Quantum Physics III (8.06) Spring 2005
Solution Set 2

February 15, 2005

1. **Fermi energy, velocity and temperature of copper**

   Griffiths 2^{nd} ed. problem 5.16 (1^{st} ed. problem 5.13).

   (a) (1 points) In order to find the Fermi energy, we need to first have the number density of electrons. Copper has one valence electron (i.e., we are taking $q = 1$) so the number density of electrons will be the same as the number density of atoms in copper. This in turn is given by

   $$\rho = \frac{8.96\,\mathrm{gm/cm^3}}{63.5\,\mathrm{gm/mole}}\,\frac{6.02\times 10^{23}\,\mathrm{atoms}}{\mathrm{mole}} = 8.49\times 10^{28}\,\mathrm{atoms}/m^3.$$

   It is now easy to calculate

   $$E_F = \frac{\hbar^2(3\pi^2\rho)^{2/3}}{2m} = 1.13\times 10^{-18}\,\mathrm{joules} = 7.05\,\mathrm{eV}.$$

   (b) (1 points) With $E_F = \frac{1}{2}mv_F^2$, we find $v_F = 1.57\times 10^6\,m/\mathrm{s}$. Although this is very fast, it is only about half a percent of the speed of light, and so it is still okay to treat the electrons as non relativistic.

   (c) (1 point) The Fermi temperature is given by $T_F = E_F/k_B = 81800\,K$. This is much larger than the melting point of copper, let alone room temperature!

   (d) (1 point) The degeneracy pressure is given by $P = \hbar^2(3\pi^2)^{2/3}\rho^{5/3}/(5m) = 3.83\times 10^{10}\,N/m^2$. This is phenomenally large; fermions *really* do not like being in the same place.

2. **The Kronig-Penney Model**

   (a) (9 points) Griffiths 2 ed. problem 5.20. When we make the periodic delta function potential attractive instead of repulsive, we find that the allowed energies (when $E > 0$) are determined through the equation

   $$\cos(Ka) = \cos(ka) - \frac{m\alpha}{\hbar^2 k}\sin(ka), \tag{1}$$

   where $k = \sqrt{2mE}/\hbar$. We only need to change the sign of α, the strength of Delta function, in Griffiths 2^{nd} ed. eqn. (5.64). Using non-dimensional variables $z \equiv ka$ and $\beta \equiv m\alpha a/\hbar^2$, we rewrite right hand side of above equation as

   $$f(z) \equiv \cos(z) - \beta\frac{\sin(z)}{z}. \tag{2}$$

   We plot it for $\beta = 1$ in figure 1 and $\beta = 3$ in figure 2. For the bands for which $f(z)$ varies from -1 to $+1$, i.e. $\cos(Ka)$ varies from -1 to $+1$, hence K varies from 0 to $2\pi/a$ and therefore band contains N states. In $\beta = 1$ case (fig.1) first allowed band has $N/2$ states because $f(z)$ varies from 0 to -1, hence K varies from $\pi/2a$ to $3\pi/2a$. For $\beta = 3$, in all bands $f(z)$ varies from -1 to $+1$ thus the bands contain N states each. Band gaps slowly decrease for subsequent bands.

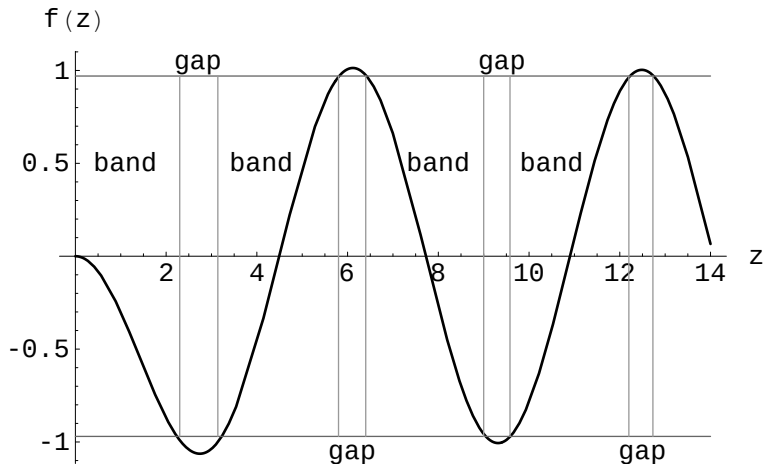

Figure 1: $f(z)$ for $\beta = 1$.

