# Quantum Physics III (8.06) Spring 2006 Solution Set 8

April 24, 2006

## 1. Tunneling and the Stark effect (20 points)

(a) (3 points) For an infinitely deep square well of width d, the energy of the ground state is  $E_{\infty,0} = \frac{\hbar^2 \pi^2}{2md^2}$  (this is the amount by which ground state energy is above the bottom of the potential well). Since the zero of energy is at the top of the well rather than the bottom in this problem, we estimate  $E_0 = \frac{\hbar^2 \pi^2}{2md^2} - V_0$ . Full credit will be given on writing only  $E_{\infty,0}$ .

Optional part: To show that true ground state is lower than this, use variational principle. Consider potential V(x)=0 for |x|< d/2 but  $V(x)=V_0$  for |x|>d/2. Take the trial wavefunctions to be  $\psi(x)=\sqrt{2/d}\cos(\pi x/d)$  for |x|< d/2 and 0 everywhere else. Of course this is the exact ground state wavefunction for the infinite well potential and indeed  $\langle \psi|H|\psi\rangle=E_{\infty,0}$ , where H is hamiltonian corresponding to the potential mentioned above, which is nothing but the square well potential of this problem shifted by  $V_0$ . Therefore the true ground state must be lower than  $E_{\infty,0}$ .

(b) (2 points) A sketch of the potential is in figure 1.

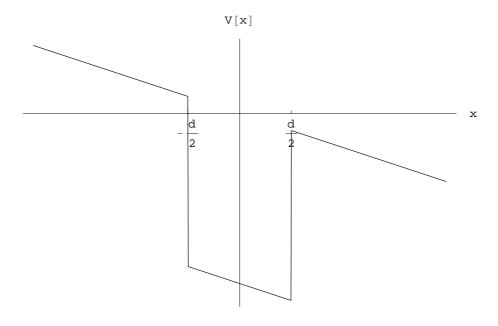


Figure 1: A square well potential in a constant electric field.

The potential no longer binds states because it is unbounded from below; a particle trapped in the well can reduce its energy by tunneling out to  $x = \infty$ .

(c) (5 points) To use semiclassical approximation to find the tunneling probability, we first

need to find the classical turning point. This occurs at

$$x_t = -\frac{E_0}{e\mathcal{E}} = \frac{V_0 - \frac{\hbar^2 \pi^2}{2md^2}}{e\mathcal{E}}.$$

The tunneling probability is given semi-classically by

$$T \simeq e^{-\frac{2}{\hbar} \int_{d/2}^{x_t} dx \, |p(x)|}.$$

The integral appearing in the exponential is

$$\int_{d/2}^{x_t} dx \sqrt{2m(V - E_0)} = \sqrt{2me\mathcal{E}} \int_{d/2}^{x_t} dx \sqrt{x_t - x}$$
$$= \frac{2}{3} \sqrt{2me\mathcal{E}} \left( x_t - \frac{d}{2} \right)^{3/2}.$$

Since  $e\mathcal{E}d \ll V_0$ , the barrier is very wide, and we do indeed have  $x_t \gg d$ :

$$\frac{x_t}{d} = \frac{V_0 - \frac{\hbar^2 \pi^2}{2md^2}}{e\mathcal{E}d} \simeq \frac{V_0}{e\mathcal{E}d} \gg 1,$$

and therefore

$$T \simeq e^{-\frac{4}{3\hbar} \frac{\sqrt{2mV_0^3}}{e\mathcal{E}}}. (1)$$

(d) (5 points) Classically, the time associated with this particle is  $t_0 = \frac{2d}{v}$ , the time it takes to bounce back and forth once. Here the velocity is  $v = \sqrt{\frac{2E_{\infty,0}}{m}} = \frac{\hbar\pi}{md}$ . So, if we have N particles in the box, all N hit the right wall in time  $t_0$ , therefore in time dt,  $Ndt/t_0$  particles hit the right wall and escape with the probability T. Hence, differential rate of loss of particle number is given by:

$$dN = -TN\frac{dt}{t_0},$$

and therefore

$$N = N_0 e^{-Tt/t_0}$$

where  $N_0$  is the initial number of particles. The lifetime of the bound state is thus,

