Quantum Physics III (8.06) Spring 2006
Solution Set 2

February 18, 2006

1. **Eigenstates of the "Translation" Operator in tight-banding model (5 points)**

   We want to find a state
   $$|\theta\rangle = \sum_{n\in\mathbb{Z}} c_n|n\rangle$$
   such that
   $$T|\theta\rangle = e^{-i\theta}|\theta\rangle.$$
   Acting with T on $|\theta\rangle$ we have
   $$T|\theta\rangle = T\sum_{n\in\mathbb{Z}} c_n|n\rangle = \sum_{n\in\mathbb{Z}} c_n|n+1\rangle = \sum_{n\in\mathbb{Z}} c_{n-1}|n\rangle.$$
   So we we see that
   $$c_{n-1} = e^{-i\theta}c_n$$
   and therefore
   $$c_n = e^{in\theta}c_0.$$
   The coefficient c_0 is a free parameter which we can set to 1. Thus
   $$|\theta\rangle = \sum_{n\in\mathbb{Z}} e^{in\theta}|n\rangle \tag{1}$$

   Appendix: energy eigenvalues

   Let us find the energy eigenvalues directly using (1) (an alternative way from that discussed in lecture). Acting with hamiltonian H on $|\theta\rangle$ and collecting terms together we have
   $$\begin{aligned} H|\theta\rangle &= \sum_{n\in\mathbb{Z}} e^{in\theta}(E_0 - \Delta e^{i\theta} - \Delta e^{-i\theta})\,|n\rangle \\ &= (E_0 - 2\Delta\cos\theta)\sum_{n\in\mathbb{Z}} e^{in\theta}|n\rangle \\ &= (E_0 - 2\Delta\cos\theta)\,|\theta\rangle. \end{aligned}$$
   Therefore the energy of $|\theta\rangle$ is
   $$E_\theta = E_0 - 2\Delta\cos\theta.$$

2. **Relativistic degenerate electron gas (10 points)**

   The dispersion relation between the energy and momentum of the ultrarelativistic particles is
   $$E = c\hbar k.$$
   At zero temperature the particles fill all the energy levels up to the Fermi energy ϵ_F.

The density of particles in momentum space, with energies below Fermi level is given by[1].

$$2V\frac{d^3k}{(2\pi)^3}.$$

Thus, the total energy of such a gas is the integral

$$E_{\rm tot} = 2V\int_0^{k_F}\frac{d^3k}{(2\pi)^3}c\hbar k = \frac{8\pi Vc\hbar}{(2\pi)^3}\int_0^{k_F}k^3dk = 2\pi Vc\hbar\frac{k_F^4}{(2\pi)^3}.$$

The total number of particles is given by

$$N = 2V\int_0^{k_F}\frac{d^3k}{(2\pi)^3} = \frac{8\pi V}{(2\pi)^3}\int_0^{k_F}k^2dk = \frac{8\pi V}{3}\frac{k_F^3}{(2\pi)^3}.$$

Therefore

$$E_{\rm tot} = \frac{3}{4}Nc\hbar k_F = \frac{3}{4}N\epsilon_F.$$

3. **White dwarfs, Neutron stars and Black holes (10 points)**

In this problem we treat the star in a constant density approximation ignoring selfconsistency which leads to a more complicated density profile. In parts a and b we assume the particles are nonrelativistic.

The equilibrium point for the white dwarf may be found from the energy balance. The zero point energy of the electron gas in the white dwarf is balanced against the gravitational energy. Let's compute both energies. Consider a thin layer of thickness dr. The mass of this layer is

$$dM(r) = M\frac{dV}{V} = M\frac{4\pi r^2dr}{\frac{4}{3}\pi R^3} = 3M\frac{r^2dr}{R^3}$$

the mass of concentrated within the radius r is

$$M(r) = M\frac{r^3}{R^3}.$$

The gravitational potential energy is given by

$$E_{\rm grav} = \int_0^R -G_N\frac{M(r)dM(r)}{r} = -\frac{3G_NM^2}{R^6}\int_0^R r^4dr = -\frac{3G_NM^2}{5R}$$

The energy of the degenerate electron gas is

$$E_{\rm gas} = 2V\int_0^{k_F}\frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m_e} = \frac{1}{(2\pi)^3}\frac{4\pi\hbar^2V}{m_e}\int_0^{k_F}k^4dk = \frac{\hbar^2k_F^5V}{10\pi^2m_e} \qquad (2)$$

The value of k_F is determined from the normalization condition

$$N = 2V\int_0^{k_F}\frac{d^3k}{(2\pi)^3} = \frac{2}{(2\pi)^3}\frac{4\pi k_F^3}{3} \qquad (3)$$

