

PROBLEM SET 4 Solutions

Physics 240A– FALL 2019

Problem 4-1

At zero temperature we fill up all the k levels up to k_f with two electrons.

$$\begin{aligned} N &= \sum_{k_x k_y} 2 = \left(\frac{L}{2\pi}\right)^2 \int dk_x dk_y 2 \\ &= 4\pi \left(\frac{L}{2\pi}\right)^2 \int_0^{k_f} k dk \\ &= L^2 \frac{1}{2\pi} k_f^2. \end{aligned} \tag{1}$$

If we define the density of electrons per unit *area*, $n = \frac{N}{A}$,

$$n = \frac{1}{2\pi} k_f^2. \tag{2}$$

This is to be compared with the form $3\pi^2 n = k_f^3$ in 3-d.

The density of states is computed by

$$\begin{aligned} N(E) &= 2 \sum_{k_x k_y} \delta(E - \epsilon(k)) \\ &= L^2 \frac{1}{\pi} \int_0^\infty k dk \delta(E - \frac{h^2 k^2}{2m}) \\ &= L^2 \frac{1}{\pi} \int_0^\pi k dk \frac{1}{\left|\frac{h^2 k}{m}\right|} \delta(k - k_0), \end{aligned} \tag{3}$$

where $k_0 = \sqrt{\frac{2mE}{h^2}}$. Thus

$$N(E) = L^2 \frac{m}{\pi h^2}. \tag{4}$$

This is independent of energy. Again, the analogous 3-d result has $N(E) \propto \sqrt{E}$.

Problem 4-2

When only a small fraction of the Brillouin zone is occupied, that is, when E is close to $-4t$, k_x and k_y will be small, and we can approximate the $\cos x \sim 1 - x^2/2$:

$$E(k) \sim -4t + t(k_x^2 + k_y^2) . \quad (5)$$

It is evident that the Fermi Surface $E = \text{constant}$ will be a circle about the origin. See Fig. 1.

Likewise if the Brillouin zone is almost completely full, the values of k_x and k_y will be close to π . Writing $k_x = \pi - \kappa_x$ and $k_y = \pi - \kappa_y$, with κ_x, κ_y small we have

$$E(k) \sim +4t - t(\kappa_x^2 + \kappa_y^2) \quad (6)$$

This is again the equation of a circle, in the κ_x, κ_y plane, and hence a circle centered at (π, π) in the (k_x, k_y) plane. The final thing to note is that one can translate points lying outside $-\pi < k_x, k_y < +\pi$. The end result is a set of four ‘hole pockets’ as shown in Fig. 1.

The final simple case is $E = 0$. It is trivial to see that if k_x and k_y are both positive (that is, in the first quadrant) then $k_y = \pi - k_x$ yields $E = 0$. Similar consideration of the other pockets will rapidly convince you that the Fermi surface is a rotated square. See Fig. 1.

Other cases can be done numerically. Given some discrete mesh of $0 < k_x < \pi$, compute

$$k_y = \cos^{-1} \left(-\frac{E}{2t} - \cos k_x \right) \quad (7)$$

and then plot the resulting (k_x, k_y) pairs to get the Fermi surface in the first quadrant. Proceed similarly with the other quadrants. You need to think for just a minute about the fact that \cos^{-1} has several solutions.

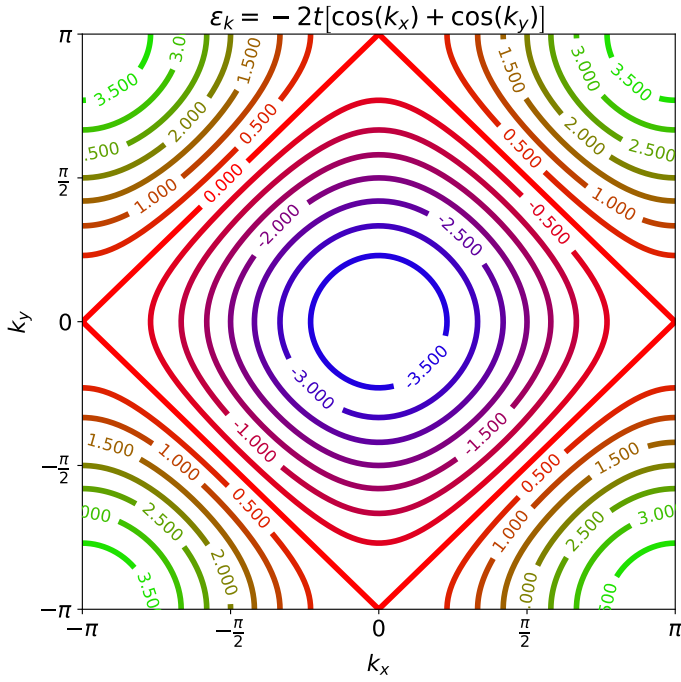


Figure 1: The Fermi surface of the two dimensional square lattice tight binding dispersion relation. For low filling, the FS are circles about the origin. These flatten increasingly along the 45 degree lines until at half-filling the surface $E = 0$ is a rotated square. For close to full fillings one gets ‘hole pockets’ at the corners of the Brillouin zone. (Figure courtesy of Ben Cohen-Stead.)

