{t_+^2 + t_-^2 - it\varepsilon_0}{tt_+} \quad \text{and} \quad R = \frac{t_+^2 - t_-^2 + it\varepsilon_0}{tt_+}. \quad (4.a.8)$$

This allows us to compute the transmission coefficient⁸

$$\mathcal{T} = \frac{|S|^2}{|A|^2} = \frac{4t_-^2 t_+^2}{\left\{ (t_+^2 + t_-^2)^2 + \varepsilon_0^2 t^2 \right\}}. \quad (4.a.9)$$

In the limit where t_{\pm} and ε_0 are much less than t , then we see that

$$\begin{aligned} 1 - \mathcal{T} &= \frac{1}{\left\{ (t_+^2 + t_-^2)^2 + \varepsilon_0^2 t^2 \right\}} \left\{ (t_+^2 + t_-^2)^2 + \varepsilon_0^2 t^2 - 4t_-^2 t_+^2 \right\}, \\ &= \frac{\left\{ (t_+^2 - t_-^2)^2 + \varepsilon_0^2 t^2 \right\}}{\left\{ (t_+^2 + t_-^2)^2 + \varepsilon_0^2 t^2 \right\}}, \\ &= \frac{t^2 \left\{ \frac{(t_+^2 - t_-^2)^2}{t^2} + \varepsilon_0^2 \right\}}{t^2 \left\{ \frac{(t_+^2 + t_-^2)^2}{t^2} + \varepsilon_0^2 \right\}}, \\ &= \left(1 + \frac{(t_+^2 - t_-^2)^2}{\varepsilon_0^2 t^2} \right) \left(1 - \frac{(t_+^2 + t_-^2)^2}{\varepsilon_0^2 t^2} + \frac{(t_+^2 + t_-^2)^4}{\varepsilon_0^4 t^4} + \dots \right), \\ &= 1 - \frac{4t_+^2 t_-^2}{\varepsilon_0^2 t^2} + \frac{4t_+^2 t_-^2 (t_+^2 + t_-^2)^2}{\varepsilon_0^4 t^4} + \dots, \\ &= 1 - \frac{4t_+^2 t_-^2}{\varepsilon_0^2 t^2} \left\{ 1 - \left(\frac{t_+^2 + t_-^2}{\varepsilon_0 t} \right)^2 + \left(\frac{t_+^2 + t_-^2}{\varepsilon_0 t} \right)^4 - \dots \right\}. \end{aligned}$$

Therefore we see that as t_{\pm}, ε_0 are taken to be small, $\mathcal{T} \rightarrow 0$.

⁸We are using sloppy notation: if we want to allow t_{\pm} , etc. to be complex, then the terms in the expression for \mathcal{T} must be interpreted as their modulus.

PHYSICS 525, CONDENSED MATTER

Homework 5

Due Tuesday, 7th November 2006

JACOB LEWIS BOURJAILY

Problem 1: Phonon Spectrum of a Diatomic One-Dimensional Crystal

Consider a one-dimensional, diatomic crystal composed of atoms of mass M_1 and M_2 , respectively. We may suppose that the interaction between nearest neighbours is a simple harmonic spring with a universal spring constant K .

a. We are to determine the full phonon spectrum of this system and sketch the dispersions $\omega(q)$.

Let a denote the lattice spacing of the Bravais lattice, and let us label the displacement functions u_1 and u_2 for the atoms with mass M_1 and M_2 , respectively. Then the harmonic contribution to the potential is given by

$$U_h = \frac{K}{2} \sum_n \left\{ \left(u_1(na) - u_2(na) \right)^2 + \left(u_2(na) - u_1((n+1)a) \right)^2 \right\}. \quad (1.a.1)$$

This immediately implies the following equations of motion:

$$M_1 \ddot{u}_1(na) = -\frac{\partial U_h}{\partial u_1(na)} = -K \left\{ 2u_1(na) - u_2(na) - u_2((n-1)a) \right\}; \quad (1.a.2)$$

$$M_2 \ddot{u}_2(na) = -\frac{\partial U_h}{\partial u_2(na)} = -K \left\{ 2u_2(na) - u_1(na) - u_1((n+1)a) \right\}. \quad (1.a.3)$$

We seek phonon solutions to these equations of motion, which have the structure of plane waves:

$$u_1(na) = \alpha e^{i(kna - \omega t)} \quad \text{and} \quad u_2(na) = \beta e^{i(kna - \omega t)}. \quad (1.a.4)$$

Inserting these test functions into the equations of motion and simplifying a bit, we find the following (independent of n),

$$M_1 \omega^2 \alpha = 2K\alpha - K(1 + e^{-ika})\beta; \quad (1.a.5)$$

$$M_2 \omega^2 \beta = 2K\beta - K(1 + e^{ika})\alpha. \quad (1.a.6)$$

This is of course equivalent to the eigenvalue equation

$$\begin{pmatrix} M_1 \omega^2 - 2K & K(1 + e^{-ika}) \\ K(1 + e^{ika}) & M_2 \omega^2 - 2K \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0, \quad (1.a.7)$$

which only has a solution if the determinant of the operator vanishes. Writing out the determinant and solving the quadratic equation for ω^2 , we find that this implies

$$\begin{aligned} \omega^2 &= K \frac{(M_1 + M_2)}{M_1 M_2} \pm \frac{1}{2} \left\{ 4K^2 \frac{(M_1 + M_2)^2}{M_1^2 M_2^2} - 8 \frac{K^2}{M_1 M_2} (1 - \cos(ka)) \right\}^{1/2}, \\ &= K \frac{M_1 + M_2}{M_1 M_2} \pm K \frac{M_1 + M_2}{M_1 M_2} \left\{ 1 - 2 \frac{M_1 M_2}{(M_1 + M_2)^2} (1 - \cos(ka)) \right\}^{1/2}; \\ \therefore \omega^2 &= \frac{K}{\mu} \left\{ 1 \pm \sqrt{1 - 4 \frac{\mu}{(M_1 + M_2)} \sin^2 \left(\frac{ka}{2} \right)} \right\}, \end{aligned} \quad (1.a.8)$$

where we have introduced the *reduced mass*: $\mu \equiv \frac{M_1 M_2}{M_1 + M_2}$.

This phonon dispersion relation is plotted in Figure 1.

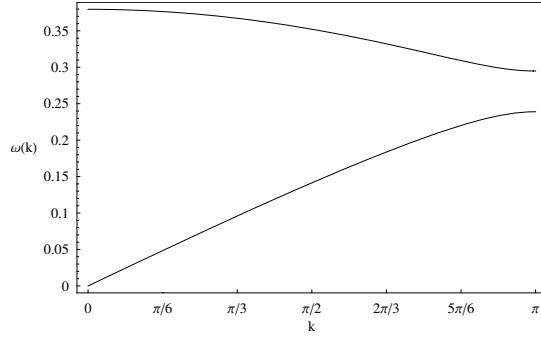


FIGURE 1. The phonon dispersion for a diatomic, one-dimensional crystal. The lower band represents acoustic mode and the upper band represents optical mode.

b. We are to describe the atomic motion associated with optical and acoustic phonons near the centre and edge of the first Brillouin zone.

Near the centre of the Brillouin zone $k \ll \pi/a$, so we may expand $\sin(ka/2) \approx (ka/2) + \mathcal{O}((ka/2)^3)$. Also Taylor expanding the square-root in equation (1.a.8), we obtain

$$\omega^2 = \frac{K}{\mu} \left\{ 1 \pm \left(1 - \frac{\mu}{2(M_1 + M_2)} (ka)^2 - \dots \right) \right\}; \quad (1.b.9)$$

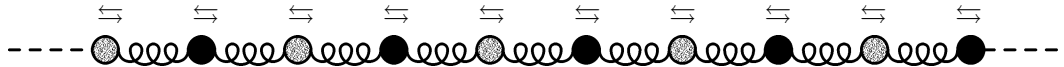
which implies

$$\omega = \begin{cases} \sqrt{\frac{K}{2(M_1 + M_2)}} (ka) + \mathcal{O}(ka)^2 & \text{acoustic} \\ \sqrt{\frac{2K(M_1 + M_2)}{M_1 M_2}} + \mathcal{O}(ka)^2 & \text{optical} \end{cases}. \quad (1.b.10)$$

If we plug this back into the eigenvalue equation (1.a.7), we find for the acoustic mode,

$$\begin{aligned} \frac{\beta}{\alpha} &= \frac{K(2 + ika + \mathcal{O}(ka)^2)}{2K^2 \left(2 - \frac{(ka)^2}{2} + \mathcal{O}(ka)^4 \right)} \left(2K - \frac{K}{2} \frac{M_2 (ka)^2}{M_1 + M_2} + \mathcal{O}(ka)^4 \right), \\ &= 1 + \mathcal{O}(ak). \end{aligned}$$

Therefore, the acoustic mode is that for which the two types of atoms are oscillating in phase:



Similarly, looking at the expansion for the optical phonons, we find

$$\begin{aligned} \frac{\beta}{\alpha} &= \frac{K(2 - ika + \mathcal{O}(ka)^2)}{2K^2 \left(2 - \frac{(ka)^2}{2} + \mathcal{O}(ka)^4 \right)} \left(2K - 2K \frac{M_1 + M_2}{M_2} + \mathcal{O}(ka)^4 \right), \\ &= -\frac{M_1}{M_2} + \mathcal{O}(ak). \end{aligned}$$

This implies that the optical phonons near low crystal momentum (modulo the reciprocal lattice) are excitations where the two types of atoms oscillate in opposite phase:



Let us now return to equation (1.a.8), only this time keeping track of M_1 and M_2 . Near the edge of the Brillouin zone, $k = \pi/a - \delta$, we may expand $\sin^2(\pi/2 - \delta a/2) =$

$1 - (\delta a)^2/4 + \mathcal{O}(\delta a)^4$. Using this, we have

$$\begin{aligned}\omega^2 &= \frac{K(M_1 + M_2)}{M_1 M_2} \left\{ 1 \pm \sqrt{1 - 4 \frac{M_1 M_2}{(M_1 + M_2)^2} \sin^2 \left(\frac{\pi}{2} - \frac{\delta a}{2} \right)} \right\}, \\ &= \frac{K(M_1 + M_2)}{M_1 M_2} \left\{ 1 \pm \sqrt{1 - 4 \frac{M_1 M_2}{(M_1 + M_2)^2} + \frac{M_1 M_2}{(M_1 + M_2)^2} (\delta a)^2 + \mathcal{O}(\delta a)^4} \right\}, \\ &= \frac{K(M_1 + M_2)}{M_1 M_2} \left\{ 1 \pm \sqrt{\frac{(M_1 - M_2)^2}{(M_1 + M_2)^2} + \frac{M_1 M_2}{(M_1 + M_2)^2} (\delta a)^2 + \mathcal{O}(\delta a)^4} \right\}, \\ &= \frac{K(M_1 + M_2)}{M_1 M_2} \left\{ 1 \pm \frac{|M_1 - M_2|}{M_1 + M_2} \sqrt{1 + \frac{M_1 M_2}{(M_1 - M_2)^2} (\delta a)^2 + \mathcal{O}(\delta a)^4} \right\}.\end{aligned}$$

Now, without loss of generality we may suppose that $M_1 > M_2$, in which case this reduces to

$$\omega = \begin{cases} \sqrt{\frac{K}{M_1}} + \mathcal{O}(ka)^2 & \text{acoustic} \\ \sqrt{\frac{K}{M_2}} + \mathcal{O}(ka)^2 & \text{optical} \end{cases}. \quad (1.b.11)$$

Notice that in this case, the matrix in equation (1.a.7) becomes diagonal, so there is no constraint on β/α . Rather, modes with momenta near the edge of the first Brillouin zone correspond to bulk-modes of lattice of M_1 atoms and the lattice of M_2 atoms oscillating independently of each-other.

c. We are to consider the concrete example of a one-dimensional NaCl lattice, for which it is observed that the highest energy optical phonon is 30 meV. We are to determine the spring constant K in reasonable atomic-physics units, and determine the minimum energy that an incoming neutron must possess to excite all phonons at all crystal momenta.