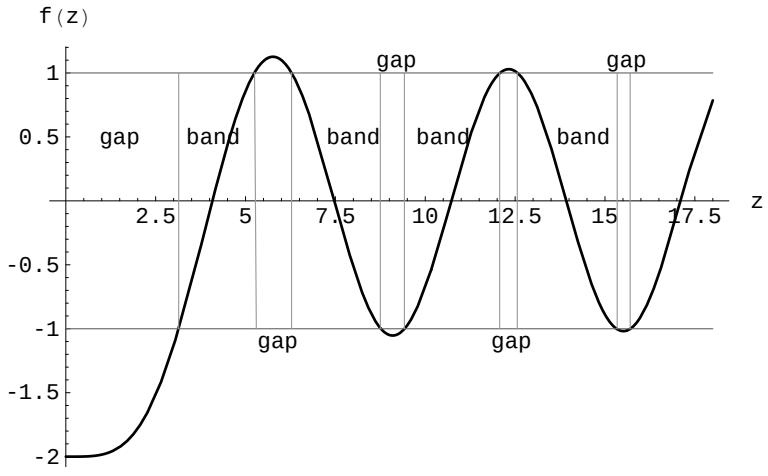

Figure 2: $f(z)$ for $\beta = 3$.

For $0 < \beta < 1$ we will have more states in the first band and for $1 < \beta \leq 2$, less states. For $\beta > 2$ (for example $\beta = 3$) we will have N states in all bands but first band won't start with $k = 0$. See figure 2.

Since we have an attractive Dirac comb we can also have negative energy states or bound states i.e. $E < 0$. Define $\kappa = \sqrt{2m|E|}/\hbar$. Since potential is 0 in the region $0 < x < a$ we can write,

$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x}. \qquad (0 < x < a)$$

From Bloch theorem we have,

$$\psi(x) = e^{-iKa}\psi(x + a). \qquad (-a < x < 0)$$

$$\Rightarrow \psi(x) = e^{-iKa}(Ae^{\kappa(x+a)} + Be^{-\kappa(x+a)}). \qquad (-a < x < 0)$$

Continuity condition for ψ at $x = 0$ gives

$$A(1 - e^{-iKa}e^{\kappa a}) = B(e^{-iKa}e^{-\kappa a} - 1).$$

While ψ' suffers a discontinuity proportional to the strength of the delta function (Griffiths 2^{nd} ed. eqn. (2.125)):

$$A\left(1 - e^{-iKa}e^{\kappa a} + \frac{2m\alpha}{\hbar^2\kappa}\right) = B\left(1 - e^{-iKa}e^{-\kappa a} - \frac{2m\alpha}{\hbar^2\kappa}\right).$$

Eliminating A and B from the above two equations and simplifying we obtain the required result,

$$\cos(Ka) = \cosh(\kappa a) - \frac{m\alpha}{\hbar^2\kappa}\sinh(\kappa a).$$

[NOTE: We can obtain the same result by substituting $k = -i\kappa$ in eqn. (1).] For $z = \kappa a$ we rewrite right hand side of the above equation as,

