Quantum Physics III (8.06) — Spring 2016
Assignment 9

Readings

The current reading assignments are:

- Supplementary notes on Canonical Quantization and Application to a Charged Particle in a Magnetic Field by Prof. Jaffe.

- Griffiths Section 10.2.3 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. Shankar's treatment is very different from the one presented in this course.

Problem Set 9

1. **The Dirac Comb (20 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 discussed in lecture and in the above problem is called the "tight binding model." The other classic example is the Dirac comb (or Kronig-Penney model), which Griffiths treats on pages 224-229. You should read through Griffiths' treatment.

   Do Griffiths problem 5.20. (Make sure you are looking at the second edition.)

2. **Analysis of a General One-Dimensional Periodic Potential (40 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:
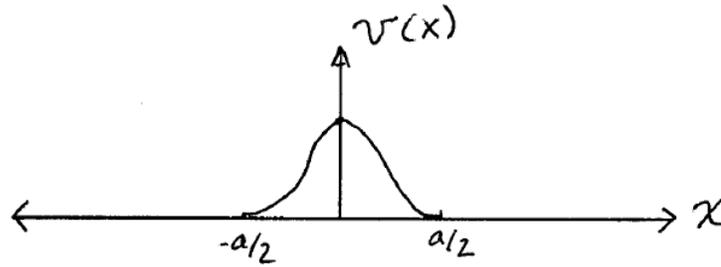
The periodic potential is then given by

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

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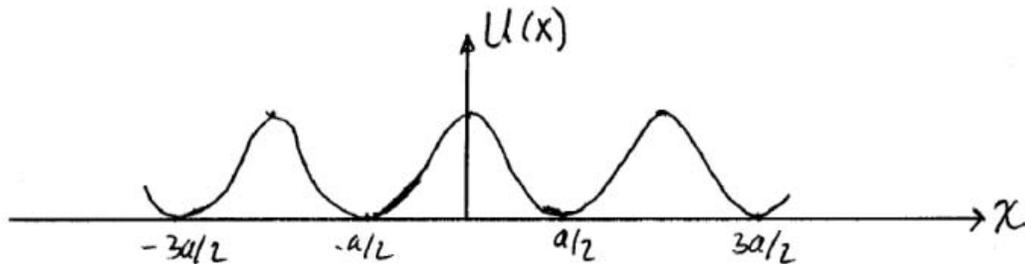
Before we analyze U, let us analyze v. For any energy $E > 0$, there are two linearly independent solutions to the Schrödinger equation with the single barrier potential $v(x)$. One, which we shall call $\psi_L(x)$ describes a plane wave incident from the left:

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

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:

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

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

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

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) 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

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

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 (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

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

3

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 $Cn|r|$ where you have to determine C. [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 — i.e. the Dirac comb model discussed in Griffiths p.224-229 — 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.

3. **Gauge Invariance and the Schrödinger Equation (15 points)**

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

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\vec{\nabla} - \frac{q}{c}\vec{A}(\vec{x},t)\right)^2 \psi(\vec{x},t) + q\phi(\vec{x},t)\psi(\vec{x},t) . \tag{9}$$

(a) Consider a gauge transformation

$$\begin{aligned}
\vec{A}'(\vec{x},t) &= \vec{A}(\vec{x},t) - \vec{\nabla}f(\vec{x},t), \\
\phi'(\vec{x},t) &= \phi(\vec{x},t) + \frac{1}{c}\frac{\partial f}{\partial t}(\vec{x},t) .
\end{aligned} \tag{10}$$

$(\vec{A}', \phi')$ 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

$$\psi'(\vec{x},t) \equiv \exp\left(-\frac{iq}{\hbar c}f(\vec{x},t)\right) \psi(\vec{x},t) \tag{11}$$

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

(b) Physical observables should be gauge invariant. Check whether the following quantities are gauge invariant or not:

    i. $\langle \psi | \hat{x}_i | \psi \rangle$

    ii. $\langle \psi | \hat{p}_i | \psi \rangle$

    iii. $\langle \psi | \hat{v}_i | \psi \rangle$, where $\hat{v}_i = \frac{1}{m} \left(\hat{p}_i - \frac{q}{c} A_i \right)$

    iv. Energy expectation values (assuming that f is time-independent)

    v. Energy eigenvalues (assuming that f is time-independent)

Gauge invariant operators are those whose expectation values in any state are gauge invariant.

4. **Term paper epilogue (25 points)** For this problem you should choose **one** of the following two possible options. Both are open-ended but we don't want you to spend too much time on this problem. Full credit will be given to any good-faith effort. This part of the assignment should be submitted electronically on stellar under the "Term Paper Epilogue" assignment, no later than **6pm** on May 8.

- **Option 1: Edit an article on wikipedia.** Create an account on wikipedia. Find an article on wikipedia concerning some topic in quantum mechanics. Make some small changes that improve the article. For example, you could add a sentence, fix an equation or two, clarify some wording, etc. More substantive changes would be even better! But not required. It might be easiest to find an article to improve that relates to your term paper, but this is not required.

  To show that you have done this, upload to stellar a text file containing a link to the diff which shows your changes. For example, this link shows the types of changes you should make and also the format of the link. You can find this link by clicking the "history" link at the top of the article and the clicking on the "prev" link next to your revision. If you make more than one change, then put one link for each change in your text file.

  Please try to follow the norms of Wikipedia when editing.

- **Option 2: Write a popular summary.** Write a 100-200 word summary of your term paper in a style that is suitable for the general, but science-interested, public. Imagine publications such as the NYT Science Times, slashdot or Wired. Your goal should be to communicate what is intellectually exciting and/or practically useful about your topic without using jargon.

8.06 Quantum Physics III

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