Quantum Physics III (8.06) Spring 2007
Assignment 2

Feb 12, 2006 **Due Wednesday Feb 21, 2007, 7pm**

- Please remember to put **your name and section time** at the top of your paper.

Readings

- The qualitative behavior of solids is dictated to a large extent simply by the fact that the electrons feel a periodic potential. The example we discussed in lecture is called the "tight binding model." The other classic example is the Dirac comb, which Griffiths treats on pages 226-228. You should read through Griffiths' treatment.

The reading assignment for the next two weeks is:

- Supplementary notes on Canonical Quantization and Application to a Charged Particle in a Magnetic Field by Prof. Jaffe.
- Griffiths Section 10.2.4 is an excellent treatment of the Aharonov-Bohm effect, but ignore the connection to Berry's phase for now. We will come back to this later.
- Quite remarkably, given its length, Cohen-Tannoudji never mentions the Aharonov-Bohm effect. It does have a nice treatment of Landau levels, however, in Ch. VI Complement E
- Those of you reading Sakurai should read pp. 130-139.

Problem Set 2

1. **More on the tight-banding model (15 points)**

   Consider an electron moving in a one-dimensional periodic potential generated by ions sitting at $x = na$ with n an integer running from $-\infty$ to $+\infty$. The quantum state $|n\rangle$ describes the wave function of the electron localized in the potential well of the ion at $x = na$. We assume that $|n\rangle$ forms an orthonormal basis, i.e

$$\langle n|m\rangle = \delta_{nm}, \qquad \sum_n |n\rangle\langle n| = 1$$

The Hamiltonian for the system is

$$H = \sum_{n=-\infty}^{n=+\infty} \Big[E_0 |n\rangle\langle n| \;-\; \Delta |n-1\rangle\langle n| \;-\; \Delta |n+1\rangle\langle n| \Big]$$

where the first term describes the energy of the electron in a given potential well and the second and the third terms describe tunnelling to neighboring ions. This is the tight-banding model discussed in lecture.

Define the "translation" operator T by:

$$T|n\rangle = |n+1\rangle \tag{1}$$

You should check for yourself that T commutes H.

(a) (3 points) Find the state $|\theta\rangle$ which is an eigenstate of T with eigenvalue $\exp(-i\theta)$, i.e.

$$T|\theta\rangle = e^{-i\theta}|\theta\rangle, \qquad -\pi < \theta \leq \pi \; . \tag{2}$$

Explain why θ is real and can be taken to lie in the range stated above. (Note: in terms of the notation of lecture $\theta \equiv ka$.)

(b) (2 points) Check that (by choosing an appropriate normalization constant for $|\theta\rangle$)

$$\langle\theta|\theta'\rangle = 2\pi\delta(\theta - \theta') \tag{3}$$

Hint: you will find the following formula useful

$$\sum_{n=-\infty}^{\infty} e^{inx} = 2\pi\delta(x) \tag{4}$$

(c) (2 points) Express $|n\rangle$ in terms of $|\theta\rangle$.

(d) (2 points) In lecture we showed that $|\theta\rangle$ are also energy eigenstates. Find their energy eigenvalues.

(e) (3 points) Suppose at $t = 0$, the wave function of the electron is given by

$$|\Psi(t=0)\rangle = |n=0\rangle \tag{5}$$

i.e. localized in the potential well of the ion at $x = 0$. Find the probability $P_n(t)$ that the electron lies in a state localized at $x = na$ at time t, i.e.

$$|\Psi(t)\rangle = |n\rangle \tag{6}$$

Hint: you will find the following formula useful

$$i^n J_n(z) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \, e^{iz\cos\theta + in\theta} \tag{7}$$

where J_n is a Bessel function.

(f) (2 points) Find the behavior of $P_n(t)$ for $t \to 0$ and $t \to \infty$ and explain why you find the behaviors physically reasonable.

(g) (1 point) Using result of (d), prove the following identity of Bessel functions

$$J_0^2(z) + 2\sum_{n=1}^{\infty} J_n^2(z) = 1 \tag{8}$$

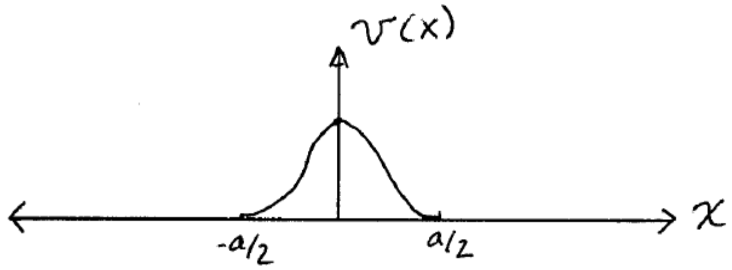
PS: (read the following only after you finish the problem)

- $|n\rangle$ are position eigenstates while $|\theta\rangle$ can be considered as "momentum" eigenstates. It is amusing that here position eigenstates are discrete while momentum eigenstates are continuous. (Compare with the situation for a particle inside an infinite square well.)
- From part (e), you should find that the time scale for an electron at $x = 0$ to tunnel to other lattice sites is of order $O(1/\Delta)$, which can be very large as Δ is typically very small. This is consistent with our intuition that if the tunnelling rate is small (i.e. tight binding), it would be hard for a trapped electron to escape.
- The energy eigenstates $|\theta\rangle$ are, however, always delocalized no matter how small Δ is (the essence of Bloch theorem). This has to do with that when $\Delta = 0$, the energy spectrum are infinite degenerate (i.e. all states $|n\rangle$ have the same energy and so do arbitrary linear superpositions of them including $|\theta\rangle$), a fact you will appreciate better after you learn degenerate perturbation theory in a few weeks.
- Although I do not ask in the problem, it will be instructive for you to plot $P_n(t)$ as a function for t for different n.

