1. More on tight binding model (15 points)

(a) (3 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
\[ T|\theta\rangle = \sum_{n \in \mathbb{Z}} c_n T|n\rangle = \sum_{n \in \mathbb{Z}} c_n |n + 1\rangle = \sum_{n \in \mathbb{Z}} c_{n-1} |n\rangle = e^{-i\theta} \sum_{n \in \mathbb{Z}} c_n |n\rangle. \]
So 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
\[ |\theta\rangle = \sum_{n \in \mathbb{Z}} e^{in\theta} |n\rangle. \]  
(1)

Note that \( T^\dagger = T^{-1} \) (because \( \langle n|T^\dagger T|n\rangle = \langle n|T^\dagger |n + 1\rangle = \langle n + 1|n + 1\rangle = 1 \). Then
\[ T^\dagger|\theta\rangle = T^{-1}|\theta\rangle \]
\[ \implies (e^{-i\theta})^* |\theta\rangle = e^{i\theta} |\theta\rangle \]
\[ \implies \theta^* = \theta, \]  
(2)
or \( \theta \in \mathbb{R} \). As \( e^{i\theta} \) is periodic, we can choose \( -\pi < \theta \leq \pi \). Note that \( \theta = ka \) in standard notation.

(b) (2 points)
\[ \langle \theta|\theta'\rangle = \sum_{n,m \in \mathbb{Z}} \langle n|e^{i(m\theta' - n\theta)}|m\rangle \]
\[ = \sum_{n \in \mathbb{Z}} e^{in(\theta' - \theta)} \]
\[ = 2\pi \delta(\theta - \theta'). \]  
(3)
Here in the last equality we have used (4) from the problem set.

(c) (2 points)

We want to express $|n\rangle$ as

$$|n\rangle = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} a(\theta)|\theta\rangle.$$  \hfill (4)

Then

$$a(\theta) = \langle \theta | n \rangle = e^{-in\theta}. \hfill (5)$$

Here we have used (1) in the second equality. Thus

$$|n\rangle = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-in\theta}|\theta\rangle. \hfill (6)$$

(d) (2 points)

Acting with hamiltonian $H$ on $|\theta\rangle$ and collecting terms together we have

$$H|\theta\rangle = \sum_{n \in \mathbb{Z}} e^{in\theta} (E_0 - \Delta e^{i\theta} - \Delta e^{-i\theta}) |n\rangle$$

$$= (E_0 - 2\Delta \cos \theta) \sum_{n \in \mathbb{Z}} e^{in\theta} |n\rangle$$

$$= (E_0 - 2\Delta \cos \theta) |\theta\rangle.$$

Therefore the energy of $|\theta\rangle$ is

$$E_\theta = E_0 - 2\Delta \cos \theta.$$  

Note:

1. For $\theta = 0$: $E_\theta = E_0 - 2\Delta$ = lowest energy, with $|0\rangle = \sum_{n \in \mathbb{Z}} |n\rangle$, which is the most symmetric wavefunction.

2. For $\theta = \pi$: $E_\theta = E_0 + 2\Delta$ = highest energy, with $|\pi\rangle = |0\rangle - |1\rangle + |2\rangle - \ldots$, where the phase changes most rapidly. In some sense $\theta$ is like a momentum.

(e) (3 points)
The probability $P_n(t)$ that the electron lies in a state localized at $x = na$ at time $t$ is

$$P_n(t) = \left| \langle \Psi(t) | e^{-iHt/\hbar} | \Psi(t = 0) \rangle \right|^2$$

$$= \left| \langle n | e^{-iHt/\hbar} | 0 \rangle \right|^2$$

$$= \int_{-\pi}^{\pi} \frac{d\theta'}{2\pi} \langle n | e^{i\theta'} e^{-iHt/\hbar} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} | 0 \rangle \right|^2$$

$$= \int_{-\pi}^{\pi} \frac{d\theta'}{2\pi} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{i\theta' - iEt\cos\theta/\hbar} 2\pi \delta(\theta - \theta') \right|^2$$

$$= e^{-itE_0/\hbar} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{in\theta + 2it\Delta \cos\theta/\hbar} \right|^2$$

$$= e^{-itE_0/\hbar} \frac{1}{2\pi} J_n(2t\Delta/\hbar) \right|^2$$

$$= J_n^2(2t\Delta/\hbar), \quad (7)$$

where in the second last inequality we have used formula (7) from the problem set.
For fixed $n = 0, 1, 2, \ldots$ and $z \to 0$

$$J_n(z) \sim \frac{(\frac{1}{2}z)^n}{n!}.$$ \hfill (8)

This and $J_{-n}(z) = (-1)^n J_n(z)$ gives that as $t \to 0$, $P_0(t) \to 1$ and $P_{|n|\neq0}(t) \to t^{2|n|}$. This makes sense because the system started with the electron at $x = 0$ and the probability of finding the electron falls of as the distance from the initial position increases.

