

Quantum Physics III (8.06) Spring 2005

Assignment 8

April 5, 2005

Due WEDNESDAY April 20, 2005

Readings

- Griffiths Chapter 8 on the semiclassical approximation.
- Griffiths Chapter 10 on the adiabatic approximation.
- The article by Wick Haxton on the Solar Neutrino Problem is *optional* extra reading.
- Note that I have not given you a problem on Berry's phase. The classic example is Griffith's Example 10.2, and I decided that it is too much to ask you to work through any example other than this one. And, I will do this example in lecture. You should make sure you understand Berry's phase and this classic example, even though it will not appear on a problem set. If you want to do another example, try Griffiths' Problem 10.6.

Problem Set 8

1. Using the Semiclassical Approximation on the Ground State (8 points)

Despite the fact that the semiclassical approximation was derived for states of large action, we shall see that it does a pretty good job on the ground states of simple potentials. For example, it gets that of the harmonic oscillator exactly right. Here is another example where the exact solution is known, and you can check how well the semiclassical approximation does. This problem is based on Griffiths' Problem 8.12.

Consider a particle of mass m moving in the potential

$$V(x) = -\frac{\hbar^2 a^2}{m} \operatorname{sech}^2(ax) .$$

- (a) Show that $\psi(x) = A \operatorname{sech}(ax)$ is the wave function for a bound state in this potential. How do you know that this bound state must be the ground state? What is the energy of this state?

- (b) Apply the semiclassical approximation to this potential to estimate the lowest energy eigenvalue. Compare your result with the exact result from part (a).

2. Quantum Mechanics of a Bouncing Ball (8 points)

The semiclassical approximation can also be used to estimate the energy eigenvalues and eigenstates for potentials that cannot be treated exactly so easily. This problem is loosely based on Griffiths' 8.6. (See Griffiths' 8.5 if you'd like to learn how to treat this quantum mechanical problem exactly, using Airy functions.)

Consider the quantum mechanical analogue to the classical problem of a ball of mass m bouncing elastically on the floor, under the influence of a gravitational potential which gives it a constant acceleration g .

- (a) Find the semiclassical approximation to the allowed energies E_n , in terms of m , g and \hbar .
- (b) Estimate the zero point energy of a neutron "at rest" (ie in the quantum mechanical ground state) on a horizontal surface in the earth's gravitational field. Express your answer in eV. [This may sound artificial to you, but the experiment has been done. See V. V. Nesvizhevsky *et al.*, Nature **415**, 297 (2002) and arXiv:hep-ph/0306198 for an experimental measurement of the quantum mechanical ground state energy for neutrons bouncing on a horizontal surface in the earth's gravitational field. This experiment got a lot of press at the time, because it involves both gravity and quantum mechanics, which made for an eye catching press release. It of course has *nothing* to do with quantum gravity.]
- (c) Now imagine dropping a ball of mass 1 gram from rest from a height of 1 meter, and letting it bounce. Do the 8.01 "calculation" of the classical energy of the ball. The quantum mechanical state corresponding to a ball following this classical trajectory must be a coherent superposition of energy eigenstates, with mean energy equal to the classical energy. How large is the mean value of the quantum number n in this state?

3. Application of the Semiclassical Method to the Double Well Potential (22 points)

Do Griffiths Problem 8.15.

This is an instructive problem in quantum dynamics. You should recall that this is the potential that we used to describe the physics of the ammonia molecule, early in 8.05. Back then, we had to wave our hands a little when we talked about tunnelling splitting the degeneracy between the even and odd states. Now, you can do this calculation for real.

What follows is an extended hint/suggestion for a slightly different way to do the problem than that which Griffiths sets up. I believe this suggestion should help you with parts (a) and (b), but you do not need to follow it, if you prefer going along with Griffiths precisely.

On page 336, there are three expressions (i), (ii) and (iii) for the wave function in three regions. (i) and (ii) are straightforward to demonstrate, and you should begin by doing so. However, I suggest that (iii) is not a particularly convenient expression for the wave function in this region, although it is correct, and you may therefore bypass showing (iii) as I now explain.

Since you know you are looking for either an even or an odd function of x , things simplify. Lets consider the even case; you can handle the odd case yourself. If the wave function is even, then in the region $-x_1 < x < x_1$ [which is region (iii) and its reflection] it must take the form:

$$\psi(x) = \frac{C}{\sqrt{\kappa(x)}} \cosh \left[\frac{1}{\hbar} \int_0^x dy \kappa(y) \right] \quad (1)$$

where $\kappa(x)$ is our standard notation for what Griffiths would call $|p(x)|$. There are then two stages to the logic of the next step of the argument:

- FIRST: apply connection formulae at $x = x_1$ to (1), and get from (1) an expression for $\psi(x)$ in region (ii), ie $x_1 < x < x_2$.
- SECOND: show that in order for the expression you have obtained to be the same as Griffiths' expression (ii) — which you remember you have already demonstrated — a certain condition must be satisfied that turns out to imply Griffiths equation (8.59), with the plus sign. When you're doing the odd case instead of the even case, you'll find (8.59) with the minus sign.

(8.59) is the key result from which the later parts of the problem all follow. By doing things as above, you get to (8.59) without ever using Griffiths form (iii). If you do things as above, you can (if you like) go back after having derived (8.59) and show that (8.59) turns (1) into Griffiths form (iii). If you do things as above, you will find that in the step labelled "SECOND" above, there is some algebra, but significantly less than doing it Griffiths' way.