$$h(z) \equiv \cosh(z) - \beta\frac{\sinh(z)}{z}. \qquad (3)$$

We plot this for $\beta = 1$ and $\beta = 3$ in figure 3. For negative energies we have only one allowed band, which can be full or partial depending on the value of β. For $\beta \geq 2$ we will have N states in the band and for $\beta < 2$ we will have less than N states. At $\beta = 1$, there are exactly $N/2$ states in this band. Band moves farther away from $E = 0$ and becomes narrower as β increases beyond 2 (for example $\beta = 3$). Now combining the results, for the case $\beta < 2$, for positive and negative E we find that, the only band for $E < 0$ and lowest band for $E > 0$ combine together and actually has exactly N states. Hence the lowest band in the full spectrum is partially above and below $E = 0$ (see figure 4). For $\beta > 2$ (for example $\beta = 3$) it is completely below $E = 0$. A rough picture of the energy spectrum for $\beta = 1$ is shown in figure 4 and that for $\beta = 3$ in figure 5. For full credit students should make graphs for one value of β and draw correct conclusions for that value.

(b) (3 points) Through the equation

$$\cos(Ka) = \cos(ka) + \beta\frac{\sin(ka)}{ka} \qquad (4)$$

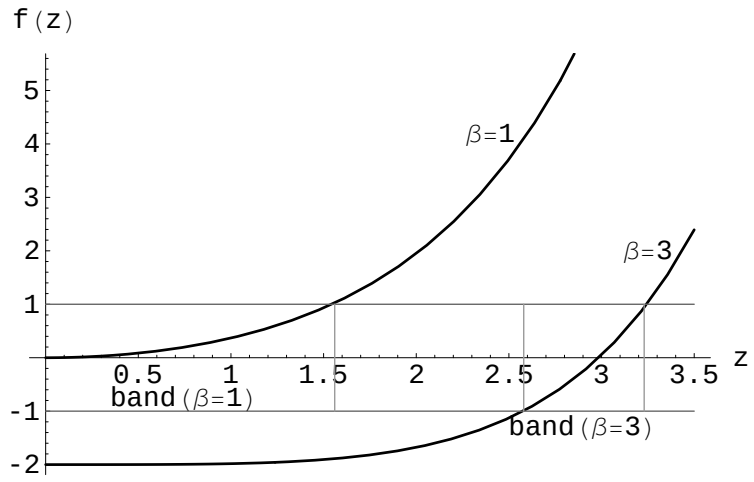

Figure 3: $h(z)$ for $\beta = 1$ and $\beta = 3$.

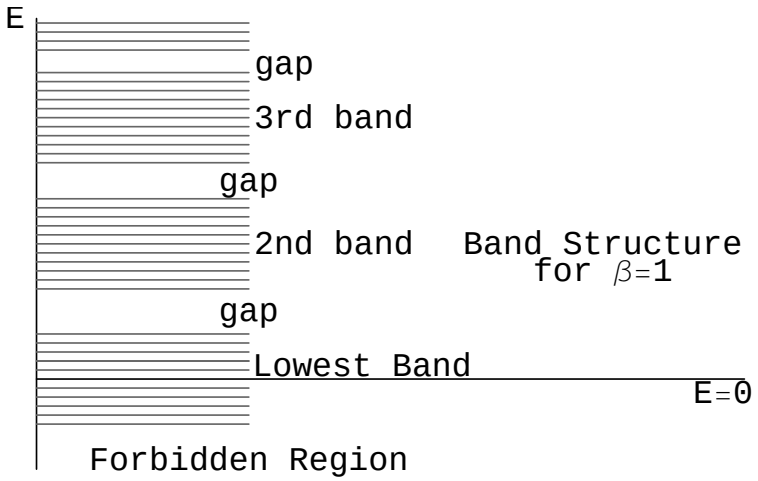

Figure 4: Schematic sketch of the energy spectrum for $\beta = 1$.