$$\tau = \frac{t_0}{T} = \frac{2md^2}{T\pi\hbar}.$$

- (e) (2 points) Plugging in the given numbers,  $T = e^{-86115}$ . This gives the lifetime of  $\tau = 4 \times 10^{37383}$  s—which is unbelievably long! The age of the universe is 13.7 billion years, which is  $4.3 \times 10^{17}$  s.
- (f) (3 points) Since we found that  $T = \exp(-\operatorname{const.}/\mathcal{E})$ , and  $\tau \propto \frac{1}{T}$ , we have already demonstrated that the lifetime goes like  $\exp(1/\mathcal{E})$ . If we Taylor expand  $e^{-1/\mathcal{E}}$  about  $\mathcal{E} = 0$ , we get zero to any finite order in  $\mathcal{E}$ , and hence you cannot see tunneling at any order in perturbation theory.

# 2. Quantum Mechanics of a Bouncing Ball (10 points)

(a) (5 points) For this potential, the appropriate quantization condition is  $\int_0^{x_t} dx \sqrt{2m(E_n - mgx)} = (n - \frac{1}{4})\pi\hbar$  (see e.g. Griffiths equation (8.47) on p. 330), as one side of the potential is a vertical wall. The classical turning point here is  $x_t = E_n/(mg)$ . Doing the integral,

$$\int_0^{x_t} dx \sqrt{2m} (E_n - mgx)^{1/2} = \sqrt{\frac{2}{m}} \frac{2}{3g} E_n^{3/2}.$$

We therefore find

$$E_n = \left(\frac{3}{4}\left(n - \frac{1}{4}\right)\pi\hbar\sqrt{2m}g\right)^{2/3}.$$

(b) (2 points) Quantum mechanical ground state of neutron  $(n = 1 \text{ and } m = 1.67 \times 10^{-27} Kg)$  will have energy

$$E_1 = \left( (3/4)^2 \pi \hbar \sqrt{2mg} \right)^{2/3} = 1.37 \times 10^{-12} \text{ eV}$$

This is tiny, as expected—gravity is a very weak force.

(c) (3 points) Classically, the energy of the dropped ball is  $E_c = mgx_0$ . With  $x_0 = 1$  m, m = 1 g, this is  $E_c = 9.8 \times 10^{-3} J$ . We would like to find n such that  $E_n = 9.8 \times 10^{-3} J$ . This works out to the huge value,  $n = 2 \times 10^{10}$ !

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

(a) and (b) (11 points) The steps suggested by Griffiths are: work out the wave function  $\psi_1$  in region (i); from  $\psi_1$  use the connection formulae at  $x_2$  to obtain the wave function  $\psi_2$  in regions (ii); use  $\psi_2$  and the connection formulae at  $x_1$  to obtain the wave function  $\psi_3$  in region (iii). (8.59) can be found by requiring that  $\psi_3$  should satisfy  $\psi_3(0) = 0$  or  $\psi'_3(0) = 0$  at x = 0.

Here we will use a slightly different approach from what Griffiths suggests. The purpose is for you to see an alternative approach, which has its own advantages. We use the symmetry condition to write down the wave function  $\psi_3$  in region (iii) directly. The wave function  $\psi_2$  in region (ii) then can be obtained using two ways: from  $\psi_1$  in region (i) via connection formulae at  $x_2$ , or from  $\psi_3$  in region (iii) via connection formulae at  $x_1$ . The equality of two wave functions leads to equation (8.59) of Griffiths. Here are details of this approach. Note that the connection formulae used below follow the convention of equations (3)-(6) in supplementary notes on connection formulae.

The wave function must satisfy two conditions, namely that (1) it must go to 0 at  $\infty$ , and (2) since the potential is even, the wave function must be either even,  $\psi(x) = \psi(-x)$ , or odd,  $\psi(x) = -\psi(-x)$ . These two conditions tell us that the WKB wave function in the three regions must have the following forms:

$$\psi_1 = \frac{A}{\sqrt{|p|}} e^{-\frac{1}{\hbar} \int_{x_2}^x dx \, |p|}, \tag{2}$$

$$\psi_2 = \frac{B}{\sqrt{p}} e^{\frac{i}{\hbar} \int_x^{x_1} dx \, p} + \frac{C}{\sqrt{p}} e^{-\frac{i}{\hbar} \int_x^{x_1} dx \, p},$$

$$\psi_3 = \frac{D}{\sqrt{|p|}} \cosh\left(\frac{1}{\hbar} \int_0^x dx \, |p|\right) \qquad \psi \text{ even}$$
 (3)

$$= \frac{D}{\sqrt{|p|}} \sinh\left(\frac{1}{\hbar} \int_0^x dx \, |p|\right) \qquad \psi \text{ odd.}$$
 (4)