Problem 4-3

We are asked to compute the density of states for a 2-dimensional tight binding dispersion relation

$$\epsilon(k) = -2t[\cos(k_x) + \cos(k_y)]. \quad (8)$$

We first comment that it is obvious that $N(E)$ will be zero except for $-4t < E < +4t$. I am going to assume $E > 0$ since it is clear that $N(E) = N(-E)$. We use the definition of the density of states:

$$\begin{aligned} N(E) &= 2 \sum_k \delta(E - \epsilon(k)) \\ &= \frac{L^2}{2\pi^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \delta(E + 2t[\cos(k_x) + \cos(k_y)]). \end{aligned} \quad (9)$$

We will first do the integral over k_y regarding k_x as fixed.

$$N(E) = \frac{L^2}{2\pi^2} \int_{k_1}^{k_2} dk_x \frac{1}{|2t\sin(k_{y0})|} \quad (10)$$

where k_{y0} is determined by

$$E + 2t(\cos[k_x] + \cos(k_{y0})) = 0 \quad (11)$$

We have to restrict the limits of integration on k_x because the above equation may not have a solution k_{y0} for any k_x . Indeed,

$$(12)$$

where $\epsilon = E/2t$ so we see that $\cos(k_x) < 1 - \epsilon$ is required for any $\epsilon > 0$. This is consistent with our original statement that $N(E)$ will vanish for $E > 4$, ($\epsilon > 2$).

Well, actually the restriction $\cos(k_x) < 1 - \epsilon$ means that the k_x integral which originally went from $-\pi$ to π now is two integrals, one from $-\pi$ to $-\cos^{-1}(1 - \epsilon)$ and the other from $\cos^{-1}(1 - \epsilon)$ to π . These give equal contributions and we find

$$N(E) = \frac{L^2}{2\pi^2 t} \int_{k_1}^{\pi} dk_x \frac{1}{\sqrt{1 - (\epsilon + \cos(k_x))^2}}. \quad (13)$$

Here $k_1 = \cos^{-1}(1 - \epsilon)$.

We now see the divergence of $N(E)$ as a possibility, since the integrand diverges at the lower limit. However, the integrand diverges there for any E . Why should $E = \epsilon = 0$ be special? The reason is rather clear. Since $\cos(k)$ has zero slope at $k = 0$, it spends a lot of time at values near 1. Other values it passes through rather quickly. Thus when $E = \epsilon = 0$ there

will be many k values contributing to the region where the integrand is large. Indeed at this point we see that

$$N(E) = \frac{L^2}{2\pi^2 t} \int_0^\pi dk_x \frac{1}{\sin(k_x)} \quad (14)$$

which clearly is infinite since $\sin(k_x) \approx k_x$ near $k_x = 0$.

To see what happens at other E , we look up in Gradshteyn and Ryzhik the definition of the elliptic integrals and find (8.111)

$$F(\phi, k) = \int_0^\phi \frac{d\alpha}{\sqrt{1 - k^2 \sin^2 \alpha}}. \quad (15)$$

This looks similar to our form, so we will not be surprised to find that our $N(E)$ is some sort of elliptic integral. We just need to cast it into the right form. Before doing this, let's evaluate the integral at small ϵ to see the manner of the divergence. If ϵ small, the big contribution will be at small k . Expanding in both of these small quantities,

$$N(E) \propto \int_{\sqrt{2\epsilon}} \frac{dk}{\sqrt{k^2 - 2\epsilon}} \propto \ln(\epsilon) \propto \ln(E). \quad (16)$$

As described in class, this divergence in $N(E)$ has been invoked in a variety of high T_c theories. The basic idea is that in the BCS form for the transition temperature

$$T_c = \omega_0 e^{-1/g(E_F)V}, \quad (17)$$

a large density of states increases T_c .

