

PHYSICS 525, CONDENSED MATTER

Homework 3

Due Tuesday, 16th October 2006

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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.

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

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

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,

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

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

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.

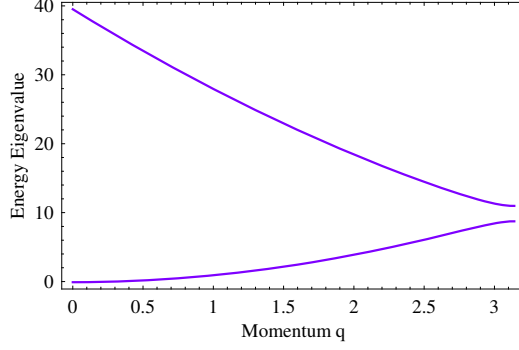


FIGURE 1. The second-order band structure for a one-dimensional system in a weak sinusoidal potential.

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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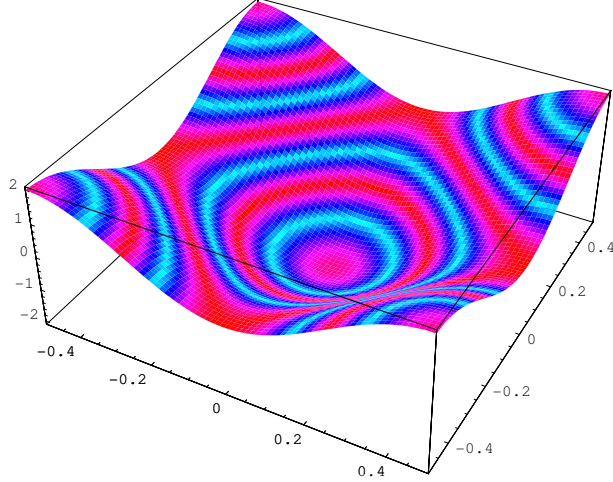


FIGURE 2. The first Brillouin zone dispersion for a tight-binding model on a two-dimensional square lattice.

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.

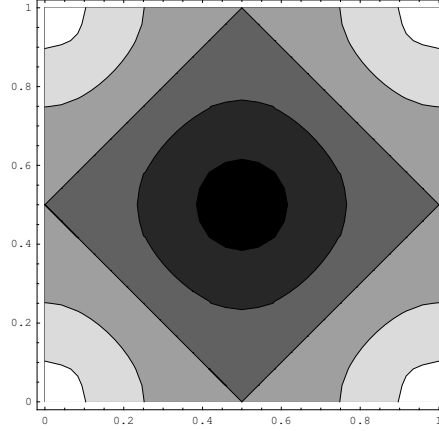


FIGURE 3. Several Fermi surfaces observed for a tight-binding square lattice model. Dark colouring indicates lower energy—Fermi surfaces are included for the band both more than and less than half filled. The half-filled Fermi surface is the clearly visible square in the plot.

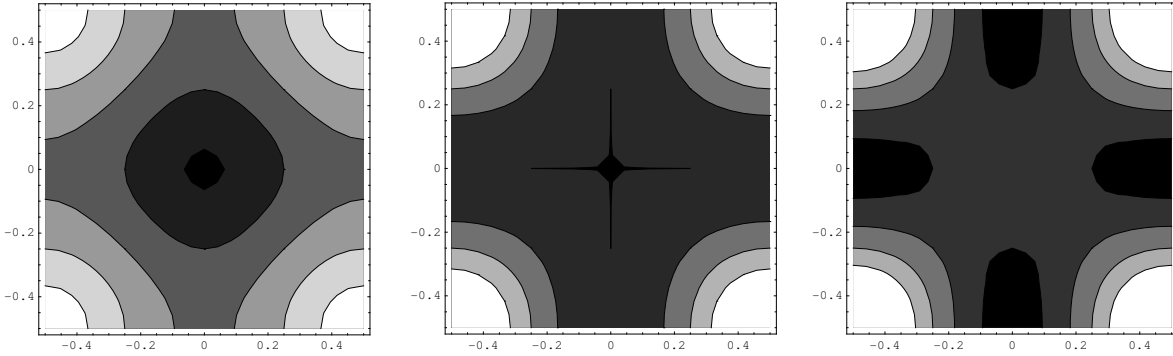


FIGURE 4. Fermi surfaces in the tight-binding square-lattice model with $t' > 0$ next-to-nearest-neighbour couplings for various values of $t'/|t|$. From left to right: $t'/|t| = 1/10$, $t'/|t| = 1/2$, and $t'/|t| = 7/10$. Notice the sharp transition at $t'/|t| = 1/2$.

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 $t' < 0$.