At the classical turning point  $x_2$ , we apply the connection formula to  $\psi_1$  (eq (2)) to find the wave function in region (ii)

$$\psi_2(x) = \frac{2A}{\sqrt{p}} \cos \left[ \int_x^{x_2} p \, dx - \frac{\pi}{4} \right].$$

Defining

$$\theta = \frac{1}{\hbar} \int_{x_1}^{x_2} p \, dx$$

and

$$I(x) = \frac{1}{\hbar} \int_{x_1}^x p \, dx,$$

we can rewrite  $\psi_2$  as

$$\psi_2(x) = \frac{2A}{\sqrt{p}}\cos\left(I + \frac{\pi}{4} - \theta\right). \tag{5}$$

We now turn our attention to the classical turning point  $x_1$ . First, we define

$$\frac{\phi}{2} = \int_0^{x_1} p \, dx.$$

In terms of  $\phi$ , the wave function (3) in region 3 is

$$\psi_3 = \frac{D}{2\sqrt{|p|}} \left[ e^{\phi/2} e^{-\frac{1}{\hbar} \int_x^{x_1} dx \, |p|} \pm e^{-\phi/2} e^{\frac{1}{\hbar} \int_x^{x_1} dx \, |p|} \right],\tag{6}$$

where the plus sign holds when the wave function is even, and the minus sign when the wave function is odd. We now use *both* connection formulae to (6) at  $x_1$  conclude that in region (ii)

$$\psi_2(x) = \frac{D}{2\sqrt{|p|}} \left[ 2e^{\phi/2} \cos\left(I - \frac{\pi}{4}\right) \pm e^{-\phi/2} \cos\left(I + \frac{\pi}{4}\right) \right]. \tag{7}$$

We are allowed to use both connection formula in this case—that is, we are allowed to use one connection formula "against the arrow"— because the symmetry of the potential tells us exactly which linear combination of growing and dying exponentials we have in region 3. Ordinarily, we are not allowed to use the second connection formula against the arrow because if the wave function contains any component which grows exponentially, then our approximation is not sensitive enough to tell whether there is also a component of the wave function which the case exponentially, and if so what the relative weight of each part of the wave function is. In this case, however, we know that we must have either a sinh or a cosh, as the potential is even.

By setting equation (5) equal to equation (7), we find

$$D\left[2e^{\phi/2}\sin\left(I+\frac{\pi}{4}\right)\pm e^{-\phi/2}\cos\left(I+\frac{\pi}{4}\right)\right] = 4A\left[\cos\left(I+\frac{\pi}{4}\right)\cos\theta + \sin\left(I+\frac{\pi}{4}\right)\sin\theta\right],$$

which tells us that  $D = e^{-\phi/2} 2A \sin \theta$ , and, more importantly, that

$$\tan \theta = \pm 2e^{\phi}$$
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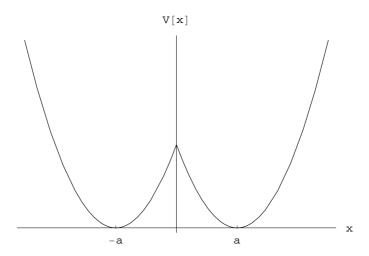


Figure 2: Double well potential

(c) (2 points) Writing  $\theta = (n + \frac{1}{2})\pi + \epsilon$ , we find

$$\tan \theta = \frac{(-1)^n \cos \epsilon}{(-1)^{n+1} \sin \epsilon} \simeq -\frac{1}{\epsilon}.$$

Therefore the quantization condition becomes

$$-\frac{1}{\epsilon} = \pm 2e^{\phi}$$

and therefore

$$\theta = (n + \frac{1}{2})\pi \mp \frac{1}{2}e^{-\phi}.$$
 (8)

(d) (3 points) The potential is sketched in figure 2. For this potential we have

$$\theta = \frac{2}{\hbar} \int_a^{x_t} dx \, m\omega \sqrt{(x_t - a)^2 - (x - a)^2}.$$

