CHAPTER 10

THE ADIABATIC APPROXIMATION

10.1 THE ADIABATIC THEOREM

10.1.1 Adiabatic Processes

Imagine a perfect pendulum, with no friction or air resistance, oscillating back and forth in a vertical plane. If I grab the support and shake it in a jerky manner, the bob will swing around in a wild chaotic fashion. But if I *very gently and steadily* move the support (Figure 10.1), the pendulum will continue to swing in a nice, smooth way, in the same plane (or one parallel to it) with the same amplitude. This *gradual change in the external conditions* characterizes an **adiabatic** process. Notice that there are two characteristic times involved: T_i, the "internal" time, representing the motion of the system itself (in this case the period of the pendulum's oscillations), and T_e, the "external" time, over which the parameters of the system change appreciably (if the pendulum were mounted on an oscillating platform, for example, T_e would be the period of the *platform's* motion). An adiabatic process is one for which $T_e \gg T_i$.[1]

The basic strategy for analyzing an adiabatic process is first to solve the problem with the external parameters held *fixed*, and only at the *end* of the calculation allow them to change with time. For example, the classical period of a pendulum of (constant) length L is $2\pi\sqrt{L/g}$; if the length is now gradually *changing*, the

[1] For an interesting discussion of classical adiabatic processes, see Frank S. Crawford, *Am. J. Phys.* **58**, 337 (1990).

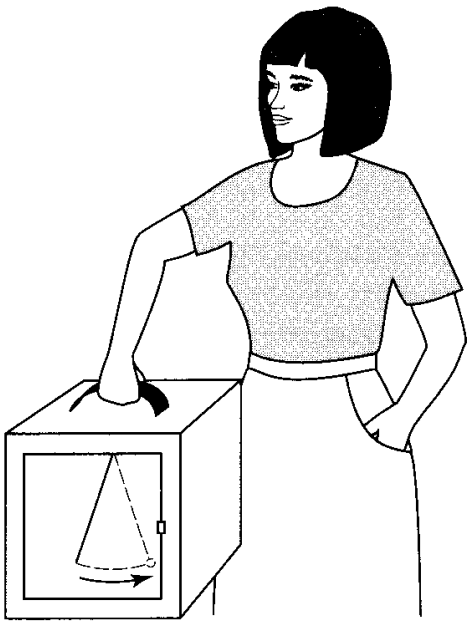

Figure 10.1: Adiabatic motion: If the case is transported very gradually, the pendulum inside keeps swinging with the same amplitude, in a plane parallel to the original one.

period will presumably be $2\pi\sqrt{L(t)/g}$. When you stop to think about it, we actually *use* the adiabatic approximation (implicitly) all the time without noticing it. A case in point is our discussion of the hydrogen molecule ion (Section 7.3). We began by assuming that the nuclei were *at rest*, a fixed distance R apart, and we solved for the motion of the electron. Once we had found the ground state energy of the system as a function of R, we located the equilibrium separation and from the curvature of the graph we obtained the frequency of vibration of the nuclei (Problem 7.10). In molecular physics this technique (beginning with nuclei at rest, calculating electronic wave functions, and using these to obtain information about the positions and—relatively sluggish—motion of the nuclei) is known as the **Born-Oppenheimer approximation**.

In quantum mechanics, the essential content of the **adiabatic approximation** can be cast in the form of a theorem. Suppose that the Hamiltonian changes *gradually* from some initial form H^i to some final form H^f (Figure 10.2). The **adiabatic theorem** states that if the particle was initially in the nth eigenstate of H^i, it will be

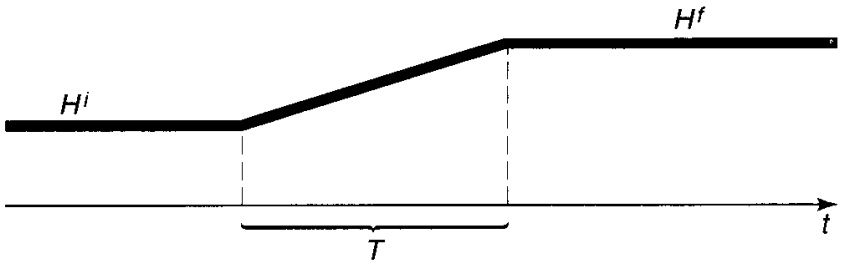

Figure 10.2: A model for adiabatic change in the Hamiltonian, from H^i to H^f.

