

# Quantum Physics III (8.06) Spring 2005

## Solution Set 8

April 20, 2005

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

(a) **(3 points)** We are given a trial wave function  $\psi(x) = A \operatorname{sech}(ax)$ . Since

$$\frac{\partial^2 \psi}{\partial x^2} = Aa^2 [\operatorname{sech}(ax) - 2\operatorname{sech}^3(ax)],$$

the Schrodinger equation becomes

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi &= -\frac{\hbar^2 a^2}{2m} A (\operatorname{sech}(ax) - 2\operatorname{sech}^3(ax) + 2\operatorname{sech}^3(ax)) \\ &= -\frac{\hbar^2 a^2}{2m} \psi. \end{aligned}$$

Therefore  $\psi$  is an eigenfunction of  $H$  with eigenvalue  $-\hbar^2 a^2/2m$ . Since  $\psi$  has no nodes, it must be the ground state.

(b) **(5 points)** Let  $b$  be the location of the classical turning point. We estimate the lowest energy eigenvalue by applying the quantization condition

$$\int_{-b}^b dx \sqrt{2m(V(b) - V(x))} = (n - \frac{1}{2})\pi\hbar, \quad (1)$$

where  $n = 1, 2, \dots$ . We need to evaluate the integral  $\int_{-b}^b dx \sqrt{\operatorname{sech}^2(ax) - \operatorname{sech}^2(ab)}$ . This integral can be done by setting  $z = \operatorname{sech}^2(ax)$  (therefore,  $dz = -2az\sqrt{1-z} dx$ ):

$$\begin{aligned} \int_{-b}^b dx \sqrt{\operatorname{sech}^2(ax) - \operatorname{sech}^2(ab)} &= \int_{z_0}^1 \frac{dz}{z} \sqrt{\frac{z - z_0}{1 - z}} \\ &= \frac{\pi}{a} (1 + \sqrt{z_0}), \end{aligned}$$

where  $0 < z_0 = \operatorname{sech}^2(ab) < 1$  and the  $z$  integral is done by using Mathematica. Since the classical turning point is

$$\operatorname{sech}(ab) = \frac{\sqrt{-E_n m}}{\hbar a},$$

our quantization condition (1) above gives us  $\sqrt{2}\hbar\pi(1 + \sqrt{-E_n m}/(\hbar a)) = (n - \frac{1}{2})\pi\hbar$ , or

$$E_n = -\frac{\hbar^2 a^2}{2m} (n - \frac{1}{2} - \sqrt{2})^2.$$

To estimate the energy of the ground state, set  $n = 1$ :

$$E_1 = -\frac{\hbar^2 a^2}{2m} \times (.914\dots)^2,$$

or, in other words, 83% of the correct answer.

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

(a) **(4 points)** For this potential, the appropriate quantization condition is  $\int_0^{x_t} dx \sqrt{2m(E_n - mgx)} = (n - \frac{1}{4})\pi\hbar$ , 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

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

(b) **(2 points)** Quantum mechanical ground state of neutron ( $n = 1$  and  $m = 1.67 \times 10^{-27} \text{ Kg}$ ) 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) **(2 points)** Classically, the energy of the dropped ball is  $E_c = mgx_0$ . With  $x_0 = 1 \text{ m}$ ,  $m = 1 \text{ g}$ , this is  $E_c = 9.8 \times 10^{-3} \text{ J}$ . We would like to find  $n$  such that  $E_n = 9.8 \times 10^{-3} \text{ J}$ . 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 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:

$$\begin{aligned} \psi_1 &= \frac{A}{\sqrt{|p|}} e^{-\frac{1}{\hbar} \int_{x_2}^x dx |p|}, \\ \psi_2 &= \frac{B}{\sqrt{p}} e^{\frac{i}{\hbar} \int_x^{x_1} dx p} + \frac{C}{\sqrt{p}} e^{-\frac{i}{\hbar} \int_x^{x_1} dx p}, \\ \psi_3 &= \frac{D}{\sqrt{|p|}} \cosh \left( \frac{1}{\hbar} \int_0^x dx |p| \right) \quad \psi \text{ even} \\ &= \frac{D}{\sqrt{|p|}} \sinh \left( \frac{1}{\hbar} \int_0^x dx |p| \right) \quad \psi \text{ odd.} \end{aligned}$$

At the classical turning point  $x_2$ , we apply the connection formula in the standard way to find

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

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

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

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 in region 3 is

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

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 conclude

$$\psi_2(x) = \frac{D}{2\sqrt{|p|}} \left[ 2e^{\phi/2} \cos\left(I - \frac{\pi}{4}\right) \pm e^{-\phi/2} \cos\left(I + \frac{\pi}{4}\right) \right]. \quad (3)$$

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 decays 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 (2) equal to equation (3), 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

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

(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

$$\theta = (n + \frac{1}{2})\pi \mp \frac{1}{2}e^{-\phi}. \quad (4)$$

(d) **(3 points)** The potential is sketched in figure 1. For this potential we have