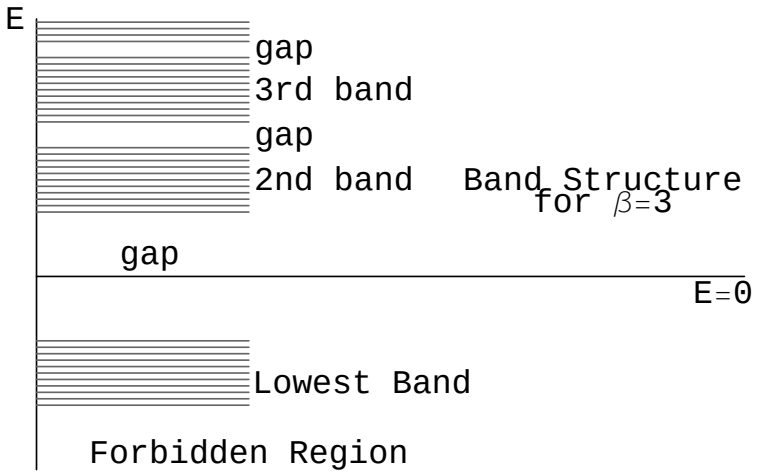

Figure 5: Schematic sketch of the energy spectrum for $\beta = 3$.

every value of $\cos(Ka)$ determines a k and therefore an energy $E = \hbar^2 k^2/2m$. Now $K = \frac{2\pi n}{Na}$, where $n = 0, 1, \ldots, N-1$. Also, $\cos\theta = \cos(2\pi - \theta)$, and therefore $\cos(\frac{2\pi n}{N}) = \cos(\frac{2\pi(N-n)}{N})$. We can therefore identify two cases: first, if $n = 0$ or $n = N/2$, then the above equality is trivial, and the energies resulting from equation (4) are non degenerate. Second, for all other values of n, n and $N - n$ give the same value of $\cos(Ka)$ (and $n \neq N - n$), and therefore the energies resulting from equation (4) are doubly degenerate.

3. **Analysis of a general one-dimensional periodic potential**

(a) (2 points) When we differentiate the Wronskian, we find

$$\frac{dW}{dx} = \psi_2\psi_1'' - \psi_1\psi_2''.$$

According to the Schrodinger equation, $\psi_1'' = -\frac{2m}{\hbar^2}(E - v)\psi_1$, and similarly for ψ_2. Therefore

$$\frac{dW}{dx} = -\frac{2m}{\hbar^2}(E - v)(\psi_2\psi_1 - \psi_1\psi_2) = 0.$$

(b) (2 points) First, we evaluate the Wronskian for $x \leq -a/2$:

$$W(x \leq -a/2) = -2ikrt^*.$$

For $x \geq a/2$, on the other hand, we have

$$W(x \geq a/2) = 2ikr^*t.$$

This tells us that $(rt^*) = -(rt^*)^*$, and therefore that rt^* is pure imaginary.

(c) (8 points) The Bloch conditions on ψ and ψ' yield the equations

$$\begin{aligned} A(e^{iKa} + re^{i(k+K)a} - te^{ika}) &= B(1 + re^{ika} - te^{i(K+k)a}) \\ A(e^{iKa} - re^{i(k+K)a} - te^{ika}) &= B(-1 + re^{ika} + te^{i(K+k)a}). \end{aligned}$$

Dividing the first equation by the second yields

$$\frac{e^{iKa}+re^{i(k+K)a}-te^{ika}}{e^{iKa}-re^{i(k+K)a}-te^{ika}}=\frac{1+re^{ika}-te^{i(K+k)a}}{-1+re^{ika}+te^{i(K+k)a}}.$$