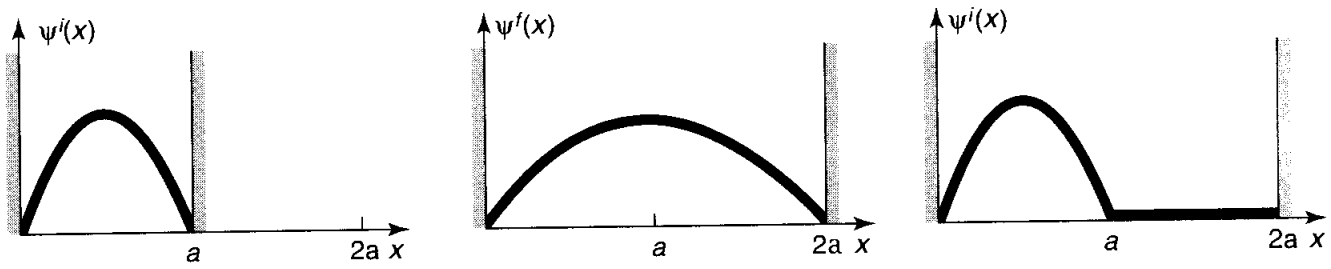

Figure 10.3: (a) Particle starts out in the ground state of the infinite square well. (b) If the wall moves *slowly*, the particle remains in the ground state. (c) If the wall moves *rapidly*, the particle is left (momentarily) in its initial state.

carried (under the Schrödinger equation) into the nth eigenstate of H^f. (I assume that the spectrum is discrete and nondegenerate throughout the transition from H^i to H^f, so there is no ambiguity about the ordering of the states; these conditions can be relaxed, given a suitable procedure for "tracking" the eigenfunctions, but I'm not going to pursue that here.)

For example, suppose we prepare a particle in the ground state of the infinite square well (Figure 10.3a):

$$\psi^i(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right). \qquad [10.1]$$

If we now gradually move the right wall out to $2a$, the adiabatic theorem says that the particle will end up in the ground state of the expanded well (Figure 10.3b):

$$\psi^f(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi}{2a}x\right) \qquad [10.2]$$

(apart, perhaps, from a phase factor). Notice that we're not talking about a *small* change in the Hamiltonian (as in perturbation theory)—this one is a *huge* change. All we require is that it happen *slowly*. By contrast, if the well expands *suddenly*, the resulting state is still $\psi^i(x)$ (Figure 10.3c), which is a complicated linear combination of eigenstates of the new Hamiltonian (Problem 3.48).

***Problem 10.1** The case of an infinite square well whose right wall expands at a *constant* velocity (v) can be solved *exactly*.[2] A complete set of solutions is

$$\Phi_n(x,t) \equiv \sqrt{\frac{2}{w}} \sin\left(\frac{n\pi}{w}x\right) e^{i(mvx^2 - 2E_n^i at)/2\hbar w}, \qquad [10.3]$$

where $w(t) \equiv a + vt$ is the width of the well and $E_n^i \equiv n^2\pi^2\hbar^2/2ma^2$ is the nth allowed

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[2] S. W. Doescher and M. H. Rice, *Am. J. Phys.* **37**, 1246 (1969).

energy of the *original* well (width a). The *general* solution is a linear combination of the Φ's:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Phi_n(x,t); \qquad [10.4]$$

the coefficients c_n are *independent of* t.

(a) Check that Equation 10.3 satisfies the time-dependent Schrödinger equation, with the appropriate boundary conditions.

(b) Suppose a particle starts out ($t = 0$) in the ground state of the initial well:

$$\Psi(x,0) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right).$$

Show that the expansion coefficients can be written in the form

$$c_n = \frac{2}{\pi} \int_0^{\pi} e^{-i\alpha z^2} \sin(nz) \sin(z)\, dz, \qquad [10.5]$$

where $\alpha \equiv mva/2\pi^2\hbar$ is a dimensionless measure of the speed with which the well expands. (Unfortunately, this integral cannot be evaluated in terms of elementary functions.)

(c) Suppose we allow the well to expand to twice its original width, so the "external" time is given by $w(T_e) = 2a$. The "internal" time is the *period* of the time-dependent exponential factor in the (initial) ground state. Determine T_e and T_i, and show that the adiabatic regime corresponds to $\alpha \ll 1$, so that $e^{-i\alpha z^2} \cong 1$ over the domain of integration. Use this to determine the expansion coefficients c_n. Construct $\Psi(x,t)$, and confirm that it is consistent with the adiabatic theorem.

(d) Show that the phase factor in $\Psi(x,t)$ can be written in the form

$$\theta(t) = -\frac{1}{\hbar} \int_0^t E_1(t')\, dt', \qquad [10.6]$$

where $E_n(t) \equiv n^2\pi^2\hbar^2/2mw^2$ is the n^{th} *instantaneous* eigenvalue, at time t. Comment on this result.

10.1.2 Proof of the Adiabatic Theorem

The adiabatic theorem is simple to state, and it *sounds* plausible, but it is not easy to prove.[3] Suppose the time-dependent part of the Hamiltonian can be written in the form[4]

$$H'(t) = Vf(t), \qquad [10.7]$$

where $f(t)$ is a function that starts out zero (at $t = 0$) and increases to 1 (at $t = T$), Figure 10.4. Assume that the particle starts out in the n^{th} eigenstate of the original Hamiltonian:

$$\Psi(0) = \psi_n^i \qquad [10.8]$$

and evolves into some state $\Psi(t)$. Our problem is to show that if the function $f(t)$ rises *very gradually*, then the probability that the particle, at time T, is in the nth eigenstate of the *final* Hamiltonian (ψ_n^f) is 1. More precisely, we must demonstrate that

$$|\langle \Psi(T)|\psi_m^f\rangle|^2 = \begin{cases} 1, & \text{if } m = n, \\ 0, & \text{if } m \neq n. \end{cases} \qquad [10.9]$$

(Of course, if the first of these is true, the second *has* to be, and vice versa. But it is not clear at this stage which condition will be easier to prove.)