From our work above we know that the highest energy phonon in the spectrum occurs at zero-crystal momentum, in the optical band¹. This was derived explicitly in equation (1.b.10). Therefore, we know that

$$E_{ph_{\max}} = \hbar\omega_{\max} = \hbar\sqrt{\frac{2K(M_1 + M_2)}{M_1 M_2}} \implies K = \frac{E_{ph_{\max}}^2 M_1 M_2}{\hbar^2 2(M_1 + M_2)}. \quad (1.c.12)$$

Using the fact that $\omega_{\max}\hbar = 30$ meV, and plugging in real numbers (with units!), we see that this gives

$$\therefore K = 1.5 \text{ eV } \text{\AA}^{-2}. \quad (1.c.13)$$

When considering a neutron inelastic scattering process, there are two constraints that must be satisfied: first, the difference between the initial and final neutron momenta must be a reciprocal lattice vector; and second, the phonon energy must equal the difference between the initial and final neutron energies. Specifically, these are²

$$p_i - p_f = n\hbar\frac{2\pi}{a} \quad \text{and} \quad E_{ph} = \frac{(p_i^2 - p_f^2)}{2m_n}. \quad (1.c.14)$$

We can combine these two equations by noting $(p_i^2 - p_f^2) = (p_i + p_f)(p_i - p_f) = (p_i + p_f)n\hbar\frac{2\pi}{a}$ to arrive at the suggestive pair of equations

$$p_i - p_f = n\frac{\hbar}{a} \quad \text{and} \quad p_i + p_f = \frac{2E_{ph}m_n a}{n\hbar}; \quad (1.c.15)$$

$$\therefore p_i = \frac{\alpha}{n} + \beta n \quad \text{where} \quad \alpha = \frac{E_{ph}m_n a}{\hbar} \quad \text{and} \quad \beta = \frac{\hbar}{2a}. \quad (1.c.16)$$

We must find the n for which p_i is minimized for the maximum phonon energy of 30 meV.

Numerically, β is about an order of magnitude larger than α , so this happens when n is small; in fact, it is minimized at $n = 3$, which gives $E_{\text{neutron}} = 30.51$ meV.

¹It may not be obvious that the global maximum occurs at zero crystal momentum in the optical band—for the one-dimensional crystal under consideration—but it turns out to be so.

²The lattice spacing for NaCl crystals is known to be $a = 5.64$ \AA.

Problem 2: Bound States of Phonons Near an Impurity (One-Dimension)

Consider a one-dimensional crystal composed almost entirely of atoms with mass M , but with one impurity atom of mass M' . We may approximate the interactions as nearest-neighbour harmonic potentials with a (universal) spring constant K . We are asked to explore the localized phonon modes that can possibly arise in this situation.

a. Let us determine the range of M' for which localized phonon modes exist.

Our intuition from Quantum Mechanics strongly hints that localized modes exist only if $M' < M$: this is because the potential energy should be lower there, giving rise to a potential well in which phonons could be entrapped. Alternatively, when $M' = M$, we know there are no localized modes because the situation is identical to a one-dimensional crystal; but when $M' < M$ wave amplitudes are locally piqued at M' so we expect localized modes. Enough intuition, let us show that our intuition isn't misguided.

The initial set-up is sufficiently similar to the previous problem (and sufficiently canonical) that we may appear brief. Given the Hooke's law harmonic potential, we can immediately write down the equations of motion for the system:

$$M\ddot{u}_{na} = -K(2u_{na} - u_{(n+1)a} - u_{(n-1)a}) \quad \forall n \neq 0 \quad \text{and} \quad M'\ddot{u}_0 = -K(2u_0 - u_a - u_{-a}). \quad (2.a.1)$$

Because we are interested in phonon modes which are localized at $n = 0$, we will try the following test functions

$$u_{n>0} = e^{-\lambda an} e^{i(kan - \omega t)} \equiv \tilde{u}_{n>0} e^{-i\omega t} \quad \text{and} \quad u_{n<0} = e^{\lambda an} e^{i(kan - \omega t)} \equiv \tilde{u}_{n<0} e^{-i\omega t}, \quad (2.a.2)$$

where $\lambda > 0$; we will use our equations of motion (2.a.1) to determine \tilde{u}_0 .

Inserting our test functions into the equations of motion, we find that virtually all of the system of equations collapses in redundancy, leaving us with

$$n \geq 2 \quad M\omega^2 = K(2 - e^{-\lambda a} e^{ika} - e^{\lambda a} e^{-ika}); \quad (2.a.3)$$

$$n = 1 \quad M\omega^2 = K(2 - e^{-\lambda a} e^{ika} - \tilde{u}_0 e^{\lambda a} e^{-ika}); \quad (2.a.4)$$

$$n = 0 \quad M'\omega^2 = K(2\tilde{u}_0 - e^{-\lambda a} e^{ika} - e^{-\lambda a} e^{-ika}); \quad (2.a.5)$$

$$n = -1 \quad M\omega^2 = K(2 - e^{-\lambda a} e^{-ika} - \tilde{u}_0 e^{\lambda a} e^{ika}); \quad (2.a.6)$$

$$n \leq -2 \quad M\omega^2 = K(2 - e^{-\lambda a} e^{-ika} - e^{\lambda a} e^{ika}). \quad (2.a.7)$$

Subtracting equation (2.a.7) from equation (2.a.3) we see that

$$e^{-\lambda a} (e^{-ika} - e^{ika}) + e^{\lambda a} (e^{ika} - e^{-ika}) = 4i \sin(ka) \sinh(\lambda a) = 0.$$

This implies that either $\lambda = 0$ —which would run contrary to our analysis: we are interested in the case when $\lambda > 0$ —or that $ka = m\pi$ for some $m \in \mathbb{Z}$. Actually, we have no need to keep this level of generality: it is $e^{\pm ika}$ that appears throughout our equations of motion, and this leaves only two possibilities: $e^{i2\pi} = e^{-i2\pi} = 1$ or $e^{i\pi} = e^{-i\pi} = -1$; labelling these possibilities as \pm , respectively, equation (2.a.3) becomes

$$M\omega^2 = 2K(1 \mp \cosh(\lambda a)). \quad (2.a.8)$$

Now, $\cosh(\lambda a) > 1$ if $\lambda > 0$. Because this would lead to negative ω^2 for the ‘-’ case above—corresponding to $ka = 2m\pi$ —we must exclude this as a possibility, leaving only $e^{ika} = e^{-ika} = -1$. Which allows us to conclude³

$$\therefore \omega = 2\sqrt{\frac{K}{M}} \cosh\left(\frac{\lambda a}{2}\right). \quad (2.a.9)$$

Inserting our expression for ω^2 into equation (2.a.4) we see that

$$\begin{aligned} 2(1 + \cosh(\lambda a)) &= 2 + e^{-\lambda a} + \tilde{u}_0 e^{\lambda a}; \\ \implies e^{-\lambda a} + e^{\lambda a} &= e^{-\lambda a} + \tilde{u}_0 e^{\lambda a}, \end{aligned}$$

³We made use of the hyperbolic identity $1 + \cosh(\xi) = 2 \cosh^2(\xi/2)$.

which of course implies that $\tilde{u}_0 = 1$. It is not hard to see that the only independent equation left for us to consider is (2.a.5). Let us see what this equation implies about M'/M .

$$\begin{aligned}
 M'\omega^2 &= K(2 + e^{-\lambda a} + e^{-\lambda a}), \\
 \implies 4K \frac{M'}{M} \cosh^2\left(\frac{\lambda a}{2}\right) &= 2K(1 + e^{-\lambda a}), \\
 \implies \frac{M'}{M} &= \frac{1 + e^{-\lambda a}}{2 \cosh^2\left(\frac{\lambda a}{2}\right)}, \\
 &= e^{-\lambda a/2} \frac{2 \cosh\left(\frac{\lambda a}{2}\right)}{2 \cosh^2\left(\frac{\lambda a}{2}\right)}, \\
 \therefore \frac{M'}{M} &= \frac{e^{-\lambda a/2}}{\cosh\left(\frac{\lambda a}{2}\right)}. \tag{2.a.10}
 \end{aligned}$$

Now, because the expression on the right hand side of (2.a.10) is strongly bounded above by 1—and is equal to one iff $\lambda = 0$ —we may conclude that localized phonon modes exist only if

$$\frac{M'}{M} < 1. \tag{2.a.11}$$

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b. We are to give explicit solutions for the frequency and displacement patterns of this localized mode and describe what happens as $M' \rightarrow M$.

Perhaps the first thing we should do is revisit equation (2.a.10) and give λ as a function of $\eta \equiv \frac{M'}{M}$. A little bit of manipulation shows that

$$\eta = \frac{2}{e^{\lambda a} + 1}, \tag{2.b.12}$$

which of course implies that

$$e^{\lambda a} = \frac{2 - \eta}{\eta} = \frac{2M - M'}{M'}. \tag{2.b.13}$$

This equation allows us to tidy up much of our previous work. For example, equation (2.a.9) can be combined with (2.a.10) using our work above,

$$\therefore \omega = 2\sqrt{\frac{KM}{M'(2M - M')}}. \tag{2.b.14}$$

We can put everything together and now give all the functions u_n at once:

$$u_{na} = \left(\frac{M'}{2M - M'}\right)^{|n|} e^{i(kan - \omega t)}. \tag{2.b.15}$$

Now, looking at these plane waves (2.b.15) and the dispersion relation (2.b.14), we see that when $M' \rightarrow M$ the ‘suppression’ term in (2.b.15) becomes 1, and the dispersion relation matches onto the solution for normal phonons in one-dimension—i.e. there are no localized modes when $M' = M$.

Problem 3: Wigner Crystals in Various Dimensions

At low temperatures and densities, electrons in an ideal semiconductor ‘crystallize’ into what is known as a Wigner crystal. This can be modelled as a crystal of electrons in a uniform background of stationary, neutralizing positive charges, where only the electrons are able to move. The long-range Coulomb repulsion between the electrons can affect the long-wavelength longitudinal acoustic phonons. We are to determine the parametric low- q behaviour of this mode (called a ‘plasmon’) in one-, two-, and three-dimensional Wigner crystals.