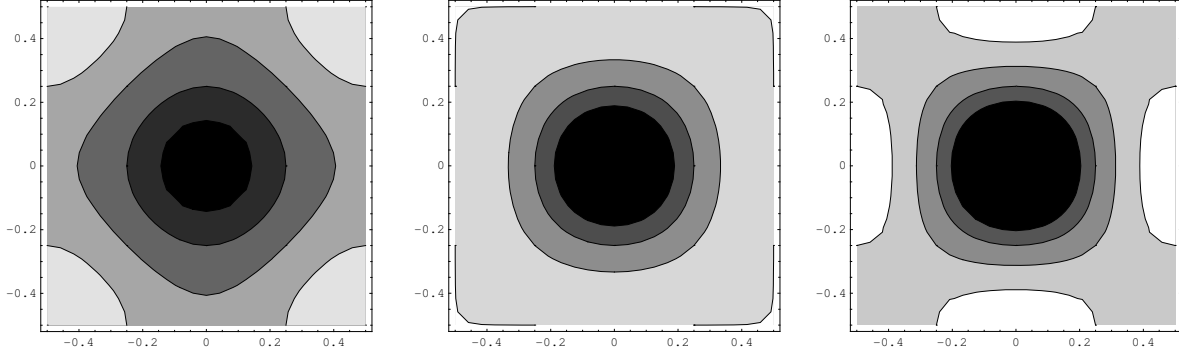


FIGURE 5. Fermi surfaces in the tight-binding square-lattice model with $t' < 0$ next-to-nearest-neighbour couplings for various values of $t'/|t|$. From left to right: $t'/|t| = -1/10$, $t'/|t| = -1/2$, and $t'/|t| = -9/10$. Notice the sharp transition at $t'/|t| = -1/2$.

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.

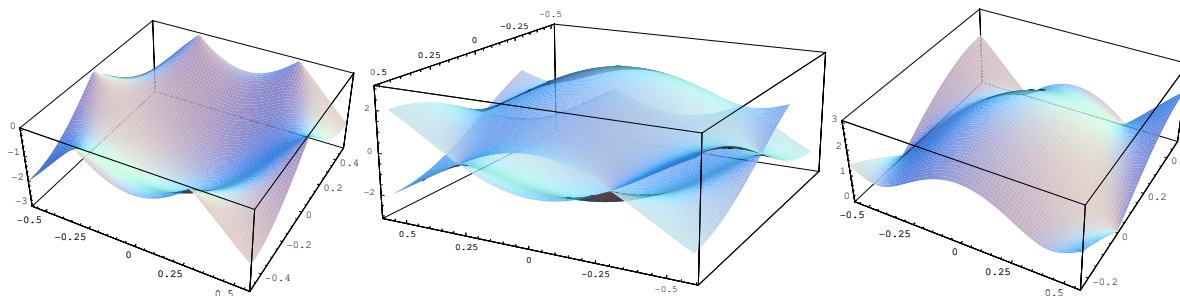


FIGURE 6. Energy bands calculated for graphene: the bands are shown separately on the right and left, and shown together in the middle. Notice there are precisely six degeneracies located in the first Brillouin zone.

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).

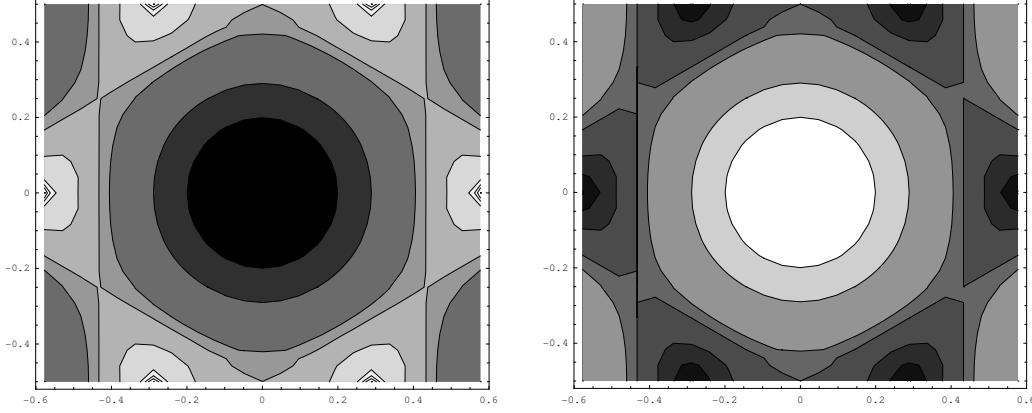


FIGURE 7. Contours indicating the Fermi surfaces for various ϵ_F in the lower (left) and upper (right) bands for the graphene tight-binding model. In both plots the energy is lower in the darker region—regions in white on the left plot match to the regions in black on the right plot.

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.