[1]we use the wavevector instead of momentum, $\vec{p} = \hbar\vec{k}$.

where N is the total number of electrons in the star equal to

$$N = f\frac{M}{m_p} \tag{4}$$

where $f = 1/2$ is the number of electrons per nucleon in the carbon atom and m_p is proton (and neutron) mass. From (3), (4) we find

$$k_F = \Big(\frac{3\pi^2 fM}{m_p V}\Big)^{1/3} = \frac{1}{R}\Big(\frac{9\pi fM}{4m_p}\Big)^{1/3}. \tag{5}$$

Plugging this back into (2) we find

$$E_{\text{gas}} = \frac{2\hbar^2}{15\pi m_e}\frac{1}{R^2}\Big(\frac{9\pi fM}{4m_p}\Big)^{5/3} \tag{6}$$

Summarizing the calculation, the total energy of the system can be written as

$$E_{\text{tot}} = -\frac{a}{R} + \frac{b}{R^2}$$

where

$$a = \frac{3G_N M^2}{5}, \qquad b = \frac{2\hbar^2}{15\pi m_e}\Big(\frac{9\pi fM}{4m_p}\Big)^{5/3}. \tag{7}$$

The white dwarf's radius may be obtained by minimizing the total energy. The extremal points are determined from

$$\frac{\partial E_{\text{tot}}}{\partial R} = \frac{a}{R^2} - \frac{2b}{R^3} = 0.$$

The solution

$$R_{\text{white dwarf}} = \frac{2b}{a} = 7496 \text{ km}$$

is the radius of the dwarf. In fact it is very close to the Earth radius (a coincidence of course).

The ratio of the mass densities of the white dwarf and the sun is

$$\frac{\rho_{\text{white dwarf}}}{\rho_{\text{Sun}}} = \left(\frac{R_{\text{Sun}}}{R_{\text{white dwarf}}}\right)^3 = 8.14 \times 10^5.$$

(b) In a neutron star the pressure is so great that the electrons have merged with protons to form neutrons, so we may assume that the star consists entirely from neutrons. The formula (7) holds if we replace m_e with m_p and use $f = 1$. The radius of the neutron star with the mass of the sun is

$$R_{\text{neutron star}} = 13.5 \text{ km}.$$

The neutron Fermi energy is

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2mR^2}\Big(\frac{9\pi fM}{4m_p}\Big)^{2/3}.$$

To find if the neutrons in the neutron star should be treated as relativistic particles we calculate the ration of the Fermi energy to the rest energy of the neutron

$$\frac{E_F}{m_p c^2} = 0.054,$$

thus the neutrons are nonrelativistic.

(c) The quantity

$$\frac{MG_N}{c^2}$$

has dimensions of length. Since it is the only quantity with the dimension of length which can be constructed out of G_N,M and c it should therefore equal to the Schwarzschild radius up to a numerical constant. Thus we estimate

$$r_s \sim \frac{MG_N}{c^2} \approx 1.48 \text{ km}.$$

4. **The Dirac comb (10 points)**

The reversed Dirac comb potential is

$$V(x) = -\alpha \sum_{j=0}^{N-1} \delta(x - ja)$$

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

$$\cos(Ka) = \cos(ka) - \frac{m\alpha}{\hbar^2 k} \sin(ka), \tag{8}$$

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

$$f(z) \equiv \cos(z) - \beta \frac{\sin(z)}{z}. \tag{9}$$

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. 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. $E < 0$. The negative energy solution within the first cell is

$$\psi(x) = Ae^{-kx} + Be^{kx}, \quad (0 < x < a)$$

where

$$k = \frac{\sqrt{-2mE}}{\hbar}.$$

By the Bloch theorem the solution in the cell immediately to the left is

$$\psi(x) = e^{-iKa}[Ae^{-k(x+a)} + Be^{k(x+a)}], \quad (-a < x < 0).$$

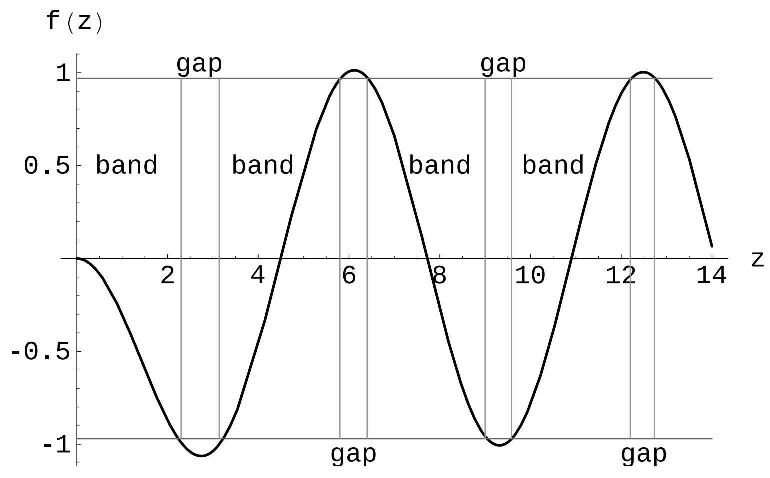

Figure 1: $f(z)$ for $\beta = 1$.