In order to determine the dispersion of plasmons, we will use the harmonic approximation for the Coulomb interaction potential⁴; for dimensions higher than one, we will have need to recall some elementary multi-dimensional calculus—namely, the generalization of Taylor’s theorem to higher dimensions,

$$f(\vec{r} - \vec{a}) = f(\vec{r}) + \vec{a} \cdot \vec{\nabla} f(\vec{r}) + \frac{1}{2} (\vec{a} \cdot \vec{\nabla})^2 f(\vec{r}) + \dots, \quad (3.a.1)$$

for any scalar function $f(\vec{r})$. Because the scalar function we are interested in is radial, it will be helpful to recall the expression for the gradient in polar and spherical coordinates in two- and three-dimensions respectively.

In one-dimension the situation is rather more elementary—there are at least no angles to worry us. Let us suppose that at zero temperature, the electrons are spaced a distance 1 apart (in appropriate units)⁵—so that the electrons are located at $r = n$ for $n \in \mathbb{Z}$. Then the equilibrium Coulomb-potential energy at the point $r = 0$ is simply

$$\varphi_{eq}(0) = -e^2 \sum_{r \neq 0} \frac{1}{|r|} = -2e^2 \sum_{r > 0} \frac{1}{r}. \quad (3.a.2)$$

It is this potential that we will Taylor-expand for the plasmon perturbations. Now, let us label the displacement from equilibrium of electron n from the point r as u_n . Then the actual potential energy at the site of the electron labeled 0—which is now located at u_0 —is given by

$$\varphi(u_0) = -e^2 \sum_{r \neq 0} \left\{ \frac{1}{|r|} - (u_r - u_0) \frac{1}{r^2} + \frac{1}{2} (u_r - u_0)^2 \frac{1}{|r|^3} - \dots \right\}. \quad (3.a.3)$$

Assuming that the values $u_r = 0$ are equilibrium, then the first term in (3.a.3) is a constant and the second term vanishes. It is the third term—the ‘harmonic’ term—that we are interested in:

$$\varphi_h(u_0) = -\frac{e^2}{2} \sum_{r=1}^{\infty} \frac{1}{r^3} \left\{ (u_r - u_0)^2 + (u_{-r} - u_0)^2 \right\}. \quad (3.a.4)$$

The equations of motion are relatively simple; for u_0 , they give

$$m\ddot{u}_0 = -\frac{\partial \varphi_h(u_0)}{\partial u_0} = e \sum_{r=1}^{\infty} \frac{1}{r^3} \left\{ 2u_0 - (u_r + u_{-r}) \right\}. \quad (3.a.5)$$

We are looking for plasmon solutions. These are

$$u_r = e^{i(kr - \omega t)}$$

where q is the momentum. Putting this into the equations of motion, we have

$$\frac{m}{e^2} \omega^2 = 2 \sum_{r=1}^{\infty} \frac{1}{r^3} (1 - \cos(kr)) \quad \implies \quad \omega^2 \propto \sum_{r=1}^{\infty} \frac{1}{r^3} \sin^2 \left(\frac{kr}{2} \right). \quad (3.a.6)$$

⁴This is actually a bit more subtle than it may seem at first: the leading order Coulomb interaction potential is a ‘strong’ effect. By taking the harmonic approximation, we are implicitly assuming that the leading Coulomb term (which is highly divergent in all dimensions—at least for infinite crystals) is completely neutralized by the positive charges; or, put another way, we ignore the machinery by which the electron system finds itself in an equilibrium distribution. Then, only the electron Coulomb interaction energy is considered as the sub-leading part of the potential. We will find that this is fine in each dimension under consideration—because it will dominate $\omega \sim cq$ in the limit of $q \rightarrow 0$ —but this was by no means obvious.

⁵Because we are only interested in the parametric q -dependence of ω , there is no reason to bother about units.

In the limit where $k \rightarrow 0$, this sum is well-approximated as an integral,

$$\omega^2 \sim \int_1^\infty dr \frac{\sin^2\left(\frac{kr}{2}\right)}{r^3}. \quad (3.a.7)$$

Now, there are two obvious regions of interest: first, if $r \lesssim 2/k$, then $\sin^2(kr/2)$ can be well-approximated by its leading Taylor expansion. When $r \gg 2/k$, the integrand is rapidly oscillating and can be well-approximated by the average value of $\sin^2(x)$ which is $\frac{1}{2}$. That is

$$\omega^2 \sim \int_1^{2/k} dr \frac{1}{r^3} \sin^2\left(\frac{kr}{2}\right) + \int_{2/k}^\infty dr \frac{1}{r^3} \sin^2\left(\frac{kr}{2}\right), \quad (3.a.8)$$

$$\sim \int_1^{2/k} dr \frac{k^2}{4r} + \int_{2/k}^\infty dr \frac{1}{2r^3}, \quad (3.a.9)$$

$$= \frac{1}{4}k^2 \log\left(\frac{2}{k}\right) - \frac{1}{16}k^2. \quad (3.a.10)$$

Now, the leading term (divergently) dominates as $k \rightarrow 0$ (and the other terms will not dominate other $\omega \sim ck$ phonons anyway), so we see that in one-dimension, Wigner-crystal plasmons have a low-momentum dispersion

$$\therefore \omega \underset{k \rightarrow 0}{\sim} k\sqrt{-\log(k)}. \quad (3.a.11)$$

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To generalize the work above requires keeping track of coordinate systems, indices, &c.

In two dimensions, we would like to use polar coordinates for the potential (because the Coulomb potential is radial), but label the points by their Cartesian coordinates. Specifically, let us denote the equilibrium locations of the electrons as \mathbf{r}_i . In two-dimensions, we will use polar coordinates (ρ, θ) to expand the potential. Doing this, we find that⁶

$$\begin{aligned} \varphi_h(u_{\vec{0}}) = & -\frac{e^2}{2} \sum_{r_x, r_y=1}^\infty \frac{1}{\rho^3} \left\{ (u_{r_x+r_y} - u_{\vec{0}})_\rho^2 + (u_{r_x-r_y} - u_{\vec{0}})_\rho^2 + (u_{-r_x+r_y} - u_{\vec{0}})_\rho^2 + (u_{-r_x-r_y} - u_{\vec{0}})_\rho^2 \right\} \\ & - \frac{e^2}{2} \sum_{r_x=1}^\infty \frac{1}{r_x^3} \left\{ (u_{r_x+0\hat{y}} - u_{\vec{0}})_x^2 + (u_{-r_x+0\hat{y}} - u_{\vec{0}})_x^2 \right\} - \frac{e^2}{2} \sum_{r_y=1}^\infty \frac{1}{r_y^3} \left\{ (u_{0\hat{x}+r_y} - u_{\vec{0}})_y^2 + (u_{0\hat{x}-r_y} - u_{\vec{0}})_y^2 \right\}, \end{aligned} \quad (3.b.1)$$

where $\rho = (r_x^2 + r_y^2)^{1/2}$. The last two terms in this expression grow only linearly with N , the number of electrons in one direction, whereas the first term grows like N^2 ; i.e. both terms in the second line of equation (3.b.1) are of measure zero in two-dimensions⁷. Therefore, it is consistent to simply ignore these contributions when taking the large- N -limit—when we will replace the sums in equation (3.b.1) by integrals over the plane.

As before, we are interested in plasmons which are longitudinal plane-waves,

$$\vec{u}_{r_x+r_y} = \hat{x} e^{i(kr_x - \omega t)}, \quad (3.b.2)$$

where we have used the longitudinality of the wave, $\vec{k} = k\hat{x}$. Inserting this test function into equation (3.b.1) we obtain the equations of motion

$$m\omega^2 = 4e^2 \sum_{r_x, r_y=1}^\infty \frac{1}{\rho^3} \left\{ 1 - \cos(kr_x) \right\} \rightarrow 8e^2 \int_0^{\pi/2} d\theta \int_1^\infty \frac{d\rho}{\rho^2} \sin^2\left(\frac{kr_x}{2}\right). \quad (3.b.3)$$

⁶The displacement functions u are of course vector quantities. The subscript ‘ ρ ’ appearing in the expression is to indicate that it is only the ρ -component of the vector-difference that is considered. This comes about because $\vec{a} \cdot \vec{\nabla} = a_\rho \frac{\partial}{\partial r} + \frac{a_\theta}{\rho} \frac{\partial}{\partial \theta}$ and the second term’s contribution vanishes when acting on a radial function.

⁷This could be a point of confusion—if it were not for the fact that the sums along the x - and y -axes gave no contribution (are of measure zero in two-dimensions) then we would of course find the one-dimensional result for this one-dimensional subsystem of the crystal. It can be checked explicitly that this term is subleading in N —but the skeptical reader should also bear in mind that k is bounded below by $1/N$.

Noting that $r_x = \rho \sin \theta$ in polar coordinates and approximating $\sin^2(x)$ by its Taylor expansion for small argument and by its average (which is $1/2$) for large argument, we see that parametrically,

$$\begin{aligned}\omega^2 &\sim \int_0^{\pi/2} d\theta \int_1^\infty \frac{d\rho}{\rho^2} \sin^2\left(\frac{k\rho \cos \theta}{2}\right), \\ &\sim \int_0^{\pi/2} d\theta \left\{ \int_1^{2/(k \cos \theta)} d\rho k^2 \cos^2(\theta) + \frac{1}{2} \int_{2/(k \cos \theta)}^\infty d\rho \frac{1}{\rho^2} \right\}, \\ &\propto \int_0^{\pi/2} d\theta \{3k \cos \theta - k^2 \cos^2 \theta\}, \\ &= 3k - \frac{\pi}{4} k^2.\end{aligned}$$

The linear term obviously dominates in the limit of $k \rightarrow 0$, in which we are interested. Therefore, we see that in two-dimensions the plasmon dispersion is parameterically given by

$$\therefore \omega \underset{k \rightarrow 0}{\sim} \sqrt{k}. \quad (3.b.4)$$

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Lastly, let us turn our attention to the case in three-dimensions. Like in the two-dimensional case, we must be mindful of coordinates. We will again choose to label the equilibrium positions⁸ by their Cartesian coordinates $\vec{r} = r_x \hat{x} + r_y \hat{y} + r_z \hat{z}$, but we will express the potential in spherical coordinates (ρ, θ, φ) . In the limit of large N , the leading contribution to the potential at $u_{\vec{0}}$ ⁹

$$\begin{aligned}\varphi(u_{\vec{0}}) &= -\frac{e^2}{2} \sum_{r_x, r_y, r_z=1}^N \frac{1}{\rho^3} \left\{ (u_{r_x+r_y+r_z} - u_{\vec{0}})^2 + (u_{r_x+r_y-r_z} - u_{\vec{0}})^2 + (u_{r_x-r_y+r_z} - u_{\vec{0}})^2 + (u_{-r_x+r_y+r_z} - u_{\vec{0}})^2 \right. \\ &\quad \left. + (u_{r_x-r_y-r_z} - u_{\vec{0}})^2 + (u_{-r_x+r_y-r_z} - u_{\vec{0}})^2 + (u_{-r_x-r_y+r_z} - u_{\vec{0}})^2 + (u_{-r_x-r_y-r_z} - u_{\vec{0}})^2 \right\}.\end{aligned} \quad (3.c.1)$$

The contributions that we are ignoring here are those from electrons in the planes normal to each of the coordinate axes. As argued before, these contribute nothing—‘are regions of measure zero’—in three-dimensions.