To continue with the explicit evaluation of the integral we do a change of variables, $u = \cos(k_x)$. Then our integral becomes

$$\begin{aligned} N(E) &= \frac{L^2}{2\pi^2 t} \int_{-1}^{1-\epsilon} \frac{du}{\sqrt{1-u^2}} \frac{1}{\sqrt{1-(\epsilon+u)^2}} \\ &= \frac{L^2}{2\pi^2 t} \int_{-1}^{1-\epsilon} \frac{du}{\sqrt{1-u}\sqrt{u+1}\sqrt{1-\epsilon-u}\sqrt{u+1+\epsilon}}. \end{aligned} \quad (18)$$

We now notice that this is precisely in the form of the definition of the elliptic integral:

$$\begin{aligned} \frac{2}{\sqrt{(a-c)(b-d)}} f(\delta, q) &= \int_{-1}^t \frac{du}{\sqrt{a-u}\sqrt{u-c}\sqrt{b-u}\sqrt{u-d}}, \\ \delta &= \sin^{-1} \left[\frac{(b-d)(t-c)}{(b-c)(t-d)} \right] \\ q &= \left[\frac{(b-c)(t-d)}{(a-c)(b-d)} \right]^{\frac{1}{2}} \end{aligned} \quad (19)$$

with the definitions $a = 1, c = -1, b = 1 - \epsilon, d = -\epsilon - 1$. These definitions satisfy the requirements $d < c < u < b \leq a$ of the definition of f . Plugging in the actual values of a, b, c, d we can explicitly evaluate

$$\begin{aligned}\delta &= \sin^{-1}(1) = \frac{\pi}{2} \\ q &= \sqrt{\frac{2 - \epsilon}{2}} = \frac{4t - E}{4t}.\end{aligned}\tag{20}$$

It is nice that q turns out to be a simple combination of E and t .

It is pretty trivial to get the DOS computationally, as discussed in class. How does such a calculation go? We use the discrete form of the summation over k -space instead of doing integrals as we have done in our analytic calculations above. Thus we take a (discrete) set of levels $E(k_x, k_y) = -2t(\cos(k_x) + \cos(k_y))$ where $k_x, k_y = 2\pi/N\{1, 2, \dots, N\}$. One approach is to divide up the interval $(-4t, 4t)$ into some set of bins and plop each $E(k_x, k_y)$ into the appropriate bin. If we look at a $10^4 \times 10^4$ lattice we have 10^8 \mathbf{k} points to loop over. Compute $E(k_x, k_y)$ and binning it is 10^1 - 10^2 operations, so, with a 3 GHz chip we expect the computation to take just a few seconds. The result is shown in Fig. 2.

In class I also mentioned that binning has the disadvantage of a bit ‘pixelated’. Another way to put its disadvantage is that it is non-linear: A small change in the value of the energy can move you to an entirely new bin. A smoother way to do things is to associate a narrow, but smooth function with each level, e.g. evaluate

$$N(E) = \frac{1}{\delta\sqrt{\pi}} \sum_{k_x, k_y} e^{-\left(E - E(k_x, k_y)\right)^2 / \delta^2}\tag{21}$$

where δ is some small number playing a similar role to that of the bin size.

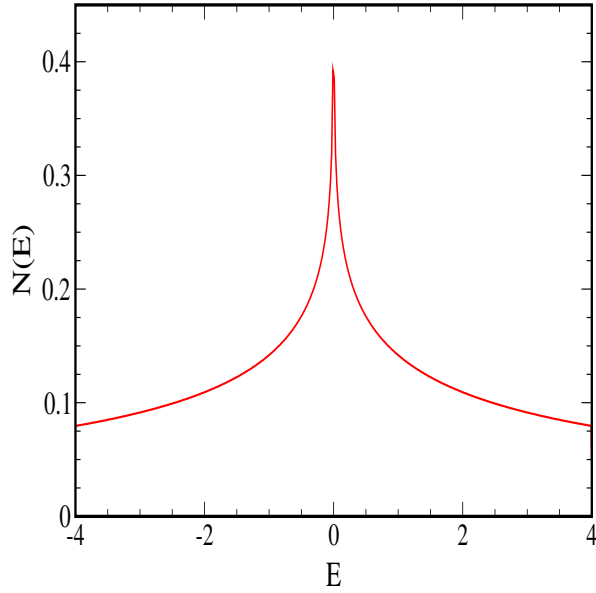


Figure 2: Numerical computation of the DOS of the two dimensional square lattice tight binding dispersion relation using 10000 bins and a $10^4 \times 10^4$ lattice. Despite my complaints about binning, the result is pretty smooth and the singularity at $E = 0$ is well-captured.

