

# PHYSICS 525, CONDENSED MATTER

## Homework 4

Due Tuesday, 24<sup>th</sup> October 2006

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### 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 equations<sup>1</sup>

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

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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<sup>1</sup>Here 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 are<sup>2</sup>

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

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

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

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

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<sup>2</sup>Just to reiterate: the solutions  $\psi_2$  and  $\psi_3$  could generically be any linear combination of what we have written.

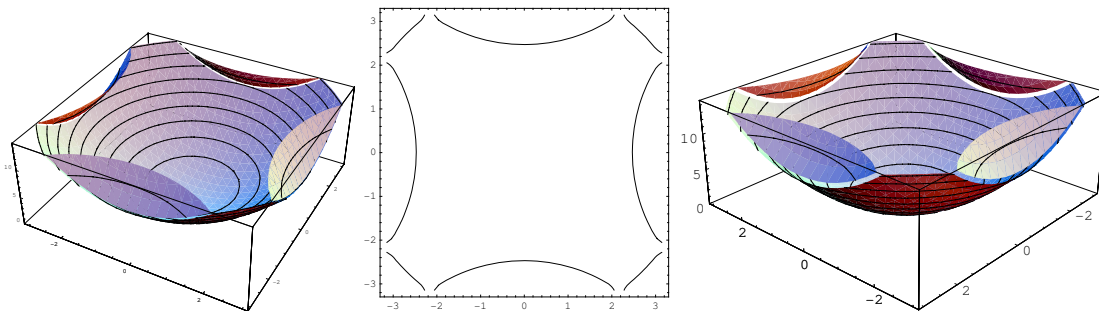


FIGURE 1. Three different views of the Fermi surfaces for the (metallic) system described in Problem 1. The figures on the left and right-hand sides show many equal-energy contours up to the Fermi energy. The middle plot shows just the Fermi surfaces. (Note that the corners of the figure are on the lower 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  $\chi$  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),  $\Delta$ ,  $m_e$ , and  $m_h$  are all positive and  $\delta$  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.  $\varepsilon_{\pm}$  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  $\varepsilon_+$  ( $\varepsilon_-$ ) 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  $\varepsilon_-$  or  $\varepsilon_+$ —*but not both*—having a third-order global maximum or minimum at  $k = 0$ , respectively.

Let us quickly find the cases when  $\varepsilon_+$  or  $\varepsilon_-$  does not have three distinct extrema. For  $\varepsilon_+$ , 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

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

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

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

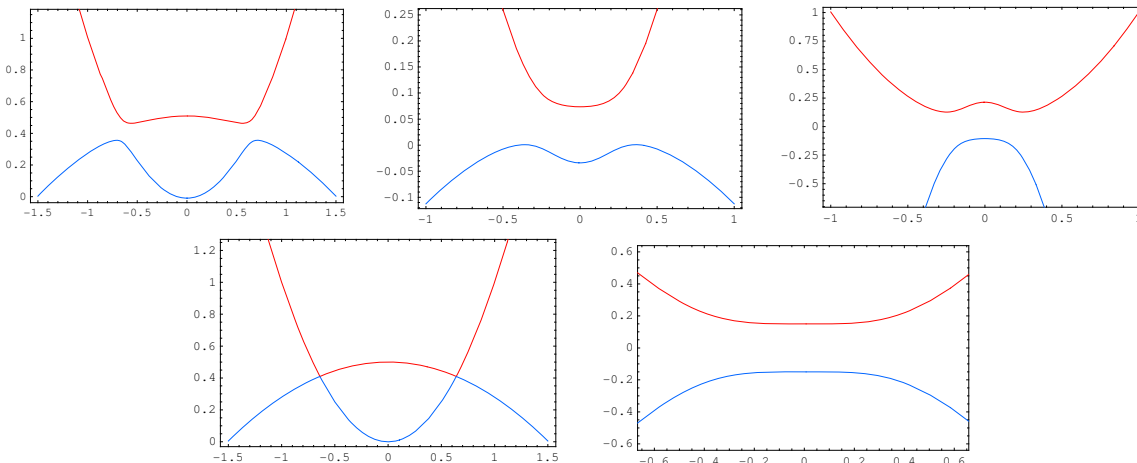


FIGURE 2. The qualitatively different possible hybridizations between particle- and hole-like bands. The possibilities are shown in the order discussed.