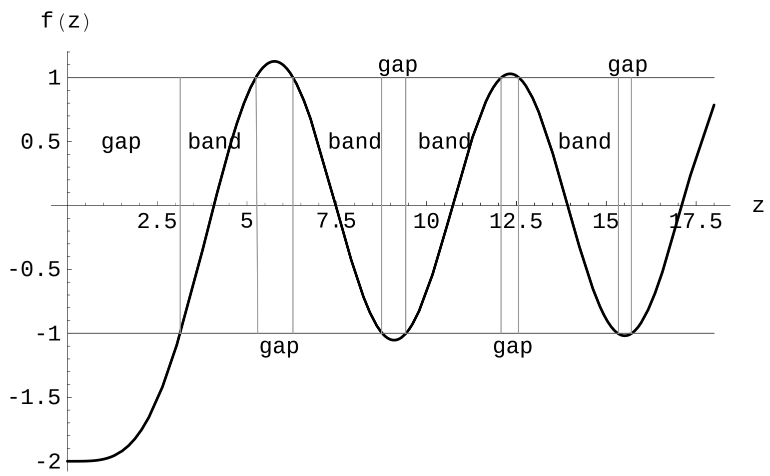

Figure 2: $f(z)$ for $\beta = 3$.

The wave function $\psi(x)$ at the spike point at $x = 0$ is continuous, therefore

$$A + B = e^{-iKa}(Ae^{-ka} + Be^{ka})$$

and the derivative of the wave function has a jump because of the delta function

$$\psi'(x+0) - \psi'(x-0) = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

which becomes

$$k(B-A) - e^{-iKa}k(Be^{ka} - Ae^{-ka}) = -\frac{2m\alpha}{\hbar^2}(B+A).$$

Collecting the terms near A and B we can write the boundary conditions as

$$A(1 - e^{-iKa-ka}) + B(1 - e^{-iKa+ka}) = 0$$
$$A\big(1 - e^{-iKa-ka} - \frac{2m\alpha}{\hbar^2 k}\big) - B\big(1 - e^{-iKa+ka} + \frac{2m\alpha}{\hbar^2 k}\big) = 0$$

This is a system of two linear equations with two unknowns and zero right hand side. To have a non-zero solution the determinant of the system must be zero. Therefore we have

$$\big(1 - e^{-iKa-ka}\big)\big(1 - e^{-iKa+ka} + \frac{2m\alpha}{\hbar^2 k}\big) + \big(1 - e^{-iKa+ka}\big)\big(1 - e^{-iKa-ka} - \frac{2m\alpha}{\hbar^2 k}\big) = 0.$$

Expanding the brackets and collecting terms with the same power of e^{-iKa} we obtain

$$2e^{-2iKa} + 2 - e^{-iKa}\left(2e^{ka} + 2e^{-ka} + \frac{2m\alpha}{\hbar^2 K}(e^{-ka} - e^{ka})\right)$$

Multiplying both sides by $\frac{1}{4}e^{iKa}$ we obtain

$$\cos Ka = \cosh ka - \frac{m\alpha}{\hbar^2 k}\sinh ka \tag{10}$$

The solution to (10) exists if the right hand side is less than one. Let's denote $z = ka$, $\beta = \frac{m\alpha a}{\hbar^2}$ and the the r.h.s. of (10) as $h(z, \beta)$. Then

$$h(z, \beta) = \cosh z - \beta\frac{\sinh z}{z} \tag{11}$$

[NOTE: We can obtain the same result by substituting $k \to -ik$ in eqn. (8).] The condition

$$|h(z, \beta)| = 1 \tag{12}$$

determines the boundaries of allowed zones.

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.

Note: For full credit students only need to make graphs for one value of β and draw correct conclusions for that value.