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

Consider a one-dimensional periodic potential $U(x)$ that we shall choose to view as the sum of lots of identical potential barriers $v(x)$ of width a, centered at the points $x = na$, where n is an integer.

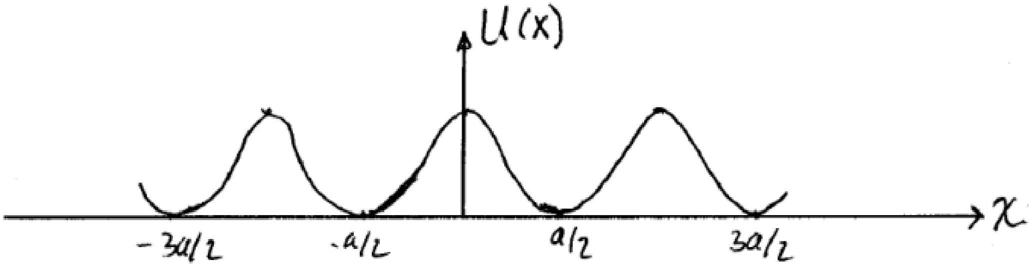
We shall require v to be even, that is $v(x) = v(-x)$, but other than that we shall allow the shape of the barrier to be arbitrary. $v(x) = 0$ for $|x| \geq a/2$. In pictures, $v(x)$ looks like:



The periodic potential is then given by

$$U(x) = \sum_{n=-\infty}^{\infty} v(x - na)$$

and looks like:



Before we analyze U, let us analyze v. For any energy $E > 0$, there are two linearly independent solutions to the Schrödinger equation with the single barrier potential $v(x)$. One, which we shall call $\psi_L(x)$ describes a plane wave incident from the left:

$$\begin{aligned} \psi_L(x) &= \exp(ikx) + r\exp(-ikx)\ , \quad x \le -a/2 \\ &= t\exp(ikx)\ , \qquad x \ge a/2\ , \end{aligned} \tag{9}$$

where k is related to E by $E = \hbar^2 k^2/2m$. We shall not need the form of ψ where the potential is nonzero. The other solution with the same energy describes a wave incident from the right:

$$\begin{aligned} \psi_R(x) &= t\exp(-ikx)\ , \qquad x \le -a/2 \\ &= \exp(-ikx) + r\exp(ikx)\ , \quad x \ge a/2\ , \end{aligned} \tag{10}$$

with the same reflection coefficient r and transmission coefficient t as in (9) because $v(x)$ is even.

We can write the complex number t in terms of its magnitude and phase as

$$t = |t|\exp(i\delta)\ , \tag{11}$$

where δ is a real number known as the phase shift since it specifies the phase of the transmitted wave relative to the incident one. Conservation of probability requires that

$$|t|^2 + |r|^2 = 1. \tag{12}$$

To this point, we have reviewed 8.04 material and established notation.

(a) (2 points) Let ψ_1 and ψ_2 be any two solutions of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_i}{dx^2} + v(x)\psi_i = E\psi_i$$

with the same energy. Define the "Wronskian" of these two solutions by

$$W(\psi_1, \psi_2) = \psi_2(x)\frac{d}{dx}\psi_1(x) - \psi_1(x)\frac{d}{dx}\psi_2(x) \; .$$

Prove that W is independent of x by showing that $dW/dx = 0$.

(b) (2 points) By evaluating $W(\psi_L, \psi_R^*)$, prove that rt^* is pure imaginary, so r must have the form

$$r = \pm i|r| \exp(i\delta) \tag{13}$$

where δ is the same as in (11).

(c) (6 points) Now, we begin our analysis of solutions of the Schrödinger equation in the periodic potential U. Since $U = v$ in the region $-a/2 \leq x \leq a/2$, in that region any solution to the Schrödinger equation with potential U must take the form

$$\psi(x) = A\psi_L(x) + B\psi_R(x) \; , \quad -a/2 \leq x \leq a/2 \; , \tag{14}$$

with ψ_L and ψ_R given by (9) and (10). Bloch's theorem tells us that

$$\psi(x+a) = \exp(iKa)\psi(x)$$

and, with $\psi' \equiv d\psi/dx$,

$$\psi'(x+a) = \exp(iKa)\psi'(x) \; .$$

By imposing these conditions at $x = -a/2$, show that the energy of the electron is related to K by

$$\cos Ka = \frac{t^2 - r^2}{2t}\exp(ika) + \frac{1}{2t}\exp(-ika) \tag{15}$$

with k specifying the energy via

$$E = \hbar^2 k^2/2m \; .$$

[Note that some of you may succeed in deriving an expression relating all the quantities in (15) — and no other quantities — but then not succeed in reducing your expression to the form (15). If so, you will not lose many points. And, make sure to use (15), rather than whatever you obtain, in the following parts.]