Multiplying through by the denominators yields

$$(e^{iKa}+re^{i(k+K)a}-te^{ika})(-1+re^{ika}+te^{i(K+k)a})=(1+re^{ika}-te^{i(K+k)a})(e^{iKa}-re^{i(k+K)a}-te^{ika}),$$

which after expansion and canceling terms gives

$$e^{iKa}(-1+(r^2-t^2)e^{2ika})+e^{2iKa}(te^{ika})+te^{ika}=0.$$

Adjusting the phases and rearranging gives the desired answer,

$$\cos(Ka)=\frac{1}{2t}(e^{-ika}+(t^2-r^2)e^{ika}). \tag{5}$$

(d) (2 points) Using the parameterizations for r and t given in the problem set, we find $\frac{t^2-r^2}{t}=e^{i\delta}\frac{1}{|t|}$. Since $\frac{1}{t}=\frac{1}{|t|}e^{-i\delta}$, equation (5) becomes

$$\cos(Ka)=\frac{\cos(ka+\delta)}{|t|}. \tag{6}$$

(e) (6 points) We want to consider situations such that $|t|\ll 1$. To be able to solve (6), we must have $\cos(ka+\delta)\leq|t|$. Since that means the cosine must be very small, its argument must be near $(n+1/2)\pi$, and therefore we can expand $\cos(ka+\delta)\simeq|ka+\delta-(n+1/2)\pi|$. This means that the largest allowed value of k is given by

$$k_{max}=\frac{1}{a}\left(\frac{(2n+1)\pi}{2}-\delta+|t|\right),$$

while the smallest allowed value of k is given by

$$k_{min}=\frac{1}{a}\left(\frac{(2n+1)\pi}{2}-\delta-|t|\right).$$

The allowed range of energies is given by $\hbar^2(k_{max}^2-k_{min}^2)/2m$, which is

$$\begin{aligned}\Delta E &= \frac{\hbar^2}{2ma^2}\left[\left(\frac{(2n+1)\pi}{2}-\delta+|t|\right)^2-\left(\frac{(2n+1)\pi}{2}-\delta-|t|\right)^2\right]\\ &= \frac{2\hbar^2}{ma^2}\left(\frac{(2n+1)\pi}{2}-\delta\right)|t|,\end{aligned}$$

which is proportional to $|t|$.

(f) (6 points) We now want to consider situations where $|r|\ll 1$. In this case, the right hand side of equation (6) is larger than one only when $\cos(ka+\delta)\geq|t|=(1-|r|^2/2)$. (We have used the binomial expansion to simplify the relationship between $|r|$ and $|t|$.) Since δ is very small, we can drop it; expanding the cosine then gives us

$$|ka-n\pi|\leq|r|.$$

In this case the largest value of k satisfying the above (or the smallest value of allowed k above $n\pi$) is given by $k_{max}a = n\pi + |r|$, while the smallest value of k (or the largest value of allowed k below $n\pi$) is given by $k_{min}a = n\pi - |r|$. From this we find that the forbidden range of energies is (to leading order in $|r|$)

$$\begin{aligned}\Delta E &= \left(\frac{\hbar^2}{2ma^2}(n^2\pi^2 + 2|r|n\pi) - \frac{\hbar^2}{2ma^2}(n^2\pi^2 - 2|r|n\pi)\right) \\ &= \frac{2\hbar^2 n\pi|r|}{ma^2}.\end{aligned}$$

(g) (6 points) We now wish to make the above discussion a bit more concrete, and we take our periodic potential to be an array of repulsive delta functions. To see what our above formulas tell us about this case, we first need to solve for r and t. To do this, it is sufficient to consider ψ_L and ψ'_L at $x = 0$. Continuity of ψ_L at $x = 0$ tells us

$$1 + r = t. \tag{7}$$

Meanwhile the continuity condition on ψ'_L at 0 is modified by the delta function (use eqn. (2.125) of Griffiths 2^{nd} ed.) to give us

$$t - (1 - r) = \frac{2m\alpha}{ik\hbar^2}t. \tag{8}$$

Recalling that $t = |t|e^{i\delta}$ and $r = \pm i|r|e^{i\delta}$, the imaginary part of (7) tells us that

$$\pm|r|\cos\delta = |t|\sin\delta,$$

while the real part gives us

$$\mp|r|\sin\delta = |t|\cos\delta - 1.$$

Combining the two above equations tells us

$$|t| = \cos\delta.$$

Meanwhile, substituting $r = t - 1$ into (8) tells us that

$$t = \frac{1 - \frac{im\alpha}{\hbar^2 k}}{1 + \left(\frac{m\alpha}{\hbar^2 k}\right)^2}.$$