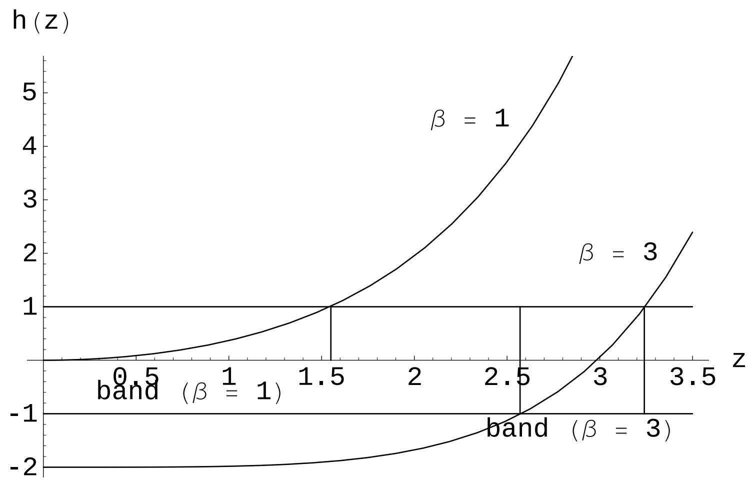

Figure 3: $h(z)$ for $\beta = 1$ and $\beta = 3$.

5. **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 $x \le -a/2$:

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

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

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

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

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

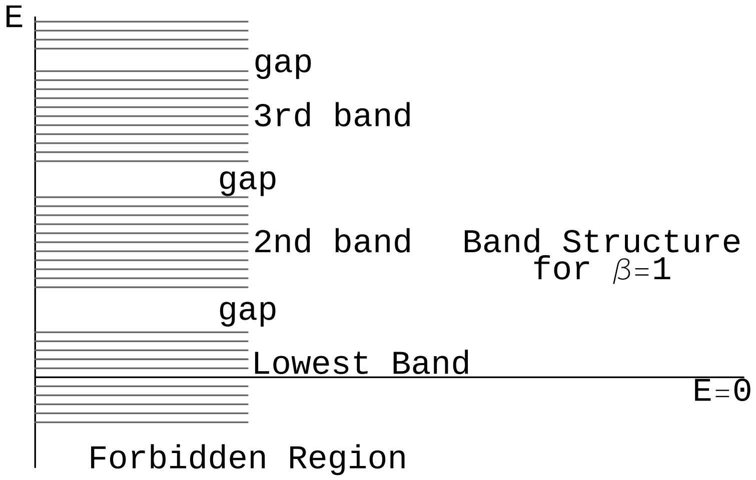

Figure 4: Schematic sketch of the energy spectrum for $\beta = 1$.

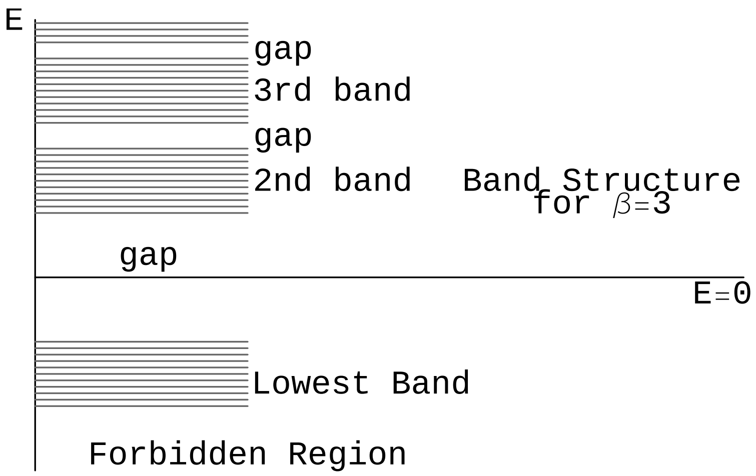

Figure 5: Schematic sketch of the energy spectrum for $\beta = 3$.

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,

$$\cos(Ka) = \frac{1}{2t}(e^{-ika} + (t^2 - r^2)e^{ika}). \tag{13}$$

(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 (13) becomes

$$\cos(Ka) = \frac{\cos(ka + \delta)}{|t|}. \tag{14}$$

(e) (6 points) We want to consider situations such that $|t| \ll 1$. To be able to solve (14), 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 (14) 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 $|r|$)

$$\begin{aligned}\Delta E &= \left(\frac{\hbar^2}{2ma^2}(n^2\pi^2 + 2|r|n\pi) - \frac{\hbar^2}{2ma^2}(n^2\pi^2 - 2|r|n\pi)\right) \\ &= \frac{2\hbar^2 n\pi|r|}{ma^2}.\end{aligned} \tag{15}$$

Note that t, r and δ are all functions of k. In particular, we expect r to decrease fast with n, i.e. faster[2] than $1/n$. Equation (15) then implies that the gaps become smaller and smaller as n increases.

(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

$$1 + r = t. \tag{16}$$

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

$$t - (1 - r) = \frac{2m\alpha}{ik\hbar^2} t. \tag{17}$$

Recalling that $t = |t|e^{i\delta}$ and $r = \pm i|r|e^{i\delta}$, the imaginary part of (16) 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 (17) 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.

[2]For example, if n is large enough that the associated energy is above the barrier we expect r falls exponentially with n.