(d) (2 points) Show that as a consequence of (12), (13) and (15) the energy and K of the Bloch electron are related by

$$\cos Ka = \frac{\cos(ka + \delta)}{|t|} \ . \tag{16}$$

Note that $|t|$ is always less than one, and becomes closer and closer to one for larger and larger k because at high incident energies, the barrier becomes increasingly less effective. Because $|t| < 1$, at values of k in the neighborhood of those satisfying $ka + \delta = n\pi$, with n an integer, the right hand side of (16) is greater than one, and no solution can be found. The regions of E corresponding to these regions of k are the energy gaps.

(e) (5 points) Suppose the barrier is very strong, so that $|t| \approx 0$, $|r| \approx 1$. Show that the allowed bands of energies are then very narrow, with widths of order $|t|$. [Note: this is the tight-binding case, discussed in lecture. This is the case that applies to a deeply bound atomic energy level which in a crystal becomes a narrow band. In this case, because the energy level is well below the top of the barrier between single-atom potential wells, "transmission" requires tunnelling, meaning that $|t|$ is small.]

(f) (5 points) Suppose the barrier is very weak (so that $|t| \approx 1$, $|r| \approx 0$, $\delta \approx 0$). Show that the energy gaps are then very narrow, the width of the gap containing $k = n\pi/a$ being $2\pi n\hbar^2|r|/ma^2$. [Note: this shows that the continuum states – namely those whose energies are above the top of the barriers – are also separated into bands. The gaps between the bands get narrower and narrower for higher and higher energy continuum states.]

(g) (6 points) Show that in the special case where $v(x) = +\alpha\delta(x)$ where $\delta(x)$ is the Dirac delta function — i.e. the Dirac comb model discussed in Griffiths p.226-228 — the phase shift and transmission coefficent are given by

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

and

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

and that (16) becomes the expression derived in Griffiths.

3. **Classical motion in a Magnetic Field (3 points)**

Consider a particle of mass m and charge q moving along a trajectory $\vec{x}(t)$ through a constant magnetic field along z-direction, i.e. $B_x = B_y = 0$, $B_z = B = \text{const}$. Classically in the $x - y$ plane the particle travels in a circle around a "center of orbit" with an angular velocity ω_L given by

$$\omega_L = \frac{qB}{mc} \ . \tag{17}$$

Suppose that the "center of orbit" has coordinates (X, Y). Show that X, Y can be expressed in terms of the coordinates (x, y) and the velocities (v_x, v_y) of the particle as

$$X = x + \frac{v_y}{\omega_L}, \qquad Y = y - \frac{v_x}{\omega_L} \ . \tag{18}$$

4. **Gauge Invariance and the Schrödinger Equation (14 points)**

The time dependent Schrödinger equation for a particle in a electromagnetic field given by

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\vec{\nabla} - \frac{q}{c}\vec{A}(\vec{x},t)\right)^2 \psi(\vec{x},t) + q\phi(\vec{x},t)\psi(\vec{x},t) \ . \tag{19}$$

(a) (4 points) Consider

$$\begin{aligned} \vec{A}'(\vec{x},t) &= \vec{A}(\vec{x},t) - \vec{\nabla} f(\vec{x},t) \\ \phi'(\vec{x},t) &= \phi(\vec{x},t) + \frac{1}{c}\frac{\partial f}{\partial t}(\vec{x},t) \ . \end{aligned} \tag{20}$$

$(\vec{A}', \phi')$ and $(\vec{A}, \phi)$ describe the same $\vec{E}$ and $\vec{B}$. Show that if $\psi(\vec{x},t)$ solves the Schrödinger equation with $\vec{A}, \phi$ (which we will call "unprimed gauge"), then

$$\psi'(\vec{x},t) \equiv \exp\left(-\frac{iq}{\hbar c} f(\vec{x},t)\right)\psi(\vec{x},t) \tag{21}$$

solves the Schrödinger equation with $\vec{A}', \phi'$ (which we will call "primed gauge").

(b) (10 points) We say an operator $\mathcal{O}$ gauge invariant if $\langle\psi|\mathcal{O}|\phi\rangle$ is gauge independent for any $|\psi\rangle$ and $|\phi\rangle$. Are the following operators gauge invariant? Give reasoning or derivation for your answers.

i. $\hat{x}_i$
ii. $\hat{p}_i$
iii. $\hat{v}_i = \frac{1}{m}\left(\hat{p}_i - \frac{q}{c}A_i\right)$
iv. the Hamiltonian H (assuming that f is time-independent)
v. Energy eigenvalues (assuming that f is time-independent)