Assume for the moment that V is *small*, so we can use first-order time-independent perturbation theory to determine ψ_m^f. From Equation 6.12,

$$\psi_m^f \cong \psi_m + \sum_{k \neq m} \frac{V_{km}}{E_m - E_k}\psi_k, \qquad [10.10]$$

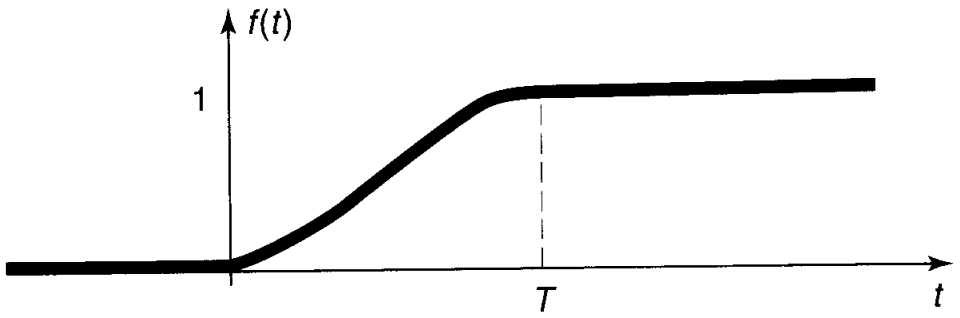

Figure 10.4: The function $f(t)$, in Equation 10.7.

[3]The adiabatic theorem is usually attributed to Ehrenfest, who studied adiabatic processes in early versions of the quantum theory. The first proof in modern quantum mechanics was given by Born and Fock, *Zeit. f. Physik* **51**, 165 (1928). Other proofs will be found in Messiah, *Quantum Mechanics* (New York: John Wiley & Sons, 1962), Vol. II, Chapter XVII, Section 12, and J-T. Hwang and Philip Pechukas, *J. Chem. Phys.* **67**, 4640 (1977). The argument given here is suggested by Gasiorowicz, *Quantum Physics* (New York: John Wiley & Sons, 1974), Chapter 22, Problem 6.

[4]The assumption that H' is the *product* of an operator (V) and a (real) function of t is not necessary for the theorem itself, but it does make the proof less cumbersome. In Section 10.1.3 we will encounter a case in which the different matrix elements of H' have *different* (complex) time dependences. As long as the adiabatic approximation (in the form of Equation 10.15) holds for *each* of them, the adiabatic theorem itself is valid.

where

$$V_{km} \equiv \langle \psi_k | V | \psi_m \rangle. \tag{10.11}$$

(To simplify the notation, I'll drop the superscript i on eigenfunctions and eigenvalues of the initial Hamiltonian; these are the "unperturbed" states for the problem.)

Meanwhile, we use first-order time-*dependent* perturbation theory to determine $\Psi(T)$. From Equation 9.81,

$$\Psi(t) = \sum_l c_l(t) \psi_l e^{-iE_l t/\hbar}, \tag{10.12}$$

where (Equation 9.84)

$$c_n(t) \cong 1 - \frac{i}{\hbar} V_{nn} \int_0^t f(t')\, dt' \tag{10.13}$$

and (Equation 9.85)

$$c_l(t) \cong -\frac{i}{\hbar} V_{ln} \int_0^t f(t') e^{i(E_l - E_n)t'/\hbar}\, dt', \quad l \neq n. \tag{10.14}$$

This last integral can be evaluated using integration by parts. Note that

$$e^{i(E_l - E_n)t'/\hbar} = \frac{-i\hbar}{E_l - E_n} \frac{d}{dt'} \left[e^{i(E_l - E_n)t'/\hbar} \right],$$

so

$$c_l(t) \cong -\frac{V_{ln}}{E_l - E_n} \int_0^t f(t') \frac{d}{dt'} \left[e^{i(E_l - E_n)t'/\hbar} \right] dt'$$

$$= -\frac{V_{ln}}{E_l - E_n} \left\{ f(t) e^{i(E_l - E_n)t/\hbar} - \int_0^t \frac{df}{dt'} e^{i(E_l - E_n)t'/\hbar}\, dt' \right\}.$$

[I dropped the lower limit in the first term, because $f(0) = 0$.] Now comes the adiabatic approximation: We want $f(t)$ to be a *very gradual* function, so that df/dt is extremely small. Specifically, we assume that

$$\frac{df}{dt} \ll \frac{|E_l - E_n|}{\hbar} f; \tag{10.15}$$

then the last term makes a negligible contribution to $c_l(t)$, and we conclude that

$$\Psi(T) \cong \left[\left(1 - i \frac{V_{nn} A}{\hbar} \right) \psi_n - \sum_{l \neq n} \frac{V_{ln}}{E_l - E_n} \psi_l \right] e^{-iE_n T/\hbar}, \tag{10.16}$$

where A is the area under the graph of $f(t)$, from 0 to T.