Also, you'll find that you have to think through and explain a subtlety in the step labelled "FIRST" above. You need to use connection formulae to get from the cosh of equation (1) into region (ii). You'll find that this means that you must use one of the connection formulae "in the direction of the arrow", ie in the legal direction, but you must use another connection formula in the ILlegal direction. You should think through the explanation I gave in lecture of why going against the arrow is in general illegal, and then see why in the specific circumstances of this problem it is in fact legal.

4. **Vibrational and Rotational Spectra in the Born-Oppenheimer Approximation (8 points)**

Consider the vibrational and rotational energy of a diatomic molecule in the Born-Oppenheimer approximation. We expand the internuclear energy about the equilibrium position R_0 and include the rotational energy:

$$\mathcal{E}(R, J) = \frac{m\omega^2}{2}(R - R_0)^2 + \frac{J(J+1)\hbar^2}{2mR^2}.$$

- (a) Find the position where the energy is a minimum.

Note: your answer will take the form $R_{\min} = R_0 + \delta R$, and you may assume throughout this problem that $\delta R \ll R_0$. This approximation is equivalent to assuming that the rotational energy is much less than $\hbar\omega$, the spacing between vibrational levels, which is the case for reasonable values of J and realistic values of ω and m and R_0 for real molecules.

- (b) If the moment of inertia of the molecule is calculated using the new internuclear separation that is, if the rotational energy is written as

$$\frac{J(J+1)\hbar^2}{2mR_{\min}^2},$$

show that the rotational energy can be written in the form

$$E_J = AJ(J+1) + BJ^2(J+1)^2 + \dots$$

Determine the coefficients A and B . The second term describes “centrifugal distortion”.

Note: By making precise measurements of the frequencies of the spectral lines emitted as the molecule makes transitions between rotational states with varying J , it is straightforward to make an experimental measurement of A and B . Given that m is known by other means, your result shows how to make an experimental determination of ω and R_0 .

5. Adiabatic Spin Rotation (6 points)

Consider a spin one-half particle at rest, with its spin free to rotate in response to a time-dependent magnetic field. The Hamiltonian of the system is

$$H = -\frac{2\mu_0}{\hbar} \vec{S} \cdot \vec{B}(t) .$$

At $t = 0$ there is a magnetic field $\vec{B}(0) = (0, 0, B_0)$, and the spin is aligned along the magnetic field, with

$$|\psi(0)\rangle = |\uparrow\rangle .$$

Now suppose that the magnetic field is very slowly decreased to zero and then increased in the opposite direction,

$$\vec{B}(t) = (0, 0, B_0 - \beta t) ,$$

until at time $t_f = 2B_0/\beta$, we have $\vec{B}(t_f) = (0, 0, -B_0)$. In addition, assume that there is a small, *constant* residual magnetic field in the xy -plane, $\delta\vec{B} = (B_x, B_y, 0)$. [After all, it would be unrealistic to assume that the magnetic field is *exactly* zero when $t = B_0/\beta$.]

Use the adiabatic theorem to show that the particle initially in the state $|\uparrow\rangle$ finishes in the state $|\downarrow\rangle$ with unit probability, regardless of the direction that $\delta\vec{B}$ points in the xy -plane. What is the condition on the parameters of the problem for the adiabatic theorem to apply?

[Aside: If the adiabatic theorem applies, the particle is in the state with spin parallel (as opposed to antiparallel) to the magnetic field at the end of the evolution just as at the beginning. This property is applied in the magnetic traps used by MIT atomic physicists to trap very cold gases of spin-polarized atoms. The magnetic field gradients are designed so that an atom which has its spin parallel to the local magnetic field $\vec{B}(x)$ experiences a force toward the center of the trap. Those atoms with spins antiparallel to $\vec{B}(x)$ feel a force which expels them from the trap. This raises a question: since $\vec{B}(x)$ varies in space, how do we ensure that as the atoms move within the trap their spins are always aligned with the local magnetic field? Answer: the atoms are moving slowly enough that the adiabatic theorem applies. You should now be able to explain the importance of the following design feature of the traps: since it is magnetic *gradients* which exert the trapping forces, you might think that there would be no problem if at one point in the trap, $\vec{B} = 0$; in fact, this *does* cause problems, and the traps are designed to have $\vec{B} \neq 0$ everywhere. Explain.]

6. **Engineering Adiabatic Transitions (8 points)**

This problem is similar to the last one, except that now the particle has spin one, and therefore has three eigenstates $|+\rangle$, $|0\rangle$ and $|-\rangle$.

The Hamiltonian is given by

$$H = -\frac{2\mu_0}{\hbar} \vec{S} \cdot \vec{B}(t) - \frac{c}{\hbar^2} S_z^2 .$$

The last term represents some small term in the environment of the spin which favors the states $|\pm\rangle$ over the state $|0\rangle$.

- (a) Write the operators S_x , S_y and S_z for this problem. (You should be able to find them in your 8.05 notes or in one of your books.)
- (b) Suppose that the magnetic field is as in the previous problem, with a small constant field in the x -direction and a large time-dependent field in the z -direction:

$$\vec{B}(t) = (B_x, 0, B_0 - \beta t) .$$

Assume the following hierarchy of energies:

$$\mu_0 B_0 \gg c \gg \mu_0 B_x \gg \hbar\beta/B_x .$$

Sketch the energy levels of this system as a function of time.

- (c) Suppose the system starts out in the state $|-\rangle$ at $t = 0$. Show that upon assuming the hierarchy of energies above, this state evolves to a state that is approximately equal to $|0\rangle$ and then evolves to $|+\rangle$. Explain how you would alter the time dependence of $\vec{B}(t)$ in order that the initial state transforms into $|0\rangle$ at late times.