Taking a longitudinal plasmon aligned in the z -direction as our test function,

$$\vec{u}_{r_x+r_y+r_z} = \hat{z} e^{i(kr_z - \omega t)} \quad \text{where} \quad \vec{k} = k \hat{z}, \quad (3.c.2)$$

we find the equations of motion to be

$$m\omega^2 = 8e^2 \sum_{r_x, r_y, r_z=1}^N \frac{1}{\rho^3} \{1 - \cos(kr_z)\} \rightarrow 16e^2 \int_0^{\pi/2} d\varphi \int_1^N d\rho \int_0^1 d \cos \theta \frac{1}{\rho} \sin^2\left(\frac{k\rho \cos \theta}{2}\right). \quad (3.c.3)$$

Notice that we’ve chosen to keep the range of the ρ integration explicit. This will come in handy later. Now, instead of doing the ρ integration first, notice that that we can exactly evaluate the angular integrals and greatly simplify the situation.

⁸We assume here, as before, a cubical lattice. This assumption is probably not accurate physically, but there are reasons to suspect that the parametric dispersions for small crystal momentum should be independent of the type of lattice.

⁹As before, the displacement $u_{\vec{r}}$ is obviously a vectorial quantity. However, for the sake of convenience—and using the foresight that we will consider plane waves for which $u_{\vec{r}}$ only has a component in the radial-direction—we will not write the vector label over $u_{\vec{r}}$. Lastly, the ‘ ρ ’ subscripts that appeared in equation (3.b.1) will be implicit in the expressions to follow.

Specifically,

$$\begin{aligned}
\omega^2 &= \frac{16e^2}{m} \int_0^{\pi/2} d\varphi \int_1^N d\rho \int_0^1 d\cos\theta \frac{1}{\rho} \sin^2\left(\frac{k\rho\cos\theta}{2}\right), \\
&= \frac{8\pi e^2}{m} \int_1^N d\rho \int_0^{k\rho/2} d\xi \frac{2}{k\rho^2} \sin^2(\xi), \\
&= \frac{8\pi e^2}{m} \int_1^N d\rho \frac{1}{k\rho^2} \left(\xi - \sin(\xi)\cos(\xi)\right)\Big|_0^{k\rho/2}, \\
&= \frac{4\pi e^2}{m} \int_1^N d\rho \frac{1}{k\rho^2} (k\rho - \sin(k\rho)), \\
&= \frac{4\pi e^2}{m} \int_k^{Nk} \frac{d\alpha}{\alpha^2} (\alpha - \sin(\alpha));
\end{aligned}$$

Here, attention to detail has paid off: the minimum (non-vanishing) crystal momentum is $k = 1/N$ so that in the limit of low crystal momentum and infinite Wigner crystal, $kN \rightarrow 1$. This means that for the entire range of integration, $\alpha \leq 1$ and we can effectively approximate the integrand by Taylor-expanding $\sin(\alpha)$. This gives

$$\begin{aligned}
\omega^2 &= \frac{2\pi e^2}{3m} \int_k^1 d\alpha \left(\alpha - \frac{\alpha^3}{20} + \frac{\alpha^5}{840} - \dots\right), \\
&= \frac{4\pi e^2}{m} \left(\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{(2n+1)!} \frac{1 - k^{2n}}{2n}\right),
\end{aligned}$$

Having come this far, we would have really like to have a closed-form expression for the constant part, but we haven't found one. To better than one part in a thousand, the constant term is

$$\omega^2 \approx \frac{983\pi e^2}{7 \cdot 3^3 \cdot 2^4 m} + k^2 \frac{\pi e^2}{3m} + \mathcal{O}(k^4). \quad (3.c.4)$$

To an accuracy of about 2%, the constant term is just $\frac{e^2}{m}$. At any rate, the important point is that as $k \rightarrow 0$, $\omega \rightarrow \text{constant}$. That is

$$\therefore \omega \underset{k \rightarrow 0}{\sim} \frac{e}{\sqrt{m}}. \quad (3.c.5)$$

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PHYSICS 525, CONDENSED MATTER

Homework 6

Due Tuesday, 21st November 2006

JACOB LEWIS BOURJAILY

Problem 1: Thermal Expansion of a One-Dimensional Crystal via Anharmonicities

Consider a simple one-dimensional crystal lattice with nearest-neighbour interaction potential

$$\varphi(y) = \frac{K}{2}y^2 - gy^3, \quad (1.1)$$

where $y = x_{i+1} - x_i - a_0$ and g is small; a is the lattice spacing. For $g = 0$ and at zero external pressure the lattice spacing $a = a_0$ and the probability distribution of y due to zero-point thermal phonons is Gaussian with root-mean-square $\sigma(T)$ at temperature T ; we are to treat $\sigma(T)$ as a known function.

By perturbatively adding the effects of the cubic anharmonicity, we are to determine the equilibrium lattice spacing a to leading order in g . We should use this to express the thermal expansion coefficient in terms of the specific heat at $g = 0$ and other parameters in the problem. We should estimate the magnitude of g for which this approximation is valid.

A lot of physics intuition leads us to expect that to leading order in g the equilibrium anharmonic lattice can be viewed as a harmonic system with modified equilibrium displacements¹. The heuristic picture we have in mind is this: if g is turned on slowly, the lattice spacing may change reaching some new equilibrium value; but the fluctuations about this new lattice spacing should still be roughly Gaussian—and the widths of the distributions shouldn't know anything about g to leading order².

Because the harmonic system amounts to a collection of N independent oscillators (each with the same Gaussian normal distribution) the entropy of the system is simply the sum of the entropies of each. This has nothing to do with the lattice spacing, so if we are allowed to view the perturbed system as identical to the original system with an 'expanded' lattice spacing, then the entropy should not be changed. We expect this argument to hold to leading order in g . This implies that the entropy is independent of g to leading order—and therefore minimization of the free energy is equivalent to minimization of the energy u .

Using our reasoning above, we see that the expectation value of the total energy per lattice site u should therefore be given by³

$$\langle u \rangle = u_0 + \frac{1}{\sigma(T)\sqrt{2\pi}} \int_{-\infty}^{\infty} dy \exp\left\{-\frac{(y - \delta a)^2}{2\sigma^2(T)}\right\} \left(\frac{K}{2}y^2 - gy^3\right) + \mathcal{O}(g^2), \quad (1.2)$$

$$= u_0 + \frac{K}{2}\sigma^2(T) - 3g\sigma^2(T)\delta a + \frac{K}{2}\delta a^2 - g\delta a^3 + \mathcal{O}(g^2). \quad (1.3)$$

Notice that the expression above makes sense when $g = 0$: then equation (1.3) reads $\langle u \rangle = u_0 + \frac{K}{2}\sigma^2 = u_0 + \frac{K}{2}\langle y^2 \rangle$ when the displacement is unchanged, i.e. $\delta a = 0$ —we will show presently that $g = 0$ implies $\delta a = 0$.

To find the modified lattice spacing for non-vanishing g , we should minimize the total energy (1.3) with respect to δa . This can be done by inspection. We find

$$K\delta a - 3g\delta a^2 - 3g\sigma^2(T) = 0, \quad (1.4)$$

which implies that

$$\delta a = \frac{3g}{K}(\sigma^2 + \delta a^2) = \frac{3g}{K}\sigma^2 + \mathcal{O}(g^2). \quad (1.5)$$

To check consistency, we observe that $g = 0$ implies δa vanishes.

¹If we think in terms of Feynman diagrams, then it takes one factor of g to communicate the anharmonicity between neighbouring lattice sites, but at least two powers of g to communicate anharmonicity between two fluctuations; so to leading order in g , we expect the distributions to be offset, but otherwise unchanged.

²Note added in revisions: this is obvious from the fact that we're considering an adiabatic process.

³The 'higher order' terms in equation (1.2) arise from, e.g., non-Gaussianity in the structure of the fluctuations past leading order.

The thermal expansion coefficient is then seen to be⁴

$$\alpha \equiv \frac{1}{a_0 + \delta a} \frac{d(\delta a)}{dT} = \frac{1}{a_0} \frac{6g}{K} \sigma \frac{d\sigma}{dT} + \mathcal{O}(g^2). \quad (1.6)$$

Setting $g \rightarrow 0$ in expression (1.3) we find the original thermal heat capacity to be

$$c_v = \frac{2}{a_0} K \sigma \frac{d\sigma}{dT}. \quad (1.7)$$

Therefore, we can write the thermal expansion coefficient α as

$$\therefore \alpha = \frac{3g}{K^2} c_v + \mathcal{O}(g^2). \quad (1.8)$$

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The leading order approximation in g is valid only when the anharmonic contribution to the potential is small compared to the harmonic contribution. Inserting our expression for δa into equation (1.3) we find that our condition is⁵

$$\begin{aligned} 3g \sigma^2 \delta a + g \delta a^3 &< \frac{K}{2} (\sigma^2 + \delta a^2); \\ \implies \frac{3}{2} g \delta a \sigma^2 &< \frac{K}{2} \sigma^2; \\ \implies g &< \frac{K^2}{9g\sigma^2}; \end{aligned}$$

and therefore our approximations are appropriate as long as

$$|g| < \frac{K}{3\sigma}. \quad (1.9)$$

Problem 2: Electrons in Two-Dimensions

Consider a two-dimensional gas of electrons (confined to, say, the xy -plane) subjected to a uniform magnetic field B in the positive \hat{z} direction and a uniform electric field $\vec{E} = E\hat{x}$, giving rise to a two-dimensional potential $U(x, y) = eEx$.⁶ We may assume for the sake of convenience that the system is of large length L in the \hat{y} -direction so that we may impose periodic boundary conditions in that direction.

a. We are to find all the single-electron eigenstates and their corresponding eigenenergies.

From our experience working with gauge fields, we know that to upgrade the Schrödinger equation for a free electron to one in a non-trivial gauge potential $A_\mu = (\varphi, -\vec{A})$,^{7, 8} all we must do is upgrade $\partial_\mu \mapsto \partial_\mu + i\frac{q}{\hbar}A_\mu$ everywhere. In our setup, the scalar potential $\varphi(x, y) = -Ex$ and we will choose the Lorentz gauge for the magnetic field so $\vec{A} = Bx\hat{y}$. This means that

$$\begin{aligned} \hat{H}\psi &= i\hbar\partial_t\psi = \frac{1}{2m} \left((-i\hbar\partial_x)^2 + (-i\hbar\partial_y)^2 \right) \psi \\ \mapsto i\hbar \left(\partial_t - i\frac{e}{\hbar}(-Ex) \right) \psi &= \frac{1}{2m} \left[(-i\hbar\partial_x)^2 + \left(-i\hbar \left(\partial_y + i\frac{e}{\hbar}Bx \right) \right)^2 \right] \psi, \\ \therefore i\hbar\partial_t\psi = \hat{H}\psi &= \frac{1}{2m} \left[-\hbar^2\partial_x^2 - \hbar^2\partial_y^2 - 2i\hbar eBx\partial_y + e^2B^2x^2 \right] \psi + eEx\psi. \end{aligned} \quad (2.a.1)$$

⁴Notice that $\frac{1}{a_0 + \delta a} = \frac{1}{a_0} + \mathcal{O}(\delta a)$ —and that the part of $\mathcal{O}(\delta a)$ is over order g and so can be neglected when multiplying terms of order g .