Putting together Equations 10.10 and 10.16, and exploiting the orthonormality of the initial eigenfunctions, we find that

$$\langle \Psi(T)|\psi_n^f\rangle = \left[1 + i\frac{V_{nn}A}{\hbar} + \sum_{k\neq n}\frac{|V_{kn}|^2}{(E_n - E_k)^2}\right] e^{iE_nT/\hbar}, \qquad [10.17]$$

while, for $m \neq n$,

$$\langle \Psi(T)|\psi_m^f\rangle = \left\{\left[1 + i\frac{V_{nn}A}{\hbar}\right]\frac{V_{nm}}{E_m - E_n} - \frac{V_{nm}}{E_m - E_n} + \sum_{n\neq k\neq m}\frac{V_{nk}V_{km}}{(E_n - E_k)(E_m - E_k)}\right\} e^{iE_nT/\hbar}$$

$$= \left[\frac{iAV_{nn}V_{nm}}{\hbar(E_m - E_n)} + \sum_{n\neq k\neq m}\frac{V_{nk}V_{km}}{(E_n - E_k)(E_m - E_k)}\right] e^{iE_nT/\hbar}. \qquad [10.18]$$

But wait: These wave functions were only accurate to *first* order in V, so the *second*-order terms in Equations 10.17 and 10.18 are spurious (we have already thrown away quantities of comparable size). To *first* order, we have

$$\langle \Psi(T)|\psi_m^f\rangle = \begin{cases} \left[1 + i\frac{V_{nn}A}{\hbar}\right] e^{iE_nT/\hbar}, & m = n, \\ 0 & m \neq n. \end{cases} \qquad [10.19]$$

It follows that

$$|\langle \Psi(T)|\psi_n^f\rangle|^2 = 1, \qquad [10.20]$$

while (for $m \neq n$)

$$|\langle \Psi(T)|\psi_m^f\rangle|^2 = 0. \qquad [10.21]$$

Ostensibly, *either* of these would suffice to establish the desired result (Equation 10.9). However, Equation 10.20 is only accurate to *first* order (in V), whereas Equation 10.21 is accurate to *second* order (and for that matter to *third* order as well).[5] In truth, Equation 10.20 tells us *nothing* (it would be valid also for a *nonadiabatic* transformation); the *crucial* point is the cancellation of the first-order terms in Equation 10.18, for this tells us that there will be no transitions to other states.[6]

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[5] See Problem 9.15 for a discussion of the analogous situation in ordinary perturbation theory.

[6] In this context the word "*transition*" means from an eigenstate ψ_n^i of the *initial* Hamiltonian (H^i) to a different eigenstate ψ_m^f of the *final* Hamiltonian (H^f). The adiabatic theorem says that if the Hamiltonian changes *gradually* from H^i to H^f, there will be *no* such transitions. By contrast, in the previous chapter we were always dealing with eigenstates of the *same* (unperturbed) Hamiltonian. At the end of the process the perturbation was (explicitly or implicitly) turned off, and a "transition" meant from one eigenstate of the unperturbed Hamiltonian to another eigenstate of the unperturbed Hamiltonian. The transition amplitudes were of *first* order in H' (Equations 9.17 and 9.85) and the transition probabilities of *second* order (for example, Equations 9.28, 9.86, and 9.87). The essence of the adiabatic theorem (as we shall see in the next paragraph) is that the transition amplitudes are only *second* order, and the transition probabilities *fourth* order in the (small) perturbation.

This shows that if the change in the Hamiltonian is both adiabatic *and* very small (so that first-order perturbation theory can be applied), then there will be no transitions. But what if the change, though gradual, is *not* small? In that case we chop the interval T into N subintervals, so that the change in the Hamiltonian during a single subinterval (ΔV) is of order V/N; if N it large, then ΔV is small, and we can apply the previous argument to each subinterval. If the transition amplitude (Equation 10.18) were *first* order in the perturbation, then the *total* transition amplitude would go like

$$N\left(\frac{V}{N}\right) \to V \qquad [10.22]$$

(N steps, each making a contribution proportional to ΔV). The net result would be of order V, and if V is large, so too would be the transition amplitude. But in *fact* the transition amplitude is *second* order, so the total goes like

$$N\left(\frac{V}{N}\right)^2 \to \frac{V^2}{N} \qquad [10.23]$$

In the limit as $N \to \infty$, the transition amplitude goes to zero, *regardless* of the size of V. QED

Problem 10.2 In the beginning of this chapter, I characterized an adiabatic process informally as one for which $T_e \gg T_i$. How is this related to the precise condition (Equation 10.15) required in the proof (in other words, what are T_e and T_i here)?