For fixed $n$ and large $z$ the principal asymptotic form of $J_n(z)$ is

$$J_n(z) = \sqrt{\frac{2}{\pi z}} \left\{ \cos \left( z - \frac{1}{2} n\pi - \frac{\pi}{4} \right) + \ldots \right\}.$$ \hfill (9)

So as $t \to \infty$ (for full credit it is enough to say that $P_n(t) \sim \frac{1}{t}$)

$$P_n(t) = \frac{\hbar}{t\Delta} \cos^2 \left( 2t\Delta/\hbar - \frac{1}{2} n\pi - \frac{\pi}{4} \right) = \frac{\hbar}{2t\Delta} (1 - (-1)^n \sin(4t\Delta/\hbar)).$$ \hfill (10)

This means that the probability of being localized at point $x = na$ oscillates (the electron moves around) and falls as $t^{-1}$ (the electron can move farther away from its initial position). The time scale of the oscillations is given by $\hbar/\Delta$.

Note: The bessel function properties can be looked up in M. Abramowitz and I. A. Stegun, "Handbook of Mathematical Functions" (http://www.math.sfu.ca/ cbm/aands/), Chapter 9, equations (9.1.7), (9.1.5) and (9.2.1). You can also search on http://mathworld.wolfram.com/ (g) (1 point)

The sum of probabilities at all points must be one, that is

$$1 = \sum_{n \in \mathbb{Z}} P_n(t)$$
$$= \sum_{n \in \mathbb{Z}} J_n^2(2t\Delta/\hbar)$$
$$= J_0^2(2t\Delta/\hbar) + 2 \sum_{n=1}^{\infty} J_n^2(2t\Delta/\hbar),$$ \hfill (11)

where in the second equality we have used (7) and in the last $J_{-n}(z) = (-1)^n J_n(z)$ when $n$ is an integer.

2. The Dirac comb (9 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

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

where $k = \sqrt{2mE/\hbar}$. We only need to change the sign of $\alpha$, the strength of Delta function, in Griffiths 2nd 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

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

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
\[
\psi(x) = e^{-iKa}[Ae^{-k(x+a)} + Be^{k(x+a)}], \quad (-a < x < 0).
\]
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, using Griffiths eq. (2.125) we get
\[
\psi'(x + 0) - \psi'(x - 0) = -\frac{2m\alpha}{\hbar^2}\psi(0)
\]
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
\[
A(1 - e^{-iKa-ka}) + B(1 - e^{-iKa+ka}) = 0
\]
\[
A(1 - e^{-iKa-ka} - \frac{2m\alpha}{\hbar^2k}) - B(1 - e^{-iKa+ka} + \frac{2m\alpha}{\hbar^2k}) = 0
\]
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
\[
(1 - e^{-iKa-ka})(1 - e^{-iKa+ka} + \frac{2m\alpha}{\hbar^2k}) + (1 - e^{-iKa+ka})(1 - e^{-iKa-ka} - \frac{2m\alpha}{\hbar^2k}) = 0.
\]
Expanding the brackets and collecting terms with the same power of \(e^{-iKa}\) we obtain
\[
2e^{-2iKa} + 2 - e^{-iKa}\left(2e^{ka} + 2e^{-ka} + \frac{2m\alpha}{\hbar^2K}(e^{-ka} - e^{ka})\right)
\]
Multiplying both sides by $\frac{1}{4}e^{iK_a}$ we obtain

$$\cos K_a = \cosh ka - \frac{m\alpha}{\hbar^2 k} \sinh ka$$ (14)

The solution to (14) exists if the right hand side is less than one. Let’s denote $z = ka$, $\beta = \frac{m\alpha}{\hbar^2 k}$ and the r.h.s. of (14) as $h(z, \beta)$. Then

$$h(z, \beta) = \cosh z - \beta \frac{\sinh z}{z}$$ (15)

[NOTE: We can obtain the same result by substituting $k \to -ik$ in eqn. (12).] The condition

$$|h(z, \beta)| = 1$$ (16)

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

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

3. Analysis of a general one-dimensional periodic potential (28 points)

(a) (2 points) When we differentiate the Wronskian, we find
\[ \frac{dW}{dx} = \psi_2'' \psi_1' - \psi_1'' \psi_2'. \]

According to the Schrödinger equation, $\psi_1'' = -\frac{2m}{\hbar^2} (E - v) \psi_1$, and similarly for $\psi_2$. 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
\[ W(x \geq a/2) = 2ikr^*t. \]

Since the Wronskian is independent of $x$, the above tells us that $(rt^*) = -(rt^*)^*$, and therefore that $rt^*$ is pure imaginary.