Now $\cot\delta = \frac{Re\, t}{Im\, t}$, so from the above

$$\cot\delta = -\frac{\hbar^2 k}{m\alpha}.$$

When we plug these expressions for $\cot\delta$ and $|t|$ into equation (8) of the problem set, we find

$$\begin{aligned}\cos(Ka) &= \frac{\cos(ka)\cos\delta - \sin(ka)\sin\delta}{\cos\delta} \\ &= \cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka),\end{aligned}$$

which is precisely the equation derived in Griffiths.

4. **An operator ordering ambiguity**

(2 points) First, we calculate $[\hat{x}^2, \hat{p}^2] = 2i\hbar(\hat{x}\hat{p} + \hat{p}\hat{x})$, and the classical Poisson bracket $\{x^2, p^2\}_{PB} = 4xp$. Using the general rule to obtain the quantum commutator from the classical Poisson bracket, $[\hat{A}, \hat{B}] = i\hbar\{A, B\}_{PB}$, would give us $[\hat{x}^2, \hat{p}^2] = 4i\hbar\hat{x}\hat{p}$. Further requiring that i times the commutator be a Hermitian operator gives us $[\hat{x}^2, \hat{p}^2] = 2i\hbar(\hat{x}\hat{p} + \hat{p}\hat{x})$, which is correct.

(4 points) We now calculate $[\hat{x}^3, \hat{p}^3] = 3i\hbar(\hat{p}^2\hat{x}^2 + \hat{p}\hat{x}^2\hat{p} + \hat{x}^2\hat{p}^2)$, and the classical Poisson bracket $\{x^3, p^3\}_{PB} = 9x^2p^2$. As in the previous case, the general rule $[\hat{A}, \hat{B}] = i\hbar\{A, B\}_{PB}$ gives us the correct quantum mechanical commutator up to operator ordering. Unlike the previous case, however, the requirement that the right hand side of the commutator be i times a Hermitian operator is not sufficient to give us the correct answer. This is because there are many different possible Hermitian combinations of two $\hat{x}$'s and two $\hat{p}$'s; two such possible combinations appear in the answer above, $\hat{p}^2\hat{x}^2 + \hat{x}^2\hat{p}^2$ and $\hat{p}\hat{x}^2\hat{p}$, but others, such as $\hat{x}\hat{p}^2\hat{x}$ do not.

5. **Landau Levels: a prelude**

(a) (3 points) When $B = 10$ tesla, then the energy spacing $\hbar\omega_L$ is given by

$$\begin{aligned} \hbar\omega_L &= \frac{\hbar ceB}{mc^2} = \frac{(197 \times 10^{-7}\,\text{eVcm})(300 \times 10^5\,\text{eV/cm})}{511\,\text{keV}} \\ &= 1.2 \times 10^{-3}\,\text{eV}. \end{aligned}$$

In natural units the length ℓ_0 is

$$\ell_0 = \sqrt{\frac{\hbar}{m\omega_L}} = \hbar c\sqrt{\frac{1}{mc^2\hbar\omega_L}} = 4.1 \times 10^{-2}\,\frac{\hbar c}{\text{eV}}.$$

Notice that this length is the inverse of the geometric average of the two energy scales of the problem: the rest energy of the electron, and the cyclotron energy $\hbar\omega_L$. Finally, in cm, $\ell_0 = 8.0 \times 10^{-7}$cm.

(b) (3 points) The magnetic flux through the area $A_B = 2\pi\ell_0^2$ is

$$\Phi_B = 2\pi\ell_0^2 B = B\frac{h}{m}\left(\frac{mc}{eB}\right) = \frac{hc}{e}.$$

As we will see, this is precisely one so-called flux quantum.