10.1.3 An Example

Imagine an electron (charge $-e$, mass m) at rest at the origin, in the presence of a magnetic field whose *magnitude* (B_0) is constant but whose *direction* sweeps out a cone, of opening angle α, at constant angular velocity ω (Figure 10.5):

$$\mathbf{B}(t) = B_0[\sin\alpha\cos(\omega t)\hat{\imath} + \sin\alpha\sin(\omega t)\hat{\jmath} + \cos\alpha\hat{k}. \qquad [10.24]$$

The Hamiltonian (Equation 4.158) is

$$H(t) = \frac{e}{m}\mathbf{B}\cdot\mathbf{S} = \frac{e\hbar B_0}{2m}[\sin\alpha\cos(\omega t)\sigma_x + \sin\alpha\sin(\omega t)\sigma_y + \cos\alpha\sigma_z]$$

$$= -\frac{\hbar\omega_1}{2}\begin{pmatrix} \cos\alpha & e^{-i\omega t}\sin\alpha \\ e^{i\omega t}\sin\alpha & -\cos\alpha \end{pmatrix}, \qquad [10.25]$$

where

$$\omega_1 \equiv -\frac{eB_0}{m}. \qquad [10.26]$$

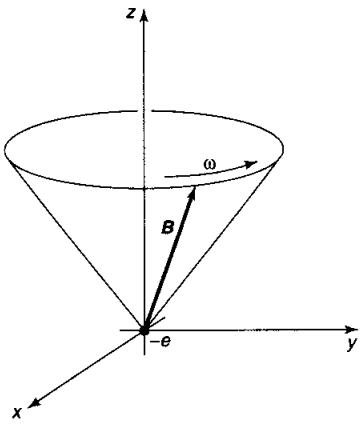

Figure 10.5: Magnetic field sweeps around on a cone, at angular velocity ω, Equation 10.24.

The normalized eigenspinors of $H(t)$ are

$$\chi_+(t) = \begin{pmatrix} \cos(\alpha/2) \\ e^{i\omega t}\sin(\alpha/2) \end{pmatrix} \quad [10.27]$$

and

$$\chi_-(t) = \begin{pmatrix} \sin(\alpha/2) \\ -e^{i\omega t}\cos(\alpha/2) \end{pmatrix}; \quad [10.28]$$

they represent spin up and spin down, respectively, *along the instantaneous direction of* $\mathbf{B}(t)$ (see Problem 4.31). The corresponding eigenvalues are

$$E_\pm = \mp\frac{\hbar\omega_1}{2}. \quad [10.29]$$

Suppose the electron starts out with spin up, along $\mathbf{B}(0)$:

$$\chi(0) = \begin{pmatrix} \cos(\alpha/2) \\ \sin(\alpha/2) \end{pmatrix}. \quad [10.30]$$

The exact solution to the time-dependent Schrödinger equation is (Problem 10.3)

$$\chi(t) = \begin{pmatrix} \left[\cos(\lambda t/2) + i\frac{(\omega_1+\omega)}{\lambda}\sin(\lambda t/2)\right]\cos(\alpha/2)e^{-i\omega t/2} \\ \left[\cos(\lambda t/2) + i\frac{(\omega_1-\omega)}{\lambda}\sin(\lambda t/2)\right]\sin(\alpha/2)e^{i\omega t/2} \end{pmatrix}, \quad [10.31]$$

where

$$\lambda \equiv \sqrt{\omega^2 + \omega_1^2 + 2\omega\omega_1\cos\alpha}, \quad [10.32]$$

or, writing it as a linear combination of χ_+ and χ_-,

$$\chi(t) = \left[\cos\left(\frac{\lambda t}{2}\right) + i\frac{(\omega_1 + \omega\cos\alpha)}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]e^{-i\omega t/2}\chi_+(t) + i\left[\frac{\omega}{\lambda}\sin\alpha\sin\left(\frac{\lambda t}{2}\right)\right]e^{-i\omega t/2}\chi_-(t). \quad [10.33]$$

Evidently the (exact) probability of a transition to spin down (along the current direction of **B**) is

$$|\langle\chi(t)|\chi_-(t)\rangle|^2 = \left[\frac{\omega}{\lambda}\sin\alpha\sin\left(\frac{\lambda t}{2}\right)\right]^2. \qquad [10.34]$$

The adiabatic theorem says that this transition probability should vanish in the limit $T_e \gg T_i$, where T_e is the characteristic time for changes in the Hamiltonian (in this case, $1/\omega$) and T_i is the characteristic time for changes in the wave function [in this case, $\hbar/(E_+ - E_-) = 1/\omega_1$]. Thus the adiabatic approximation means $\omega \ll \omega_1$: The field rotates slowly, in comparison with the phase of the (unperturbed) wave functions. In the adiabatic regime $\lambda \cong \omega_1$, and therefore

$$|\langle\chi(t)|\chi_-(t)\rangle|^2 \cong \left[\frac{\omega}{\omega_1}\sin\alpha\sin\left(\frac{\lambda t}{2}\right)\right]^2 \to 0, \qquad [10.35]$$

as advertised. The magnetic field leads the electron around by its nose, with the spin always pointing in the direction of **B**. By contrast, if $\omega \gg \omega_1$ then $\lambda \cong \omega$, and the system bounces back and forth between spin up and spin down (Figure 10.6).