⁵A quicker calculation, using equation (1.1), would give $g < \frac{K}{\sqrt{6}\sigma}$ which is a bit stronger than what we obtain above—but the difference is not very substantive.

⁶To avoid confusion—which is not easy to do in this problem— e will always be taken to be the absolute value of the electron's charge. This ensures that the E -field points in the positive x -direction, but it forces us to systematically alter the equations copied in lecture (where 'e' was often used to denote the charge q).

⁷We are going to set $c = 1$ to avoid lots of confusion. If at the end units are desired, there is always a unique way of adding c to the expressions.

⁸However, I am quite sure that the spatial components of A_μ come with a minus sign: this important fact comes about via the metric. Many textbooks disappointingly do not clarify how all these signs work out. (Indeed, it is a common practice of field theory textbooks to define the gauge covariant derivative of QED oppositely to all other gauge fields so that a familiar minus sign is present for the electron.)

We may suppose that ψ is separable—specifically, of the form $\psi(x, y) = \tilde{\varphi}(x)e^{-iky}$. Periodic boundary conditions of course require that $k \equiv k_n = \frac{2\pi n}{L}$ for some nonnegative integer n ⁹. Inserting this into the Schrödinger equation (2.a.1), we find that

$$\hat{H}\varphi(x) = \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{\hbar^2}{2m}k_n^2 - \frac{\hbar k_n e B x}{m} + \frac{e^2}{2m}B^2 x^2 + e E x \right] \tilde{\varphi}(x). \quad (2.a.2)$$

To make this conceptually easier, we should try as hard as we can to simplify the structure. Although not apparently obvious, it may prove useful to define the cyclotron frequency ω_c and magnetic length ℓ_B :

$$\omega_c \equiv \frac{eB}{m} \quad \text{and} \quad \ell_B^2 \equiv \frac{\hbar}{eB}. \quad (2.a.3)$$

Making use of these constants, we see that equation (2.a.2) becomes

$$\begin{aligned} \hat{H}\varphi &= \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega_c^2}{2}\ell_B^4 k_n^2 - m\omega_c^2 \ell_B^2 k_n x + \frac{m\omega_c^2}{2}x^2 + e E x \right] \tilde{\varphi}(x), \\ &= \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega_c^2}{2} \left(x - k_n \ell_B^2 + \frac{E}{B\omega_c} \right)^2 + e E \left(k_n \ell_B^2 - \frac{E}{B\omega_c} \right) + \frac{m}{2} \left(\frac{E}{B} \right)^2 \right] \tilde{\varphi}(x), \\ &= \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega_c^2}{2} (x - x_n)^2 + e E x_n + \frac{m}{2} \left(\frac{E}{B} \right)^2 \right] \tilde{\varphi}(x), \end{aligned} \quad (2.a.4)$$

where in the last line we have introduced

$$x_n \equiv k_n \ell_B^2 - \frac{E}{B\omega_c}.$$

Notice that equation (2.a.4) is the Schrödinger equation for simple harmonic oscillator with a displaced origin and a ‘lifted’ energy:

$$\hat{H}\varphi(x) = \left[-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega_c^2}{2} (x - x_n)^2 \right] \tilde{\varphi}(x) + \left[e E x_n + \frac{m}{2} \left(\frac{E}{B} \right)^2 \right] \tilde{\varphi}(x), \quad (2.a.5)$$

$$= \left(m + \frac{1}{2} \right) \hbar \omega_c + e E x_n + \frac{m}{2} \left(\frac{E}{B} \right)^2. \quad (2.a.6)$$

If we let $\varphi_m(x)$ denote the canonical simple harmonic oscillator wave function at level m , then the eigenenergies (2.a.6) correspond to eigenfunctions

$$\psi_{m,n}(x) = \varphi_m(x - x_n) e^{-ik_n y} \quad (2.a.7)$$

where m labels the Landau level and n labels the \hat{y} -momentum.

Now, the $\varphi_m(x - x_n)$ are Hermite polynomials centred at x_n . For a sample with a finite width W in the \hat{x} -direction, it should be the case that x_n lies within the sample. This implies that

$$\frac{E}{B\omega_c} < k_n \ell_B^2 < W + \frac{E}{B\omega_c}. \quad (2.a.8)$$

Because this confines k_n to a (finite) range of positive values, this agrees with our choice of signs earlier.

⁹See the discussion following equation (2.a.7) for an explanation.

b. Using the wavefunctions found above, we are to determine the total current carried by each state and compare this to the classical result for a particle undergoing cyclotron motion in perpendicular E and B fields and to the result obtained by using the semiclassical velocity $\vec{v} = \frac{1}{\hbar} \frac{d\epsilon}{dk}$.

It is rather straight-forward to compute the current of the wave functions found above.

Indeed, using equation (2.a.7) we find for the \hat{x} -component of the current¹⁰

$$\begin{aligned} \vec{j}_x &= -ev_x = -\frac{e}{m} \Re \left\{ \psi_{m,n}^* \hat{\Pi} \psi_{m,n} \right\}, \\ &= -\frac{e}{m} \Re \left\{ \varphi_m^*(x - x_n) e^{-ik_n y} (-i\hbar) \partial_x \varphi_m(x - x_n) e^{ik_n y} \right\}, \\ &= 0 \end{aligned}$$

because we can choose the simple harmonic oscillator wave functions $\varphi_m(x)$ to be real. The \hat{y} -component of the current is found similarly,

$$\vec{j}_y = -\frac{e}{m} \Re \left\{ \varphi_m^*(x - x_n) e^{ik_n y} (-i\hbar \partial_y + eBx) \varphi_m(x - x_n) e^{-ik_n y} \right\}, \quad (2.b.9)$$

$$= \frac{e}{m} (\hbar k_n - eBx) \varphi_m^2(x - x_n) \hat{y}. \quad (2.b.10)$$

Considering the range of k_n allowed, this seems to give a current in the $+\hat{y}$ -direction, as we would expect. The minimum value of $k_n > \frac{Em}{B\hbar}$.

The classical solution to crossed electric and magnetic fields is of course a cycloid. Indeed, if we consider the trajectory of an individual electron classically, we find it to be

$$x(t) = \frac{E}{\omega_c B} \left((\cos(\omega_c t) - 1), (\sin(\omega_c t) - \omega_c t) \right), \quad (2.b.11)$$

which gives rise to a net current in the positive \hat{y} -direction

$$\vec{j} = -e \langle \dot{y}(t) \rangle = \frac{E}{B} \hat{y}. \quad (2.b.12)$$

Semiclassically, we take the derivative of the energy (2.a.6) with respect to $-k_n$ to obtain

$$\vec{j} = (-e) \frac{1}{\hbar} \frac{-\hbar E}{eB} = \frac{E}{B} \hat{y}. \quad (2.b.13)$$

¹⁰Recall that the gauge-covariant momentum operator $\Pi = -i\hbar \vec{\nabla} + \frac{e}{\hbar} \vec{A}$.

PHYSICS 525, CONDENSED MATTER

Homework 7

Due Tuesday, 5th December 2006

JACOB LEWIS BOURJAILY

Problem 1: BCS Mean-Field Theory

The mean-field BCS Hamiltonian is

$$\bar{H}_{BCS} = \sum_{\mathbf{k}} \left\{ \epsilon_{\mathbf{k}} (n_{\mathbf{k},\uparrow} + n_{-\mathbf{k},\downarrow}) + c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger \Delta + \Delta^* c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \right\}. \quad (1)$$

When the mean-field ansatz was made to write the Hamiltonian in terms of the gap energy Δ , it was necessary that Δ obey the consistency-condition

$$\Delta = \frac{U}{V} \sum_{\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle, \quad (2)$$

where U is the effective attraction between unlike spins and V is the sample volume.

We are to determine all of the eigenenergies and eigenstates of this Hamiltonian, and study its properties at finite temperature. We will do this using the method introduced by Bogoliubov¹.

The key insight of Bogoliubov is that although the mean-field Hamiltonian (1) is clearly not diagonal in the space of states created by the operators $c_{\mathbf{k},\uparrow/\downarrow}^\dagger$, it may be diagonal in a basis of states created by operators related to these via a simple SU_2 transformation. Indeed, it may be the case that ‘electrons’ and ‘holes’ are the wrong degrees of freedom to consider; we should at least look to see if the Hamiltonian is simpler in terms of any collective degrees of freedom.

Along these lines, we define the rotated, ‘collective’ or ‘Bogoliubov’ creation and annihilation operators $b_{\mathbf{k},\uparrow/\downarrow}$ and $b_{\mathbf{k},\uparrow/\downarrow}^\dagger$ given by

$$\begin{aligned} b_{\mathbf{k},\uparrow} &= A_k c_{\mathbf{k},\uparrow} + B_k c_{-\mathbf{k},\downarrow}^\dagger; \\ b_{-\mathbf{k},\downarrow} &= A_k c_{-\mathbf{k},\downarrow} - B_k c_{\mathbf{k},\uparrow}^\dagger. \end{aligned} \quad (3)$$

It is clear that we desire this to be an SU_2 transformation, which implies that $|A_k|^2 + |B_k|^2 = 1$. As an SU_2 -related basis of fermionic operators, these Bogoliubov operators obey the normal anticommutation relations $\{b_j, b_k\} = \{b_j^\dagger, b_k^\dagger\} = 0$ and $\{b_j^\dagger, b_k\} = \delta_{jk}$. To clarify, we merely propose the transformations (3) and hope that an appropriate choice of A_k and B_k will bring \bar{H}_{BCS} into diagonal form. Therefore, the first thing we must do is re-cast the Hamiltonian in terms of ‘Bogoliubons’—and to do this, the first thing we must do is invert the relationship (3).