Similar algebra in the case of the  $\varepsilon_-$  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  $\varepsilon_+$  will not lie over the global maxima of  $\varepsilon_-$ .
- (2) When the upper band,  $\varepsilon_+$ , 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,  $\varepsilon_-$ , 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  $\varepsilon_1$ <sup>3</sup> 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  $\varepsilon_{\pm}$ . 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  $\varepsilon_{\pm}$ . In problem (a) we calculated the values of  $k$  for which  $\varepsilon_{\pm}$  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

<sup>3</sup>Here  $\varepsilon_1$  refers to the particle-like band.

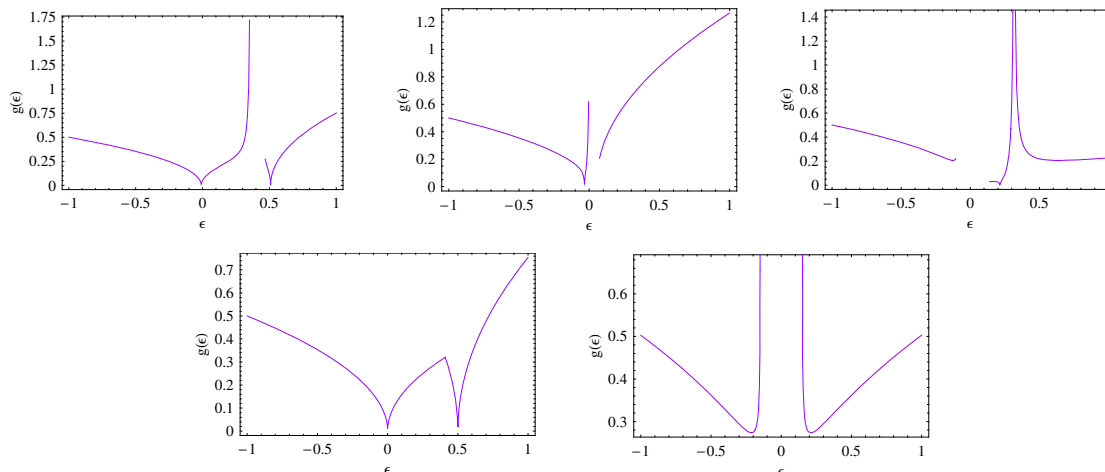


FIGURE 3. The densities of states for the band structures illustrated in Figure 2.

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 1,2,3<sup>4</sup> 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  $2\delta$ . To see this, consider zooming in near where the two bands cross; locally, this is to order  $\delta$  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  $\varepsilon_+$  ( $\varepsilon_-$ ) 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

<sup>4</sup>We 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  $\Delta$  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 weak<sup>5</sup>, 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  $2 \times 10^{-9}$  Gauss<sup>-1</sup>. 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<sup>-1</sup>.  $A_e$  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  $\pi k_F^2$ —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  $\ell$  is given by

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

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<sup>5</sup>Ashcroft 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  $\rho_\mu$  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  $\varepsilon_0$ ,  $t_-$ , 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  $-q$ <sup>6</sup> 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  $q = \pm \frac{\pi}{2}$ <sup>7</sup>. 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

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

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

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

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

<sup>7</sup>We 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  $\varepsilon_0$ . 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 coefficient<sup>8</sup>

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

In the limit where  $t_{\pm}$  and  $\varepsilon_0$  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  $t_{\pm}, \varepsilon_0$  are taken to be small,  $\mathcal{T} \rightarrow 0$ .

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<sup>8</sup>We 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.