(c) (6 points) The Bloch conditions on $\psi$ and $\psi'$ yield the equations
\[
\begin{align*}
A(e^{iKa} + re^{i(k+K)a} - te^{ika}) &= B(1 + re^{ika} - te^{i(K+k)a}) \\
A(e^{iKa} - re^{i(k+K)a} - te^{ika}) &= B(-1 + re^{ika} + te^{i(K+k)a}).
\end{align*}
\]
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
\[
e^{iKa}(-1 + (r^2 - t^2)e^{2ika}) + e^{2iK}(te^{ika}) + te^{ika} = 0.
\]

Adjusting the phases and rearranging gives the desired answer,
\[
\cos(Ka) = \frac{1}{2t}(e^{-ika} + (t^2 - r^2)e^{ika}).
\]

(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 (17) becomes
\[
\cos(Ka) = \frac{\cos(ka + \delta)}{|t|}.
\]

(e) (5 points) We want to consider situations such that \(|t| \ll 1\). To be able to solve (18), 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
\[
k_{\text{max}} = \frac{1}{a} \left(\frac{(2n + 1)\pi}{2} - \delta + |t|\right),
\]
while the smallest allowed value of $k$ is given by

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

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

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

which is proportional to $|t|$.

(f) (5 points) We now want to consider situations where $|r| \ll 1$. In this case, the right hand side of equation (18) 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 $\delta$ 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 $k_{\text{max}}a = n\pi + |r|$, while the smallest value of $k$ (or the largest value of allowed $k$ below $n\pi$) is given by $k_{\text{min}}a = n\pi - |r|$. From this we find that the forbidden range of energies is (to leading order in $|r|$)

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

$$= \frac{2\hbar^2 n\pi |r|}{ma^2}. \quad (19)$$

Note that $t$, $r$ and $\delta$ are all functions of $k$. In particular, we expect $r$ to decrease fast with $n$, i.e. faster than $1/n$. Equation (19) 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 $\psi_L$ and $\psi'_L$ at $x = 0$. Continuity of $\psi_L$ at $x = 0$ tells us

$$1 + r = t. \quad (20)$$

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

$$t - (1 - r) = \frac{2ma}{\imath \hbar^2} t. \quad (21)$$

\footnote{For example, if $n$ is large enough that the associated energy is above the barrier we expect $r$ falls exponentially with $n$.}
Recalling that $t = |t|e^{i\delta}$ and $r = \pm |r|e^{i\delta}$, the imaginary part of (20) 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 (21) tells us that

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

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 (16) of the problem set, we find

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

which is precisely the equation derived in Griffiths.

4. **Classical motion in a Magnetic Field (8 points)**

(a) (3 points) The force that a particle feels in a magnetic field is given by $\vec{F} = q(\vec{v}/c) \times \vec{B}$. This force is perpendicular to the particle’s velocity $v$ and to the magnetic field $B$, so it acts like a centrifugal force in the $x - y$ plane, forcing the particle to move in a circle in this plane. This can be seen from:

$$\vec{v} \cdot \frac{d\vec{v}}{dt} = q(\vec{v}/c) \times \vec{B} \cdot \vec{v} \Rightarrow \vec{v} \cdot \frac{d\vec{v}}{dt} = 0.$$ 

Denoting the circle’s radius as $R$ and using Newton’s second law in the radial direction ($F = ma$), we find

$$F = q(\vec{v}/c)B = \frac{mv^2}{R} \Rightarrow \omega_L = \frac{v}{R} = \frac{qB}{mc}.$$ 

(b) (3 points) In this part we will assume that $q > 0, B > 0$. Consider the vector $\vec{R}$ pointing from the center of the circle to the particle (with coordinates $(x, y)$) which is perpendicular to $\vec{v}$ and has length $v/\omega_L$, so

$$\vec{R} = \left(-\frac{v_x}{\omega_L}, \frac{v_y}{\omega_L}\right).$$
where the correct choice of sign is determined by the right hand rule. Therefore

\[ X = x + \frac{v_y}{\omega_L}, \quad Y = y - \frac{v_x}{\omega_L}. \]

(c) (2 points) Using \( F = ma \) in the \( x \) and \( y \) directions we obtain (with \( v_y = \dot{y} = dy/dt \) and similarly for \( v_x \)):

\[ F_x = q(\dot{y}/c)B = m\ddot{x}, \quad (26) \]

\[ F_y = -q(\dot{x}/c)B = m\ddot{y}. \quad (27) \]

Now differentiating \( X \) and \( Y \) with respect to time and using (26), (27) we get:

\[ \dot{X} = \dot{x} + \frac{\dot{y}}{\omega_L} = -\frac{mc}{qB}\ddot{y} + \frac{\dot{y}}{\omega_L} = 0. \quad (28) \]

Similarly, \( \dot{Y} = 0 \) and hence \( X \) and \( Y \) are constants of the motion.