Using the definitions (3) together with their Hermitian conjugates we obtain the system

$$\begin{aligned} c_{\mathbf{k},\uparrow} &= \frac{1}{A_k} b_{\mathbf{k},\uparrow} - \frac{B_k}{A_k} c_{-\mathbf{k},\downarrow}^\dagger & \text{and} & & c_{-\mathbf{k},\downarrow}^\dagger &= \frac{1}{B_k} b_{\mathbf{k},\uparrow} - \frac{A_k}{B_k} c_{\mathbf{k},\uparrow}^\dagger \\ c_{\mathbf{k},\uparrow} &= -\frac{1}{B_k^*} b_{-\mathbf{k},\downarrow}^\dagger + \frac{A_k^*}{B_k^*} c_{-\mathbf{k},\downarrow}^\dagger & & & c_{-\mathbf{k},\downarrow}^\dagger &= \frac{1}{A_k^*} b_{-\mathbf{k},\downarrow}^\dagger + \frac{B_k^*}{A_k^*} c_{\mathbf{k},\uparrow}^\dagger \end{aligned} \quad (4)$$

By subtracting the related identities, we find that

$$\begin{aligned} c_{\mathbf{k},\uparrow} &= A_k^* b_{\mathbf{k},\uparrow} - B_k b_{-\mathbf{k},\downarrow}^\dagger; \\ c_{-\mathbf{k},\downarrow}^\dagger &= B_k^* b_{\mathbf{k},\uparrow} + A_k b_{-\mathbf{k},\downarrow}^\dagger. \end{aligned} \quad (5)$$

Now, writing the mean-field Hamiltonian in terms of the Bogoliubov operators, we encounter

$$\begin{aligned} \bar{H}_{BCS} = \sum_{\mathbf{k}} \left\{ \epsilon_{\mathbf{k}} \left[\left(A_k b_{\mathbf{k},\uparrow}^\dagger - B_k^* b_{-\mathbf{k},\downarrow} \right) \left(A_k^* b_{\mathbf{k},\uparrow} - B_k b_{-\mathbf{k},\downarrow}^\dagger \right) + \left(B_k^* b_{\mathbf{k},\uparrow} + A_k b_{-\mathbf{k},\downarrow} \right) \left(B_k b_{\mathbf{k},\uparrow}^\dagger + A_k^* b_{-\mathbf{k},\downarrow} \right) \right] \right. \\ \left. + \Delta \left(A_k b_{\mathbf{k},\uparrow}^\dagger - B_k^* b_{-\mathbf{k},\downarrow} \right) \left(B_k^* b_{\mathbf{k},\uparrow} + A_k b_{-\mathbf{k},\downarrow} \right) + \Delta^* \left(B_k b_{\mathbf{k},\uparrow}^\dagger + A_k^* b_{-\mathbf{k},\downarrow} \right) \left(A_k^* b_{\mathbf{k},\uparrow} - B_k b_{-\mathbf{k},\downarrow}^\dagger \right) \right\}, \end{aligned}$$

¹This is the method discussed the course textbook, Tinkham’s *Introduction to Superconductivity*. Our analysis will closely follow the discussion in that text.

which at first-sight appears horrendous to expand. Using anti-commutation relations to simplify things a bit,

$$\begin{aligned}
\bar{H}_{BCS} &= \sum_{\mathbf{k}} \left\{ \epsilon_k \left[(|A_k|^2 - |B_k|^2) \left(b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow} + b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow} \right) + 2|B_k|^2 - 2A_k B_k b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger - 2A_k^* B_k^* b_{-\mathbf{k},\downarrow} b_{\mathbf{k},\uparrow} \right] \right. \\
&\quad + \Delta \left[A_k B_k^* \left(b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow} + b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow} \right) - A_k B_k^* + A_k^2 b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger - B_k^{*2} b_{-\mathbf{k},\downarrow} b_{\mathbf{k},\uparrow} \right] \\
&\quad \left. + \Delta^* \left[A_k^* B_k \left(b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow} + b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow} \right) - A_k^* B_k + A_k^{*2} b_{-\mathbf{k},\downarrow} b_{\mathbf{k},\uparrow} - B_k^2 b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger \right] \right\} \\
&= \sum_{\mathbf{k}} \left\{ 2\epsilon_k |B_k|^2 - 2 \Re(\Delta A_k B_k^*) + \left[\epsilon_k (|A_k|^2 - |B_k|^2) + 2 \Re(\Delta A_k B_k^*) \right] \left(b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow} + b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow} \right) \right. \\
&\quad \left. + b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger \left(\Delta A_k^2 - \Delta^* B_k^2 - 2\epsilon_k A_k B_k \right) + b_{-\mathbf{k},\downarrow} b_{\mathbf{k},\uparrow} \left(\Delta^* A_k^{*2} - \Delta B_k^{*2} - 2\epsilon_k A_k^* B_k^* \right) \right\}. \quad (6)
\end{aligned}$$

Now, because we are free to choose A_k and B_k any way we'd like—so long as the transformation is SU_2 —we would obviously like to define them so that the off-diagonal contributions to \bar{H}_{BCS} vanish—these are the last two terms in (6). Now, the off-diagonal terms will vanish if the Bogoliubov coefficients are chosen to satisfy

$$\Delta A_k^2 - \Delta^* B_k^2 - 2\epsilon_k A_k B_k = 0. \quad (7)$$

This is a simple quadratic equation, the solution to which is simply²

$$A_k = \frac{B_k}{\Delta} \left(\epsilon_k \pm \sqrt{\epsilon_k^2 + |\Delta|^2} \right) \equiv \frac{B_k}{\Delta} (\epsilon_k \pm E_k). \quad (8)$$

With this condition, the last line of (6) vanishes. But we actually have a bit more than that: the additional constraint $|A_k|^2 + |B_k|^2 = 1$ allows us to eliminate these coefficients all-together³. Notice that (8) implies that, after a bit of algebra,

$$|A_k|^2 = \frac{|B_k|^2}{|\Delta|^2} (\epsilon_k \pm E_k)^2 = (1 - |A_k|^2) \frac{1}{|\Delta|^2} (\epsilon_k \pm E_k)^2 = \frac{(\epsilon_k \pm E_k)^2}{|\Delta|^2 + (\epsilon_k \pm E_k)^2} = \dots = \frac{1}{2} \left(1 \pm \frac{\epsilon_k}{E_k} \right). \quad (9)$$

And, similarly,

$$|B_k|^2 = \frac{1}{2} \left(1 \mp \frac{\epsilon_k}{E_k} \right). \quad (10)$$

Notice also that $\Delta A_k B_k^*$ is manifestly real and specifically

$$\Re(\Delta A_k B_k^*) = \Delta A_k B_k^* = |B_k|^2 (\epsilon_k \pm E_k). \quad (11)$$

Let us define the quasi-particle ('Bogoliubon') number operators $\tilde{n}_{\mathbf{k},\uparrow} \equiv b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow}$ and $\tilde{n}_{-\mathbf{k},\downarrow} \equiv b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow}$. Putting all of this together, we may re-express the BCS Hamiltonian completely in terms of the Bogoliubov operators.

$$\begin{aligned}
\bar{H}_{BCS} &= \sum_{\mathbf{k}} \left\{ 2\epsilon_k |B_k|^2 - 2|B_k|^2 (\epsilon_k \pm E_k) + \left[\epsilon_k (|A_k|^2 - |B_k|^2) + 2|B_k|^2 (\epsilon_k \pm E_k) \right] (\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow}) \right\}, \\
&= \sum_{\mathbf{k}} \left\{ \mp 2|B_k|^2 E_k + (\epsilon_k \pm 2|B_k|^2 E_k) (\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow}) \right\}, \\
&= \sum_{\mathbf{k}} \left\{ \epsilon_k \mp E_k \pm E_k (\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow}) \right\}.
\end{aligned}$$

The physical requirement that the total energy be bounded below demands that ' \pm ' \mapsto ' $+$ ': otherwise, the creation of Bogoliubons would lower the energy of the system without bound. Therefore, we have shown that in terms of the Bogoliubon quasi-particles,

$$\therefore \bar{H}_{BCS} = \sum_{\mathbf{k}} \left\{ \epsilon_k - E_k + E_k (\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow}) \right\}. \quad (12)$$

²We have not made use of the freedom to make A_k real—nor will we: it never is necessary.

³To be precise, there is still an arbitrary (unphysical) phase between A_k and B_k , and there is an insofar unspecified sign in A_k . This sign will be determined below—until then, however, we'll keep it unspecified.

Notice that the Hamiltonian is diagonal in terms of the quasi-particles—it manifestly commutes with the Bogoliubon number operators. Eigenstates are therefore labeled by their momenta \mathbf{k} and quasi-particle numbers: for a given momentum, let $|\mathbf{k}\rangle$ be defined as that which is annihilated by both $b_{\mathbf{k},\uparrow}$ and $b_{-\mathbf{k},\downarrow}$; clearly, $|\mathbf{k}\rangle$ has both quasi-particle numbers 0. Because the quasi-particles are fermions, there can be at most one of each kind at a given momentum. Therefore, the eigenstates of \bar{H}_{BCS} for a given \mathbf{k} are exactly

$$|\mathbf{k}\rangle, \quad b_{\mathbf{k},\uparrow}^\dagger |\mathbf{k}\rangle, \quad b_{-\mathbf{k},\downarrow}^\dagger |\mathbf{k}\rangle, \quad \text{and} \quad b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger |\mathbf{k}\rangle, \quad (13)$$

with eigenenergies, respectively,

$$\epsilon_k - E_k, \quad \epsilon_k, \quad \epsilon_k, \quad \text{and} \quad \epsilon_k + E_k. \quad (14)$$

Now, recall that the consistency of the mean-field Hamiltonian requires that

$$\Delta = \frac{U}{V} \sum_{\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle.$$

To find the expectation value of the operator $c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow}$ at a given momentum \mathbf{k} , we'll need the partition function

$$\mathcal{Z} = \sum_{\text{states}} e^{-\beta H} = e^{-b(\epsilon_k - E_k)} + 2e^{-\beta \epsilon_k} + e^{-\beta(\epsilon_k + E_k)} = 2e^{-\beta \epsilon_k} (1 + \cosh(\beta E_k)). \quad (15)$$

Now, we should express the operator $(c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow})$ in terms of the Bogoliubov operators,

$$\begin{aligned} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} &= \left(B_k b_{\mathbf{k},\uparrow}^\dagger + A_k^* b_{-\mathbf{k},\downarrow} \right) \left(A_k^* b_{\mathbf{k},\uparrow} - B_k b_{-\mathbf{k},\downarrow}^\dagger \right), \\ &= A_k^* B_k (\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow} - 1) + A_k^{*2} b_{-\mathbf{k},\downarrow} b_{\mathbf{k},\uparrow} - B_k^2 b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger. \end{aligned}$$

Because the last two terms do not commute with the Hamiltonian, they will not contribute anything to the expectation value $\langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle$. Therefore⁴,

$$\begin{aligned} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle &= \frac{1}{\mathcal{Z}} \sum_{|\psi\rangle} A_k^* B_k \langle \psi | (\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow} - 1) e^{-\beta H} | \psi \rangle, \\ &= \frac{\Delta e^{\beta \epsilon_k}}{4E_k (1 - \cosh(\beta E_k))} \left\{ -e^{-\beta(\epsilon_k - E_k)} + e^{-\beta(\epsilon_k + E_k)} \right\}, \\ &= -\frac{\Delta \sinh(\beta E_k)}{2E_k (1 - \cosh(\beta E_k))}, \\ &= -\frac{\Delta \tanh(\beta E_k/2)}{2 E_k}. \end{aligned}$$

So in the large-volume limit, the consistency demands that

$$-\Delta \frac{V}{U} = \Delta \frac{1}{2} \int_{\text{fermi surface}} \frac{\tanh\left(\frac{\beta}{2} \sqrt{\epsilon_k^2 + |\Delta|^2}\right)}{\sqrt{\epsilon_k^2 + |\Delta|^2}} d\epsilon_k \quad \implies \quad \Delta = 0 \quad \text{or} \quad -\frac{V}{U} = \int_0^{\hbar\omega_c} \frac{\tanh\left(\frac{\beta}{2} \sqrt{\epsilon_k^2 + |\Delta|^2}\right)}{\sqrt{\epsilon_k^2 + |\Delta|^2}} d\epsilon_k. \quad (16)$$

We were asked to argue that for low enough temperature, $\Delta > 0$ is consistent, but for high enough temperatures only $\Delta = 0$ is possible. We will actually do a bit more and determine the critical temperature, T_c , above which $\Delta = 0$ is required for consistency. However, before we do that calculation, let us argue generally to understand the results qualitatively.

