Quantum Physics III (8.06) Spring 2005
Assignment 2

Feb 8, 2005 **Due Tuesday Feb 15, 2005, 6pm**

Readings

The readings assigned last week should suffice for all of this problem set except Problem 4.

The reading assignment for the next two weeks is:

- 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. **Fermi energy, velocity and temperature of copper (4 points)**

   Do Griffiths, Problem 5.16. [Unless otherwise noted, Griffiths page and problem numbers refer to the 2nd Edition, the one with the blue cover. If some of you are using Griffiths' 1st Edition, with a black cover, in that edition this problem is Problem 5.13.]

2. **The Kronig-Penney Model (12 points)**

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 will discuss in lecture (and whose essence you worked out in the last problem of Problem Set 1) is called the "tight binding model." The other classic example, worked out in many books, is the Kronig-Penney model, which Griffiths treats on pages 224-228. [Pages 198-202 in the 1st Edition.] You should work carefully through Griffiths' treatment, including all details.

   (a) Do Griffiths problem 5.20. [This problem has been modified since the 1st Edition.]

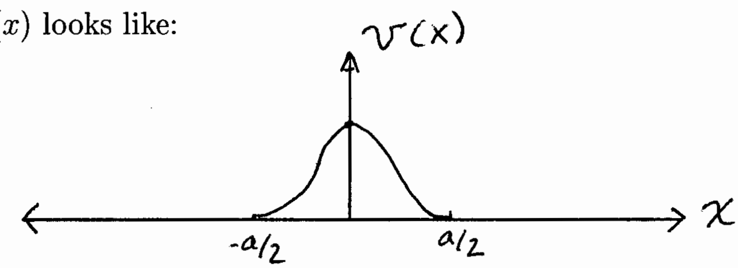
   (b) Do Griffiths problem 5.21. [Problem 5.18 in the 1st Edition.]

   (c) Optional: Griffiths' problems 5.18 and 5.19 are worth doing also, but I will not assign them. [These are Problems 5.15 and 5.16 in the 1st Edition.]

3. **Analysis of a general one-dimensional periodic potential (32 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 $x = \pm na$, where n is an integer.

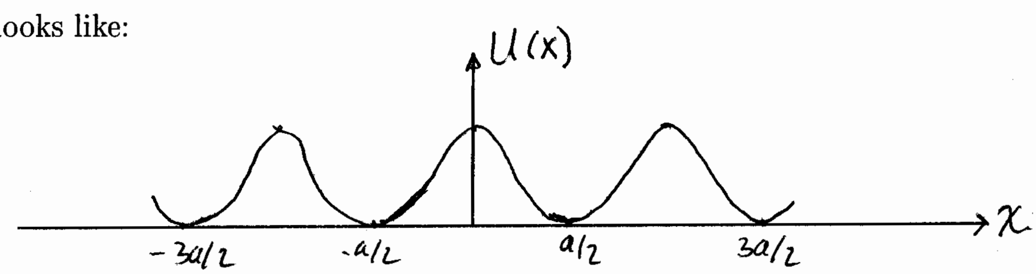
In pictures, $v(x)$ looks like:



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 $|x| \geq a/2$. 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:

$$\begin{aligned}\psi_L(x) &= \exp(ikx) + r\exp(-ikx)\ , \quad x \le -a/2 \\ &= t\exp(ikx)\ , \qquad x \ge a/2\ ,\end{aligned} \tag{1}$$

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:

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

with the same reflection coefficient r and transmission coefficient t as in (1) because $v(x)$ is even.

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

$$t = |t|\exp(i\delta)\ , \tag{3}$$

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

$$|t|^2 + |r|^2 = 1. \tag{4}$$

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

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

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

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

$$r = \pm i|r|\exp(i\delta) \tag{5}$$

where δ is the same as in (3).

(c) 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

$$\psi(x) = A\psi_L(x) + B\psi_R(x) \ , \quad -a/2 \leq x \leq a/2 \ , \tag{6}$$

with ψ_L and ψ_R given by (1) and (2). 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

$$\cos Ka = \frac{t^2 - r^2}{2t} \exp(ika) + \frac{1}{2t} \exp(-ika) \ . \tag{7}$$

[Recall that k specifies the energy via $E = \hbar^2 k^2/2m$. Note that you do not need to use (3), (4) or (5) to derive (7). Note also that some of you may succeed in deriving an expression relating all the quantities in (7) — and no other quantities — but then not succeed in reducing your expression to the form (7). If so, you will not lose many points. And, make sure to use (7), rather than whatever you obtain, in the following parts.]

(d) Show that as a consequence of (4), (5) and (7) the energy and K of the Bloch electron are related by

$$\cos Ka = \frac{\cos(ka + \delta)}{|t|} \ . \tag{8}$$

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 (8) 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) 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) 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) Show that in the special case where $v(x) = +\alpha\delta(x)$ where $\delta(x)$ is the Dirac delta function — ie the Kronig Penney model as in Griffiths' problem 5.17 — the phase shift and transmission coefficent are given by

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

and

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

and that (8) becomes the expression derived in Griffiths.

4. **An Operator Ordering Ambiguity (6 points)**

Evaluate $[\hat{x}^2, \hat{p}^2]$. Now, evaluate the Poisson bracket $\{x^2, p^2\}_{PB}$ from classical mechanics. Show that the rules of canonical quantization and the requirement that $i[\hat{x}^2, \hat{p}^2]$ must be a Hermitian operator are sufficient to correctly guess the result for $[\hat{x}^2, \hat{p}^2]$ from the result for $\{x^2, p^2\}_{PB}$. Now, repeat this exercise for $[\hat{x}^3, \hat{p}^3]$ and $\{x^3, p^3\}_{PB}$. Show that in this case, the requirement that $i[\hat{x}^3, \hat{p}^3]$ be Hermitian is NOT sufficient to allow one to guess the correct quantum mechanical result from the classical result.

5. **Landau Levels: a Prelude (6 points)**

When we analyze the problem of a charged particle in a magnetic field, we shall find that the energy eigenvalues are separated by a spacing $\hbar\omega_L$, where ω_L (the Larmor or cyclotron frequency) is proportional to the magnetic field B and is given by

$$\omega_L = \frac{eB}{mc} \ ,$$

with m the mass of the electron.

Furthermore, we shall find that the length

$$\ell_0 = \sqrt{\frac{\hbar}{m\omega_L}}$$

and the area

$$A_B = 2\pi\ell_0^2$$

play an important role.

(a) Suppose B is a field of 10 Tesla. (This is a very strong magnetic field but is certainly one which can be created in the laboratory. I am actually not sure what the strongest laboratory magnetic fields achieved to date are, but I believe they are less than 100 Tesla.) In a 10 Tesla magnetic field, what is $\hbar\omega_L$ in eV? What is ℓ_0 in natural units? What is ℓ_0 in cm?

(b) Lets see whether we can get some sense of how the area A_B may arise in this problem. In a magnetic field of strength B, the flux Φ through an area A perpendicular to B is $\Phi = BA$. What is the flux through the area A_B? Express your answer in units of hc/e. (Note: hc/e, not $\hbar c/e$.)

Useful facts: 1 Tesla $= 10^4$ gauss. The gauss is the cgs unit of B. This turns out to mean that if B is 1 gauss, then the force eB is 300 eV/cm. Also, $\hbar c = 197 \times 10^{-7}$eV cm. And, the mass of the electron is $m = 0.511\text{MeV}/c^2$.