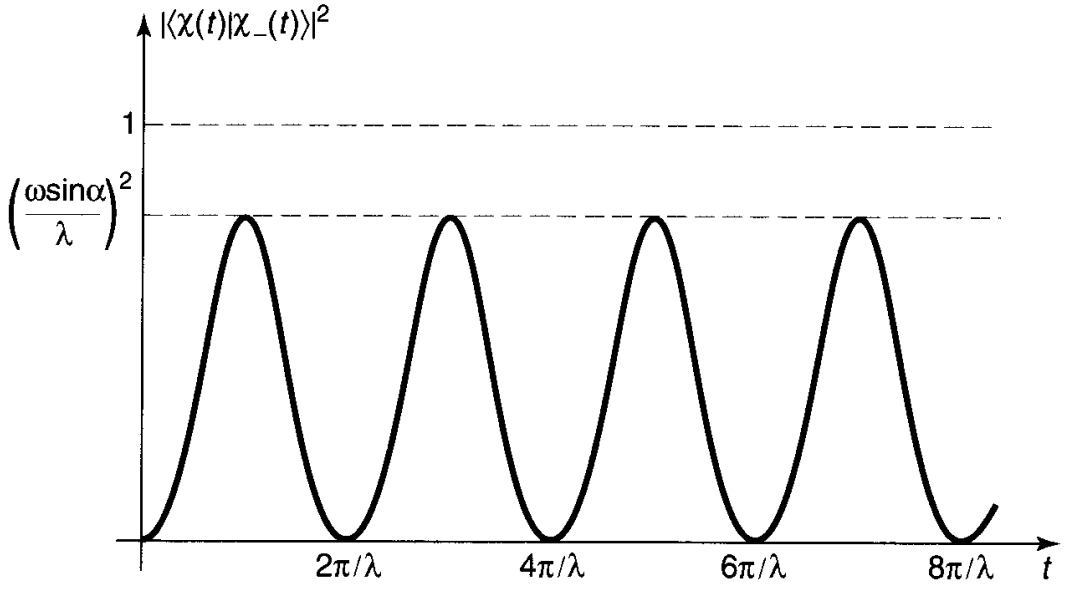

Figure 10.6: Plot of the transition probability, Equation 10.34, in the *nonadiabatic* regime ($\omega \ll \omega_1$).

****Problem 10.3** Check that Equation 10.31 satisfies the time-dependent Schrödinger equation for the Hamiltonian (Equation 10.25). *Note*: This is the same as Problem 9.19(b), except that now the electron starts out with spin up along **B**, whereas in Equation 9.90 it started out with spin up along z. Also confirm Equation 10.33, and show that the sum of the squares of the coefficients is 1, as required for proper normalization.

10.2 Berry's Phase

10.2.1 Nonholonomic Processes

Let us return to the classical model I used (in Section 10.1.1) to develop the notion of an *adiabatic* process: a perfectly frictionless pendulum whose support is carried around from place to place. I claimed that as long as the motion of the support is *very slow*, compared to the period of the pendulum (so that the pendulum executes many oscillations before the support has moved appreciably), it will continue to swing in the same plane (or one parallel to it), with the same amplitude (and, of course, the same frequency).

But what if I took this ideal pendulum up to the North Pole, and set it swinging—say, in the direction of Portland (Figure 10.7). (For the moment, I'll pretend the earth is not rotating.) Very gently (that is, *adiabatically*), I carry it down the longitude line passing through Portland, and on beyond, down to the equator. At this stage it is swinging north-south. Now I carry it (still swinging north-south) partway around the equator. And finally, I carry it back up to the North Pole, along the new longitude line. It is clear that the pendulum will no longer be swinging in the same plane as it was when I set out—indeed, the new plane makes an angle Θ with the old one, where Θ is the angle between the southbound and the northbound longitude lines. Now Θ is equal to the *solid angle* (Ω) subtended (at the center of the earth) by the path around which I carried the pendulum. For this path surrounds a fraction $\Theta/2\pi$ of the northern hemisphere, so its area is $A = (1/2)(\Theta/2\pi)4\pi R^2 = \Theta R^2$ (where R is the radius of the earth), and hence

$$\Theta = A/R^2 \equiv \Omega. \qquad [10.36]$$

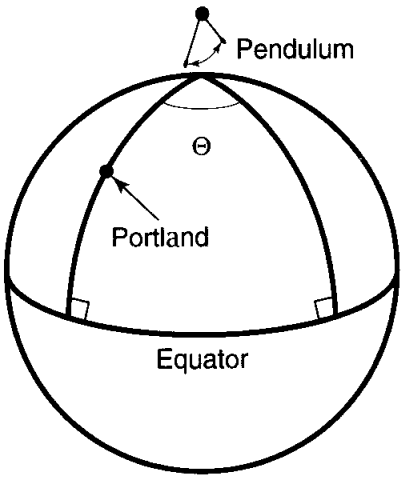

Figure 10.7: Itinerary for adiabatic transport of a pendulum on the surface of the earth.

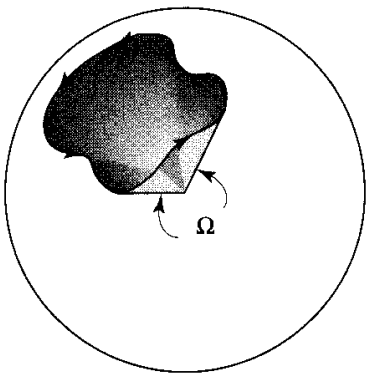

Figure 10.8: Arbitrary path on the surface of a sphere, subtending a solid angle Ω.