At zero temperature, $\tanh(\beta E_k/2) \rightarrow 1$ so that a non-zero Δ would be determined by the equation

$$-\frac{V}{U} = \int_0^{\hbar\omega_c} \frac{dx}{\sqrt{x^2 + |\Delta|^2}} = \log\left(\hbar\omega_c \left(1 + \sqrt{1 + \frac{|\Delta|^2}{(\hbar\omega_c)^2}}\right)\right) - \log(\Delta) \approx \log\left(\frac{2\hbar\omega_c}{|\Delta|}\right). \quad (17)$$

Solving for $\Delta(T=0)$ we find

$$|\Delta(T=0)| \approx 2\hbar\omega_c e^{V/U}. \quad (18)$$

⁴On the borderline of triviality, we recall the identities $\sinh(\xi) = 2 \sinh(\xi/2) \cosh(\xi/2)$ and $1 + \cosh(\xi) = 2 \cosh^2(\xi/2)$.

Therefore, we know that for small enough temperature, $\Delta \neq 0$ is consistent. However, for temperatures greater than about $kT > \frac{1}{2}\sqrt{(\hbar\omega_c)^2 + |\Delta|^2}$, we may Taylor-expand the integrand of the consistency equation, yielding

$$-\Delta \frac{U}{V} = \Delta \int_0^{\hbar\omega_c} d\epsilon_k \frac{1}{E_k} \left(\frac{\beta}{2} E_k - \frac{\beta^3}{24} E_k^3 + \frac{\beta^5}{240} E_k^5 - \dots \right). \quad (19)$$

Parametrically, if we suppose that $\Delta \neq 0$ then the constraint equation becomes a polynomial linear in β and with a leading Δ term of order $\beta^3 \Delta^2$. Regardless of the details of integration, the general solution to a polynomial equation of the form $c_1 \Delta^2 \beta^3 + c_2 \beta = c_3$ has Δ parametrically of the form $\Delta \sim 1/\beta^{3/2}$. But as β becomes small, Δ must therefore grow very large to compensate, immediately in contradiction with the hypothesis that $kT > \frac{1}{2}\sqrt{(\hbar\omega_c)^2 + |\Delta|^2}$. —*—

Therefore, we know that at sufficiently high temperatures the only consistent mean-field Hamiltonian is one for which $\Delta = 0$. But we have shown also that at zero temperature, $\Delta > 0$ is consistent and given by the expression above. Let us find the temperature T_c where Δ first vanishes.

When $\Delta \rightarrow 0$, $E_k \rightarrow \epsilon_k$ so that the consistency equation becomes

$$-\frac{V}{U} = \int_0^{\beta_c \hbar\omega_c / 2} \frac{\tanh(x) dx}{x} = \log(2e^{\gamma_E} \pi \beta_c \hbar\omega_c); \quad (20)$$

the integral was evaluated using a computer algebra package, and γ_E is Leonhard Euler's constant⁵. Combining this with the above, we find

$$\therefore kT_c = e^{\gamma_E} \pi \Delta(0). \quad (21)$$

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⁵For fun, $\gamma_E = \lim_{n \rightarrow \infty} \frac{\Gamma(\frac{1}{n})\Gamma(n+1)n^{1+1/n}}{\Gamma(2+n+\frac{1}{n})} - \frac{n^2}{n+1}$.

PHYSICS 525, CONDENSED MATTER

Homework 8

Due Thursday, 14th December 2006

JACOB LEWIS BOURJAILY

Problem 1: Little-Parks Experiment

Consider a long, thin-walled, hollow cylinder of radius R and thickness d made of a superconductor subjected to an external magnetic field H which is parallel to the axis of the cylinder. If the wave function for superconducting electron pairs $\Psi(r)$ is taken as the order parameter for a Landau-Ginzburg theory, the free energy density is then

$$f = f_n + a(T - T_{c0})|\Psi|^2 + \frac{\beta}{2}|\Psi|^4 + \frac{\hbar^2}{2m} \left| \left(-i\vec{\nabla} + \frac{2e}{\hbar c} \vec{A} \right) \Psi \right|^2 + \frac{1}{8\pi} (\vec{H} - \vec{B})^2. \quad (1.1)$$

Here, we have made the additional assumption that the leading coefficient is a linear function in T that vanishes at the zero-field critical temperature T_{c0} . To lowest order in the induced current, $\vec{H} = \vec{B}$ everywhere, and the last term of the free energy may be ignored.

a. We are to find the lowest free-energy state as a function of both T and H , for H such that the total flux through the interior of the cylinder is no more than a few flux quanta. We are to give the values of $|\Psi(r)|$ and $\vec{v}_s(r)$ and calculate the shifted critical temperature as a function of applied field.

Let the cylinder lie with its axis in the \hat{z} -direction in cylindrical coordinates. We may write choose our gauge so that the vector potential is

$$\vec{A} = \frac{rH}{2} (0, 1, 0), \quad (1.2)$$

which is easily seen to give rise to $\vec{H} = H\hat{z}$.

Before we try to find the minimum of the free energy, it will be helpful to cut away generality of our analysis for the conveniences offered by the case at hand. Recall that the field within a thin-walled superconductor is well approximated by London theory; this is because gradient terms in the magnitude $|\Psi|$ cost too much free energy when the field must vanish outside of the thin cylinder. Therefore, we may write

$$\Psi(r) = \psi e^{i\varphi(r)}, \quad \text{for } \psi \in \mathbb{R}. \quad (1.3)$$

Of course, Ψ must be taken to vanish outside the superconductor, but this will not really complicate our analysis. Observe that

$$(-i\vec{\nabla}\Psi) = \Psi \left(\vec{\nabla}\varphi(r) \right), \quad (1.4)$$

which encourages us to write the fourth term in (1.1) as

$$\frac{\hbar^2}{2m} \left| \left(-i\vec{\nabla} + \frac{2e}{\hbar c} \vec{A} \right) \Psi \right|^2 = \frac{\hbar^2}{2m} |\Psi|^2 \left(\vec{\nabla}\varphi(r) + \frac{2e}{\hbar c} \vec{A} \right) \equiv \frac{1}{2} m \psi^2 \vec{v}_s^2, \quad \text{where } \vec{v}_s \equiv \frac{\hbar}{m} \left(\vec{\nabla}\varphi(r) + \frac{2e}{\hbar c} \vec{A} \right). \quad (1.5)$$

Using the symmetry of the problem it is obvious that there are only currents in the θ -direction; this implies that $\partial_r(\varphi) = \partial_z(\varphi) = 0$ ¹; so φ is only a function of θ . Furthermore, single-valuedness of the wave function requires that

$$\oint \nabla\varphi = 2\pi r \frac{1}{r} \partial_\theta\varphi = 2\pi n, \quad \implies \quad \partial_\theta\varphi = n, \quad \implies \quad \varphi(\theta) = n\theta. \quad (1.6)$$

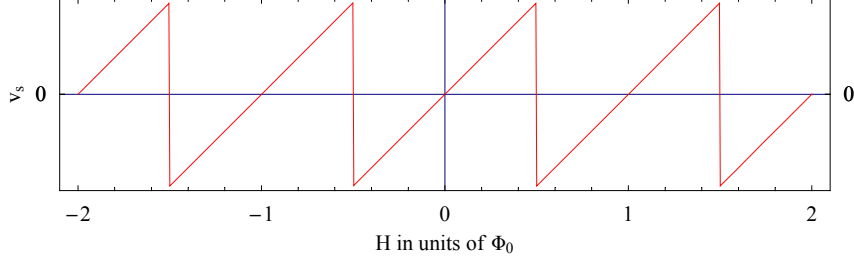
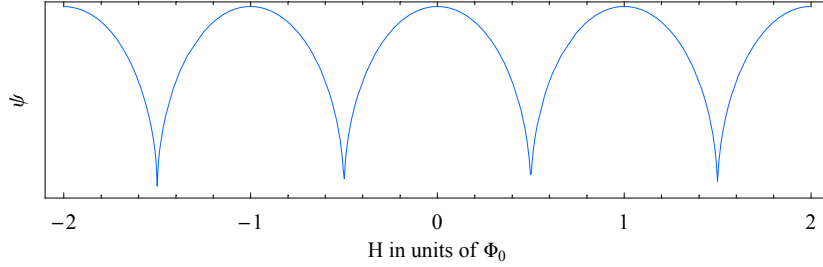
Using this together with the definition

$$\Phi_0 \equiv \frac{hc}{2e}, \quad (1.7)$$

and the fact that the flux through the cylinder is $\Phi = H\pi R^2$, we can write

$$v_s = \frac{\hbar}{mR} \left(n + \frac{\Phi}{\Phi_0} \right). \quad (1.8)$$

¹Actually, symmetry does not exclude currents in the \hat{z} -direction: these are excluded because they raise the free energy unnecessarily—so that the ground state will have no vertical components.

FIGURE 1. The velocity operator v_s as a function of the applied field H .FIGURE 2. The magnitude of the wave function $\psi(H)$.

Putting everything together, we find the free energy of the superconductor to be

$$f_s = a(T - T_{c_0})\psi^2 + \frac{\beta}{2}\psi^4 + \frac{1}{2}mv_s^2\psi^2. \quad (1.9)$$

Notice that the free energy is naturally lowered by seeking the smallest possible value of v_s . This is done by choosing the integer n so that $n - \frac{\Phi}{\Phi_0}$ is minimized. This is shown in Figure 1. Minimizing this with respect to the field magnitude ψ , we obtain the Landau-Ginzburg equation

$$\left\{ a(T - T_{c_0}) + \beta\psi^2 + \frac{1}{2}mv_s^2 \right\} \psi = 0. \quad (1.10)$$

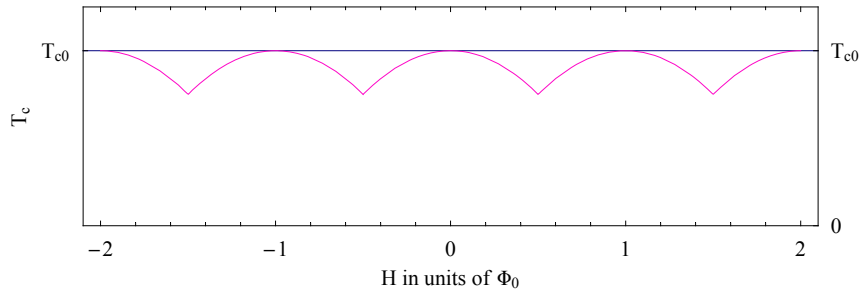
$$\therefore \psi^2 = \frac{1}{\beta} \left(a(T_{c_0} - T) - \frac{1}{2}mv_s^2 \right). \quad (1.11)$$

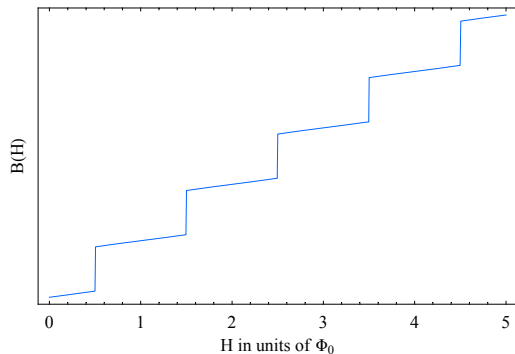
The parametric dependence on H is shown in Figure 2.