Using the result

$$\int dz \sqrt{\alpha^2-z^2} = \frac{1}{2} z \sqrt{\alpha^2-z^2} - \frac{1}{2} \alpha^2 \mathrm{arctan} \left( -\frac{z}{\sqrt{\alpha^2-z^2}} \right),$$

we find

$$\theta = \frac{2m\omega}{\hbar} \left( \frac{E}{m\omega^2} \mathrm{arctan}(\infty) \right) = \frac{\pi E}{\hbar \omega}.$$

Here we have taken  $\arctan(\infty) = \pi/2$ , as the multivaluedness of the inverse tangent is taken care of below. Equation (8) is now

$$\frac{\pi E}{\hbar \omega} = (n + \frac{1}{2})\pi \mp \frac{1}{2}e^{-\phi},$$

or

$$E = (n + \frac{1}{2})\hbar\omega \mp \frac{\hbar\omega}{2\pi}e^{-\phi}.$$

The first part of this expression is, of course, the familiar harmonic oscillator energy levels; the second part is an offset due to the barrier.

(e) (3 points) The wave function for a particle that starts out in the right well is

$$\psi(x,t) = \frac{1}{\sqrt{2}} \left( \psi_n^+ e^{-iE_n^+ t/\hbar} + \psi_n^- e^{-iE_n^- t/\hbar} \right).$$

The probability density coming from this wave function is

$$|\psi(x,t)|^2 = \frac{1}{2} \left( |\psi_n^+|^2 + |\psi_n^-|^2 + 2\psi_n^+ \psi_n^- \cos\left(\frac{\omega e^{-\phi}t}{\pi}\right) \right).$$

When  $\cos\left(\frac{\omega e^{-\phi_t}}{\pi}\right) = -1$ , then the particle has hopped to the other well, since at that time  $t_{-1} |\psi(x,t_{-1})|^2 = \frac{1}{2}|\psi_n^+(x,0) - \psi_n^-(x,0)|^2$ .

The period of oscillation between the two wells is therefore  $\tau = \frac{2\pi^2}{\omega} e^{\phi}$ . Note that a large barrier corresponds to a very long period, which makes physical sense.

(f) (3 points) We have for this specific potential

$$\phi = \frac{2m\omega}{\hbar} \int_0^{x_1} dx \sqrt{(x-a)^2 - (x_1 - a)^2}.$$

Using the integral

$$\int dz \sqrt{z^2 - \alpha^2} = \frac{1}{2} z \sqrt{z^2 - \alpha^2} - \frac{1}{2} \alpha^2 \ln \left( z + \sqrt{z^2 - \alpha^2} \right),$$

we find

$$\phi = \frac{m\omega}{\hbar} \left[ a\sqrt{a^2 - \frac{2E}{m\omega}} - \frac{2E}{m\omega} \ln \frac{2E/m\omega}{-a + \sqrt{a^2 - \frac{2E}{m\omega}}} \right].$$

In the limit where  $V(0) = \frac{1}{2}m\omega^2 a^2 \gg E$ , the above expression reduces to

$$\phi \simeq \frac{m\omega a^2}{\hbar}.$$

# 4. Vibrational and rotational Spectra in Born-Oppenheimer Approximation (8 points)

(a) (5 points) Define a convenient dimensionless variable  $y \equiv (R - R_0)/R_0$ . In terms of this new variable  $\mathcal{E}(y, J)$  is given by,

$$\mathcal{E}(y,J) = \frac{m\omega^2 R_0^2}{2} y^2 + \frac{J(J+1)\hbar^2}{2mR_0^2(y+1)^2}$$
$$= ay^2 + \frac{b}{(y+1)^2}.$$

Notice that the ratio,

$$\frac{b}{a} \sim \frac{\text{rotational energy}}{\text{vibrational energy}} \ll 1.$$