This is a particularly nice way to express the answer, because it turns out to be independent of the *shape* of the path (Figure 10.8).[7]

Incidentally, the **Foucault pendulum** is an example of precisely this sort of adiabatic transport around a closed loop on a sphere—only this time instead of *me* carrying the pendulum around, I let the *rotation of the earth* do the job. The solid angle subtended by a latitude line θ_0 (Figure 10.9) is

$$\Omega = \int \sin\theta \, d\theta d\phi = 2\pi(-\cos\theta)\Big|_0^{\theta_0} = 2\pi(1 - \cos\theta_0). \qquad [10.37]$$

Relative to the earth (which has meanwhile turned through an angle of 2π), the daily precession of the Foucault pendulum is $2\pi \cos\theta_0$—a result that is ordinarily obtained by appeal to Coriolis forces in the rotating reference frame,[8] but is seen in this context to admit a purely *geometrical* interpretation.

A system such as this, which does not return to its original state when transported around a closed loop, is said to be **nonholonomic**. (The "transport" in question need not involve physical *motion*: What we have in mind is that the external parameters of

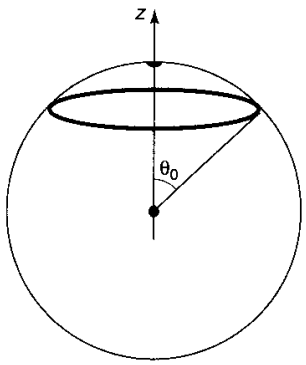

Figure 10.9: Path of a Foucault pendulum in the course of one day.

[7] You can prove this for yourself, if you are interested. Think of the circuit as being made up of tiny segments of great circles (geodesics on the sphere); the pendulum makes a fixed angle with each geodesic segment, so the net angular deviation is related to the sum of the vertex angles of the spherical polygon.

[8] See, for example, Jerry B. Marion, *Classical Dynamics*, 2nd ed. (New York: Academic Press, 1970), Section 11.4. Geographers measure latitude (λ) up from the equator, rather than down from the pole, so $\cos\theta_0 = \sin\lambda$.

the system are changed in some fashion that eventually returns them to their initial values.) Nonholonomic systems are ubiquitous—in a sense, every cyclical engine is a nonholonomic device: At the end of each cycle the car has moved forward a bit, or a weight has been lifted slightly, or something. The idea has even been applied to the locomotion of microbes in fluids at low Reynolds number.[9] My project for the next section is to study the *quantum mechanics of nonholonomic, adiabatic processes*. The essential question is this: How does the final state differ from the initial state, if the parameters in the Hamiltonian are carried adiabatically around some closed cycle?

10.2.2 Geometric Phase

If the Hamiltonian is *independent* of time, then a particle which starts out in the nth eigenstate $\psi_n(x)$,

$$H\psi_n(x) = E_n\psi_n(x),$$

remains in the n^{th} eigenstate, simply picking up a phase factor:

$$\Psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar}. \qquad [10.38]$$

If the Hamiltonian *changes* with time, then the eigenfunctions and eigenvalues themselves are time dependent:

$$H(t)\psi_n(x,t) = E_n(t)\psi_n(x,t). \qquad [10.39]$$

But the adiabatic theorem tells us that when H changes very *gradually*, a particle which starts out in the nth eigenstate will *remain* in the n^{th} eigenstate—picking up at most a time-dependent phase factor—even as the eigenfunction itself evolves. That is to say,

$$\Psi_n(x,t) = \psi_n(x,t)e^{-\frac{i}{\hbar}\int_0^t E_n(t')dt'}e^{i\gamma_n(t)}. \qquad [10.40]$$

The term

$$\theta_n(t) \equiv -\frac{1}{\hbar}\int_0^t E_n(t')\,dt' \qquad [10.41]$$

is known as the **dynamic phase**; it generalizes the "standard" factor $(-E_nt/\hbar)$ to the case where E_n is a function of time. (You will have encountered dynamical phase factors already, if you worked Problems 9.16 and and 10.1.) Any "extra" phase, $\gamma_n(t)$, is called the **geometric phase**. At the moment we don't know what it *is*, or what physical significance (if any) it carries; all we can say is that the adiabatic theorem does not *rule out* such a factor, since the particle is still "in the n^{th} eigenstate", *whatever* the value of γ_n. [More precisely, a measurement of the energy at time t would be certain to return the value $E_n(t)$.] Indeed, since the eigenvalue equation (Equa-

[9]The pendulum example is an application of **Hannay's angle**, which is the classical analog to Berry's phase. For a collection of papers on both subjects, see Alfred Shapere and Frank Wilczek, eds., *Geometric Phases in Physics*, (Singapore: World Scientific, 1989).

tion 10.39) and the normalization condition only determine $\psi_n(x, t)$ up to an arbitrary phase, and since this arbitrary phase could in principle be chosen independently at each instant of time [though in practice we shall always take $\psi_n(x, t)$ to be a *smooth* function of t], we *have* to allow for an arbitrary phase factor in Equation [10.40].[10] Notice, incidentally, that energy is not conserved here. Of *course* not: Whoever is changing the Hamiltonian is pumping energy into or out of the system.