If we define $T_c(H)$ to be the field temperature at which ψ^2 vanishes for a given H (which enters our expression via v_s), we see that

$$T_c(H) = T_{c_0} - \frac{mv_s^2}{2a}. \quad (1.12)$$

This was one of the principle experimental results of Little and Parks. The dependence of T_c on H is shown in Figure 3.

FIGURE 3. The critical temperature as a function of H .

FIGURE 4. The qualitative structure of $B(H)$.

b. We are to obtain the field $\vec{B}(H)$ to leading order in the current of the cylinder and describe when this approximation is valid.

Recall that the current density is

$$J = -2e\psi^2 v_s = -\frac{2e}{\beta} v_s \left(a(T_{c_0} - T) - \frac{mv_s^2}{2} \right). \quad (1.13)$$

We can find the (upper bound on) the maximum of J by differentiating with respect to v_s ; we find

$$v_s^2 = \frac{2a(T_{c_0} - T)}{3m}, \quad (1.14)$$

will maximize J . The reason why one could be worried is that v_s is of course bounded. However, the bound on v_s extends beyond the v_s required to saturate the maximum of J ,

$$v_s^2 \leq \frac{2a(T_{c_0} - T)}{m}. \quad (1.15)$$

Anyway, we may use this to find the maximum current,

$$J_{max} = -4e \frac{a(T_{c_0} - T)}{\beta} \sqrt{\frac{2a(T_{c_0} - T)}{3m}}. \quad (1.16)$$

Using the equation above for the current as a function of v_s , we can compute the induced B -field as a function of H . The total field is shown in Figure 4.

Problem 2: Plane Waves on Thin Superconductors

Consider a thin-sheet superconductor with the same Landau-Ginzburg free energy expansion as discussed in problem 1. We are to determine the spatially uniform configurations of $\Psi(r)$ which are minima of the free energy under variation of ψ . We should determine the maximum current that can be carried by the wave—and especially describe the behaviour as T_{c_0} is approached from below.

Similar to the situation above, we notice that solutions will necessarily have no spatial variation in magnitude—again, because this gradient term costs too much in the free energy. Therefore, we may write (approximate) any solution which minimizes the Landau Ginzburg free energy as $\Psi(r) = \psi e^{i\varphi(r)}$ for $\psi \in \mathbb{R}$. And also like above we find that—ignoring the magnetic fields induced by the supercurrent—

$$\psi^2 = \frac{1}{\beta} \left(a(T_{c_0} - T) - \frac{1}{2}mv_s^2 \right), \quad (2.1)$$

where

$$\vec{v}_s(r) \equiv \frac{\hbar}{m} \vec{\nabla}(\varphi(r)). \quad (2.2)$$

Notice that this time there is no contribution from the vector potential.

A spatially uniform solution must therefore be one such that $\vec{v}_s(r) = k \cdot x$ for some constant vector k inside the thin-sheet superconductor and \hat{x} is a direction in the

plane—which we may take as one of the coordinate axes for convenience. Such a solution will manifestly generate a spatially uniform velocity,

$$\vec{v}_s = \frac{\hbar}{m} k \hat{x}. \quad (2.3)$$

Recalling some standard notation,

$$\psi_0^2 = \frac{a(T_{c_0} - T)}{\beta}, \quad \text{and} \quad \xi^2(T) = \frac{\hbar^2}{2ma(T_{c_0} - T)}, \quad (2.4)$$

we can rewrite the minimization condition as

$$\psi^2 = \psi_0^2 \left(1 - \frac{\hbar^2 k^2}{2ma(T_{c_0} - T)} \right) = \psi_0^2 (1 - \xi^2 k^2). \quad (2.5)$$

Therefore, we see that spatially uniform solutions are of the form

$$\Psi(r) = \psi_0 \sqrt{1 - \xi^2 k^2} e^{ikx}. \quad (2.6)$$

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Notice that this requires that

$$k < \frac{1}{\xi} \quad (2.7)$$

for a superconducting solution.

This gives us a current of

$$J = -2e\psi^2 v_s = -2e\psi_0^2 k \frac{\hbar}{m} (1 - \xi^2 k^2). \quad (2.8)$$

The extreme current can be found via differentiation

$$1 - 3\xi^2 k^2 = 0 \quad \implies \quad k = \frac{1}{\sqrt{3}\xi}; \quad (2.9)$$

which of course implies that

$$\therefore J_{max} = \psi_0^2 \frac{1}{\xi} \frac{2\hbar}{3\sqrt{3}m}. \quad (2.10)$$

Near $T = T_{c_0}$ from below, we know that

$$\psi_0 \sim 1 - \frac{T}{T_{c_0}}, \quad \text{and} \quad \xi(T) \sim \frac{1}{\sqrt{1 - T/T_{c_0}}}, \quad (2.11)$$

and therefore the maximum current vanishes according to

$$J_{max} \sim \left(1 - \frac{T}{T_{c_0}} \right)^{3/2}. \quad (2.12)$$

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Problem 3: Superconducting Spheres and Monopoles

Aluminium is a type-I superconductor with coherence length $\xi = 1.5 \times 10^{-6}$ m and a magnetic penetration length $\lambda = 2 \times 10^{-8}$ m at low temperature.

a. At zero temperature, a spherical piece of aluminium of radius $r \gg \lambda$ is placed in a magnetic field $\vec{B} = B(z)\hat{z}$ with a small field gradient ($r \gg dB/dz$) and $B < H_c$. We are to state $H_c(T = 0)$ and compute the force on the sphere for the specific case $r = 10^{-3}$ m, $B = 10^{-3}$ T, and $dB/dz = 10^{-2}$ T/m and compare this to the case if $B \mapsto 1$ T while keeping everything else the same.

First, we notice that

$$H_c = \frac{\Phi_0}{2\sqrt{2}\pi\xi(0)\lambda(0)} = 7.8 \times 10^{-3} \text{ T} = 78 \text{ gauss}. \quad (3.1)$$

To compute the force of the sphere of superconducting aluminium from the B -field, we need to find the external field. This is done by first finding the field inside the superconductor. There, we know that \vec{B} must vanish. Because gradient is small

compared to the radius of the sphere, we can approximate the solution by considering the field to be constant throughout the sphere. It is clear that the superconducting currents on the surface must cancel this field exactly inside. Therefore, we can quickly discover the required field arrangement if we know of a system which gives rise to a uniform magnetic inductance within the volume of a sphere.

Now, if we remember our electrodynamics as much as any student studying for Preliminary exams should, then we recall at once that such a field distribution is obtained by a rotating, insulating sphere of uniform surface charge density. We could derive this solution but, for the sake of brevity, we will refer the reader to homework solutions prepared many years ago by the author². Alternatively, we draw the reader's attention to section (5.10) of Jackson's *Classical Electrodynamics*.

The principle result was that if a sphere has a uniform magnetic field in its interior given by

$$B\hat{z} = \frac{2\mu_0}{3}M\hat{z}, \quad (3.2)$$

then the field outside the sphere is precisely that of a dipole with dipole moment

$$m\hat{z} = \frac{4\pi r^3}{3}M\hat{z}. \quad (3.3)$$

In our present situation, we need the field within the sphere to exactly cancel that of the ambient B -field. This tells us that currents which generate a uniform $B_{in} = -B(z)$ give rise to a perfect dipole field outside the sphere with dipole moment

$$m\hat{z} = \frac{4\pi r^3}{3} \frac{3}{2\mu_0} (-B(z)) = -\frac{2\pi r^3}{\mu_0} B(z). \quad (3.4)$$

Making use again of the fact that the sphere is small compared to the gradient of B , we will not lose much by considering the interaction between B and the sphere therefore to be that between a any magnetic inductance and a dipole—namely,

$$\vec{F} = \vec{\nabla}(\vec{m} \cdot \vec{B}) = -\frac{2\pi r^3}{\mu_0} B(z) \frac{\partial B(z)}{\partial z}. \quad (3.5)$$

$$\dot{\gamma}\pi\epsilon\rho \quad \dot{\epsilon}\delta\epsilon\iota \quad \rho\iota\eta\hat{\sigma}\alpha\iota$$

Putting in the numbers for our problem, we find

$$F(10^{-3} \text{ T}) = 10^{-2} \text{ dyne}, \quad \text{and} \quad F(1 \text{ T}) = 10 \text{ dyne}. \quad (3.6)$$

b. Consider a Dirac monopole/anti-monopole pair 10^{-2} m apart within a much larger piece of superconducting aluminium at zero temperature. The monopole emits magnetic flux hc/e . We are to give a rough estimate of the force between these two hypothetical particles.

The physical picture to have in mind is the following. If the two monopoles were separated in free-space, their flux lines would be exactly analogous electrostatics. However, magnetic flux by definition cannot exist within a superconducting state—the superconductor will do all that it can to confine the magnetic flux to a very small region in the superconductor. Therefore, it is easy to imagine that *all* of the flux connecting the two monopoles is *confined* to a narrow ‘sting’ between the two monopoles. The width of this string is roughly 2λ —because this is as narrow a region as a Type-I superconductor can confine a region of non-critical state.

We may approximate the situation as there being a cylindrical band connecting the two monopoles in which there is confined all of the magnetic flux between them and completely normal-state Aluminium. In terms of energy costs, the flux lines must

²If the grader truly desires to see this calculation, please see the homework prepared during a course in the fall of 2004 at: <http://www.umich.edu/~jbourj/jackson/5-13.pdf>.

pay a debt of free energy of³

$$F_{mag} = \frac{1}{8\pi} d\pi\lambda^2 \left(\frac{2hc}{e\pi\lambda^2} \right)^2 = \frac{2d\Phi_0^2}{\pi^2\lambda^2}, \quad (3.7)$$

where we have made use of the flux quantum Φ_0 . Also, we must pay the energy debt of raising the superconducting minimum to the normal state over the volume of the ‘flux tube’ of force. Using some identities from work elsewhere, we have as the leading term in the Landau Ginzburg free-energy potential,

$$F_s = d\pi\lambda^2\alpha\psi_0^2 = d\pi\xi^2 \frac{2e^2 H_c^2(T)\lambda^2}{mc^2} \frac{mc^2}{8\pi e^2\lambda^2} = d\frac{\xi^2}{4} H_c^2. \quad (3.8)$$

Notice that this energy is linear with distance: this is as expected: the energy content of the flux tube is proportional to its length. We find the force then to be

$$F = - \left(\frac{2\Phi_0^2}{\pi^2\lambda^2} + \frac{\xi^2}{4} H_c^2 \right). \quad (3.9)$$

This is an attractive force on the order of a dyne.

³I’m not sure exactly the choice of units here, but if I compute Φ_0 in Tesla-meters², then there needs to be a $1/\mu_0$ to get the units right. I suspect that $\frac{1}{8\pi} \mapsto 1/\mu_0$, but it doesn’t really matter: we are only asked to qualitatively describe the force.