Now we minimize  $\mathcal{E}$  w.r.t. y, to get the equation

$$y_{min}(1+y_{min})^3 = \frac{b}{a}.$$

Since both  $b/a \ll 1$  and  $y_{min} = \delta R/R_0 \ll 1$ , we can slove the equation above order by order in b/a. To the least order in the ratio b/a we get,  $y_{min} = b/a$ . [Note: To the next leading we solve the quadratic equation  $3y^2 + y = b/a$  to get  $y_{min} = b/a - 3b^2/a^2$ . This comment is for illustration purpose only. Result only upto leading order in b/a is required for part (b). Full credit must be provided for solutions upto leading order in b/a.] Therefore,

$$R_{min} = R_0 + y_{min}R_0 = R_0 + \frac{J(J+1)\hbar^2}{m^2\omega^2 R_0^3}.$$

(b) (3 points) Using the form  $R_{min} = R_0(1 + b/a)$ , we get

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

$$= \frac{J(J+1)\hbar^{2}}{2mR_{0}^{2}(1+b/a)^{2}}$$

$$= \frac{J(J+1)\hbar^{2}}{2mR_{0}^{2}} \left(1 - \frac{2b}{a} + \mathcal{O}\left(\frac{b^{2}}{a^{2}}\right)\right).$$

Substituting for  $b = J(J+1)\hbar^2/2mR_0^2$  and  $a = m\omega^2R_0^2/2$  in the above expression we obtain,

$$E_J = \frac{J(J+1)\hbar^2}{2mR_0^2} - \frac{J^2(J+1)^2\hbar^4}{m^3\omega^2R_0^6} + \dots$$

From this we readily obtain  $A = \hbar^2/2mR_0^2$  and  $B = -\hbar^4/m^3\omega^2R_0^6$ 

## 5. Adiabatic Spin Rotation (8 points)

The adiabatic theorem tells us that, provided we change the magnetic field slowly enough, the particle will remain in the same (slowly varying) energy level provided that the particle never reaches a point in its trajectory where energy levels become degenerate. (The proof of the adiabatic theorem relies on being able to choose timescales larger than  $\hbar/(\Delta E)$ ; when  $\Delta E = 0$ , this is impossible. There is no way to suppress the transition amplitudes between exactly degenerate states.) The residual field  $\delta \vec{B} = (B_x, B_y, 0)$  ensures that at  $t = B_0/\beta$ , the two spin states are still non degenerate. This is all that we need to know to conclude that at  $t_f$  the particle's final state is  $|\downarrow\rangle$ , independent of the details of  $\delta \vec{B}$ , provided that we change  $B_z$  slowly enough.

The closest splitting between the two energy levels occurs at  $t = B_0/\beta$ . Here the difference in the energy between the two states is  $\Delta E = 2\mu_0 |\delta B|$ , and so the shortest timescale of the system is  $t_s = \hbar/(2\mu_0 |\delta B|)$ . The amount of time that the system spends in this "dangerous" region is of the order of  $t_d = \frac{2|\delta B|}{\beta}$ , since this is the length of time during which the residual magnetic field  $\delta B$  is larger than the magnetic field  $B_0 - \beta t$ . We therefore identify the adiabatic timescale as  $t_d$ . For the adiabatic theorem to apply, we must have  $t_d \gg t_s$ , or

$$\beta \ll \frac{\mu_0 |\delta B|^2}{\hbar}.$$

(Here I have dropped numerical factors of order unity.) This result shows why, in magnetic traps, one does not allow the magnetic fields to be 0. When B=0, the two spin states become

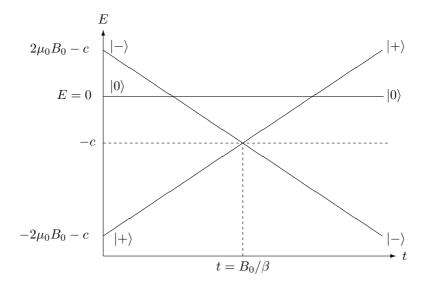


Figure 3: The energy levels of the system without  $B_x$ .

degenerate, and the adiabatic theorem breaks down. This means that the spins can flip, and atoms can leak out of the traps.

## 6. Engineering Adiabatic Transitions (12 points)

(a) (3 points) In the basis  $\{|+\rangle, |0\rangle, |-\rangle\}$ , the spin matrices are

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad S_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad S_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

These matrices satisfy  $[S_i, S_j] = i\epsilon_{ijk}\hbar S_k$ , as any self-respecting set of angular momentum matrices must.