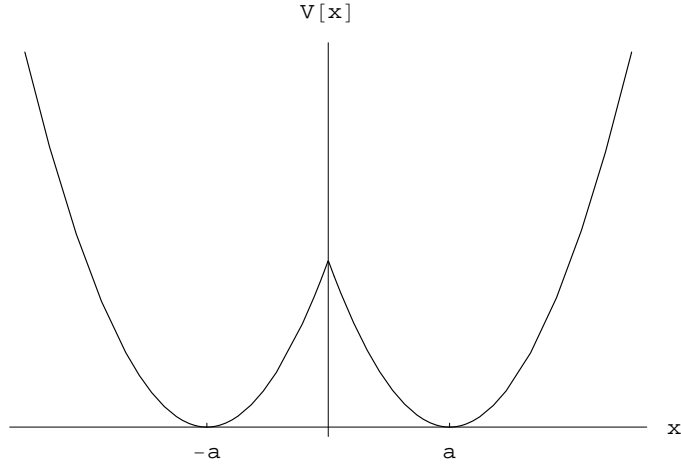


Figure 1: Double well potential

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

Using the result

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

we find

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

Here we have taken  $\arctan(\infty) = \pi/2$ , as the multivalued-ness of the inverse tangent is taken care of below. Equation (4) 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,

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

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 solve 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

$$\begin{aligned} E_J &= \frac{J(J+1)\hbar^2}{2mR_{min}^2} \\ &= \frac{J(J+1)\hbar^2}{2mR_0^2(1 + b/a)^2} \\ &= \frac{J(J+1)\hbar^2}{2mR_0^2} \left( 1 - \frac{2b}{a} + \mathcal{O}\left(\frac{b^2}{a^2}\right) \right). \end{aligned}$$

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

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

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

### 5. Adiabatic Spin Rotation (6 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 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 (8 points)

(a) **(2 points)** In the basis  $\{|+\rangle, |0\rangle, |-\rangle\}$ , the spin matrices are

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

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

(b) **(4 points)** The Hamiltonian has the form

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

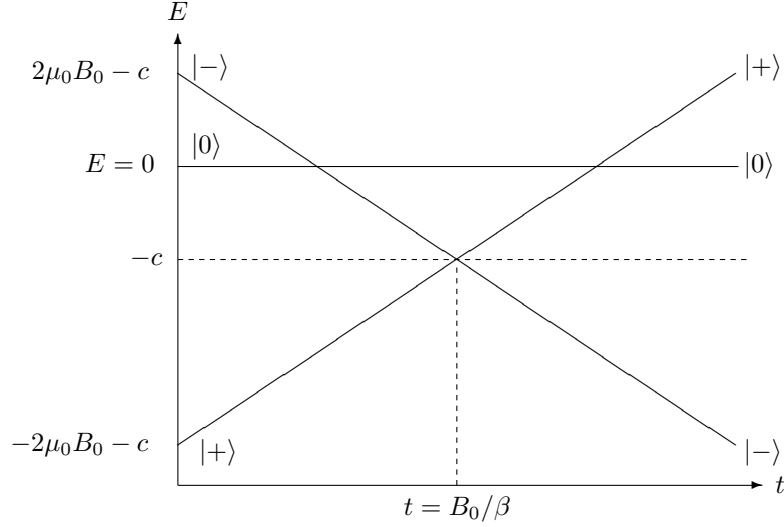


Figure 2: The energy levels of the system without  $B_x$ .

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 2. 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.

The contributions of the  $B_x$  term (which we can treat as a perturbation) become important when the differences between the eigenvalues of  $H_0 = -\frac{2\mu_0}{\hbar} S_z B_z - \frac{c}{\hbar^2} S_z^2$  are small. We can see from figure 2 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,

$$H = -\sqrt{2}\mu_0 B_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The eigenvalues of the above Hamiltonian are  $\pm\sqrt{2}\mu_0 B_x$ , and therefore the effect of the nonzero  $B_x$  here is to open up a gap of width  $2\sqrt{2}\mu_0 B_x$  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  $c \gg \mu_0 B_x$ .

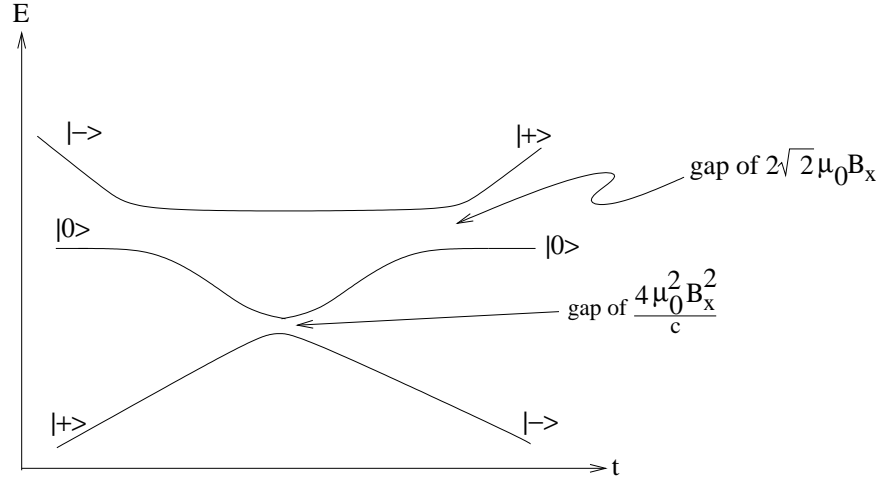


Figure 3: Sketch of the evolution of the energy levels.

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 3.

(c) **(2 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  $\Delta E = 2\sqrt{2}\mu_0 B_x$ . The statement  $\mu_0 B_x \gg \hbar\beta/B_x$  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 3 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  $t = B_0/\beta$ .