A little fortran code:

```

implicit none
integer ix,iy,N,ibin,Nbin
real*8 kx,ky,E,tpiN,dos(0:10000)

write (6,*) 'enter N,Nbin'
read (5,*)      N,Nbin
tpiN=8.d0*datan(1.d0)/dfloat(N)

do 10 ibin=0,Nbin
    dos(ibin)=0.d0
10  continue

do 110 iy=-N/2+1,N/2
    ky=tpiN*dfloat(iy)
do 100 ix=-N/2+1,N/2
    kx=tpiN*dfloat(ix)
    E=-2.d0*dcos(kx)-2.d0*dcos(ky)
    ibin=int( dfloat(Nbin)*(E+4.d0)/8.d0 )
    dos(ibin)=dos(ibin)+1.d0
100  continue
110  continue

do 200 ibin=0,Nbin
    E=-4.d0+8.d0*dfloat(ibin)/dfloat(Nbin)
    E= E  +4.d0/dfloat(Nbin)
    write (82,990) E,dfloat(Nbin)*dos(ibin)/dfloat(N*N)/8.d0
200  continue

990  format(2f12.6)

end

```

Problem 4-4

In class we derived the relation between the energy and density $n = \frac{N}{V}$ at $T = 0$:

$$E = \frac{3}{5}NE_F = \frac{3}{5}N \frac{\hbar^2}{2m} \left(3\pi^2 \frac{N}{V} \right)^{2/3} \quad (22)$$

Taking the derivative with respect to volume,

$$P = -\frac{\partial E}{\partial V} = \frac{2E}{3V} \quad (23)$$

Compare this to the (mon-atomic) ideal gas case

$$\begin{aligned} PV &= Nk_{\text{B}}T \\ E &= \frac{3}{2}Nk_{\text{B}}T \\ P &= \frac{2E}{3V} \end{aligned} \quad (24)$$

Note, however, that despite this apparent similarity the energy of electrons in a metal is *much* higher than that of atoms in a gas at STP, so the pressure of electrons in a metal is also very large.

Problem 4-5

A good derivation of the Sommerfeld expansion is given in the appendix to Ashcroft and Mermin. Here I just want to summarize the features that everyone should know. We are interested in calculating integrals like

$$\begin{aligned}
 I_A &= \int_{-\infty}^{\infty} A(E)f(E)g(E)dE \\
 f(E) &= [e^{-\beta(E-\mu)} + 1]^{-1} \quad (\text{the Fermi function}) \\
 g(E) &= \text{the density of states} \\
 A(E) &= \text{some physical quantity}
 \end{aligned}
 \tag{25}$$

The Sommerfeld expansion provides a procedure for doing this which is based on the special structure of the Fermi function. At zero temperature, $f(E)$ is unity for $E < \mu = E_F$ and zero for $E > \mu$. When $T \neq 0$ there is some rounding of the sharp step. This rounding has a width set by T . Meanwhile $A(E)$ and $g(E)$ are presumed to be relatively smooth. μ typically has values in the electron volt range, that is 10^4 degrees Kelvin. Thus $\mu \gg T$. The two most important applications are when $A(E) = 2$, in which case we are just counting the number of electrons in the solid, and to $A(E) = 2E$, in which case we obtain the average energy.

This mathematics embodies some of the most important physics of electrons in solids, namely that the Pauli principle forbids the scattering of most of the electrons, since thermal excitations cannot take them to unoccupied states unless they lie near the Fermi energy. Thus the specific heat of the electrons in a metal is reduced by two orders of magnitude, the ratio of $k_B T$ to E_F , from its classical equipartition value and, indeed, picks up a nontrivial temperature dependence discussed below.

These simple ideas are somewhat complicated by the fact that the chemical potential μ depends on the temperature. Remember we regard μ as an adjustable parameter which gives us the correct number N of electrons in the solid. If we want the specific heat, we want to compute the change in energy keeping, among other things, N constant. Thus we must begin by computing $N(T, \mu)$ and inverting the relation to get $\mu(N, T)$. We are then in a position to compute other quantities keeping N fixed.

The important results are summarized here:

$$\begin{aligned}
 \mu &= E_F \left[1 - \frac{1}{3} \left(\frac{\pi k_B T}{2E_F} \right)^2 \right], \\
 \frac{E}{N} &= \frac{E_0}{N} + \frac{\pi^2}{6} (k_B T)^2 g(E_F).
 \end{aligned}
 \tag{26}$$

The Fermi energy E_F is the energy up to which one fills states at $T = 0$ to get the desired number of particles, so that the chemical potential μ equals E_F at $T = 0$. As T increases, μ shifts downward. This is sometimes a useful general fact for doing numerical work. Recall also the form for the density of states $g(E_F) = 3n/2E_F$.

The most important consequence of Eq. (2.3.2) is the linear contribution of the electronic degrees of freedom to the specific heat of a solid. As we shall see next quarter, lattice vibrations contribute with a T^3 dependence. Thus when one plots C/T vs. T^2 one gets a straight line whose intercept measures the electronic part of C and whose slope measures the part due to the phonons.