(b) (6 points) The Hamiltonian has the form

$$H = \begin{pmatrix} -2\mu_0(B_0 - \beta t) - c & -\sqrt{2}\mu_0 B_x & 0\\ -\sqrt{2}\mu_0 B_x & 0 & -\sqrt{2}\mu_0 B_x\\ 0 & -\sqrt{2}\mu_0 B_x & 2\mu_0(B_0 - \beta t) - c \end{pmatrix}.$$

We need to sketch the behavior of the energy levels of the system as we vary the time t. The hierarchy of energies that we are given,  $\mu_0 B_0 \gg c \gg \mu_0 B_x$ , tells us that we can get a rough picture of the energy levels by temporarily ignoring  $B_x$ . Without the contributions of the  $B_x$  fields, the energy levels of the system vary with time as shown in figure 3. Notice that if  $B_x$  were 0, we could not use the adiabatic theorem to analyze this system, because it is not applicable when the eigenvalues cross each other.

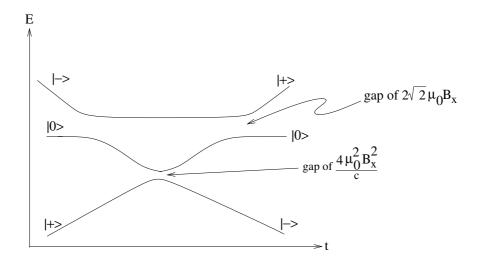


Figure 4: Sketch of the evolution of the energy levels.

The contributions of the  $B_x$  term (which we can treat as a perturbation) become important when the differences between the eigenvalues of  $H_0 = -\frac{2\mu_0}{\hbar}S_zB_z - \frac{c}{\hbar^2}S_z^2$  are small. We can see from figure 3 that we will need to take the  $B_x$  perturbation into account at all three places where the unperturbed energy levels intersect; the effect of the perturbation will be to lift the (instantaneous) degeneracies at these intersections.

When  $\beta t = B_0 - c/(2\mu_0)$ ,  $|0\rangle$  and  $|-\rangle$  are degenerate. To find the correction to the energy levels from the nonzero  $B_x$ , we need to diagonalize the instantaneous Hamiltonian within the degenerate subspace at this crossing point,

$$H = -\sqrt{2}\mu_0 B_x \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right).$$

The eigenvalues of the above Hamiltonian are  $\pm\sqrt{2}\mu_0B_x$ , and therefore the effect of the nonzero  $B_x$  here is to open up a gap of width  $2\sqrt{2}\mu_0B_x$  between the two energy levels.

When  $\beta t = B_0$ , the energy levels  $|+\rangle$  and  $|-\rangle$  are degenerate. Diagonalizing the Hamiltonian at  $t = B_0/\beta$  tells us that a gap of  $4\mu_0^2 B_x^2/c$  opens up between the degenerate energy levels at this point. Notice that this is only a small gap when  $c \gg \mu_0 B_x$ .

Therefore, the effect of the magnetic field  $B_x$  is to open up gaps between energy levels that, in the absence of  $B_x$ , would intersect. The energy levels of the system as a function of time look like the sketch in figure 4.

(c) (3 points) If we begin in the state  $|-\rangle$  at t=0, then the smallest gap we will encounter as we vary the magnetic field has a width of  $\Delta E=2\sqrt{2}\mu_0B_x$ . The statement  $\mu_0B_x\gg\hbar\beta/B_x$  in the given hierarchy of energies is precisely the adiabatic condition for this gap, as we can see by reasoning similar to what we used on problem 5. As before, the adiabatic timescale is the amount of time that the system spends traversing the dangerous region near the small gap,  $t_a=B_x/\beta$ . This time needs to be much larger than the timescale determined by the energy

difference,  $t_s = \hbar/\Delta E$ . This condition,  $t_a \gg t_s$ , is precisely the statement that  $\mu_0 B_x \gg \hbar \beta/B_x$ . Therefore, the variation of the magnetic field is sufficiently slow compared to the gap for the adiabatic theorem to apply. Thus, a particle that begins in the state  $|-\rangle$  initially will follow the top level in the sketch of figure 4 without making any transitions to other energy levels. We can conclude that this particle will evolve to a state first approximately equal to  $|0\rangle$  and then  $|+\rangle$ .

To have this particle end up in the state  $|0\rangle$ , we could stop varying the magnetic field once we reach the point  $t = B_0/\beta$ .