If we plug Equation 10.40 into the (time-dependent) Schrödinger equation,

$$i\hbar\frac{\partial\Psi}{\partial t} = H(t)\Psi, \qquad [10.42]$$

there emerges a simple formula for the time development of the geometric phase:

$$i\hbar\left[\frac{\partial\psi_n}{\partial t}e^{i\theta_n}e^{i\gamma_n} - \frac{i}{\hbar}E_n\psi_n e^{i\theta_n}e^{i\gamma_n} + i\frac{d\gamma_n}{dt}\psi_n e^{i\theta_n}e^{i\gamma_n}\right]$$
$$= [H\psi_n]e^{i\theta_n}e^{i\gamma_n} = E_n\psi_n e^{i\theta_n}e^{i\gamma_n},$$

whence

$$\frac{\partial\psi_n}{\partial t} + i\psi_n\frac{d\gamma_n}{dt} = 0. \qquad [10.43]$$

Taking the inner product with ψ_n (which I assume has been normalized), we obtain

$$\frac{d\gamma_n}{dt} = i\langle\psi_n|\frac{\partial\psi_n}{\partial t}\rangle. \qquad [10.44]$$

Now $\psi_n(x, t)$ depends on t because there is some parameter $R(t)$ in the Hamiltonian that is changing with time. [In Problem 10.1, $R(t)$ would be the width of the infinite square well, whose right wall is expanding.] Thus

$$\frac{\partial\psi_n}{\partial t} = \frac{\partial\psi_n}{\partial R}\frac{dR}{dt}, \qquad [10.45]$$

so that

$$\frac{d\gamma_n}{dt} = i\langle\psi_n|\frac{\partial\psi_n}{\partial R}\rangle\frac{dR}{dt},$$

and hence

$$\gamma_n(t) = i\int_0^t\langle\psi_n|\frac{\partial\psi_n}{\partial R}\rangle\frac{dR}{dt'}\,dt' = i\int_{R_i}^{R_f}\langle\psi_n|\frac{\partial\psi_n}{\partial R}\rangle\,dR, \qquad [10.46]$$

where R_i and R_f are the initial and final values of $R(t)$. In particular, if the Hamiltonian returns to its original form after time T, so that $R_f = R_i$, then $\gamma_n(T) = 0$ —nothing very interesting *there*!

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[10] For this reason, most people assumed until quite recently that the geometric phase was of no conceivable physical significance. It was Michael Berry's inspiration to realize that if you carry the Hamiltonian around a closed *cycle*, bringing it back to its original form at the end, the relative phase at the beginning and at the end of the process is a *nonarbitrary* quantity, with profound physical implications.

However, I assumed (in Equation 10.45) that there is only *one* parameter in the Hamiltonian that is changing. Suppose there are N of them: $R_1(t)$, $R_2(t)$, ..., $R_N(t)$; in that case

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R_1}\frac{dR_1}{dt} + \frac{\partial \psi_n}{\partial R_2}\frac{dR_2}{dt} + \cdots + \frac{\partial \psi_n}{\partial R_N}\frac{dR_N}{dt} = (\nabla_R \psi_n) \cdot \frac{d\mathbf{R}}{dt}, \quad [10.47]$$

where $\mathbf{R} \equiv (R_1, R_n, \ldots, R_N)$, and ∇_R is the gradient with respect to these parameters. This time we have

$$\gamma_n(t) = i \int_{\mathbf{R}_i}^{\mathbf{R}_f} \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\mathbf{R}, \quad [10.48]$$

and if the Hamiltonian returns to its original form after a time T, the net geometric phase change is

$$\boxed{\gamma_n(T) = i \oint \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\mathbf{R}.} \quad [10.49]$$

This is a *line* integral around a closed loop in parameter space, and it is *not*, in general, zero. Equation 10.49 was first obtained by Berry in 1984,[11] and $\gamma_n(T)$ is called **Berry's phase**. Notice that $\gamma_n(T)$ depends *only on the path taken*, not on how *fast* that path is traversed (provided, of course, that it is slow enough to validate the adiabatic hypothesis). By contrast, the accumulated *dynamic* phase,

$$\theta_n(T) = -\frac{1}{\hbar}\int_0^T E_n(t')\,dt',$$

depends critically on the elapsed time.

The derivation of Berry's phase raises several questions, which I would like to address before turning to some examples and applications.

1. Is $\gamma_n(t)$ real? If it's *not*, then $e^{i\gamma_n}$ is not a phase factor at all, but an *exponential* factor, and the normalization of Ψ_n (in Equation 10.40) is lost. Since the time-dependent Schrödinger equation conserves probability, it must preserve normalization. It would be comforting to *check* this, by showing explicitly that Equation 10.48 yields a real γ_n. In fact, this is very easy to do. First note that

$$\nabla_R \langle \psi_n | \psi_n \rangle = 0 \quad [10.50]$$

(because by assumption ψ_n is normalized). So

$$\langle \nabla_R \psi_n | \psi_n \rangle + \langle \psi_n | \nabla_R \psi_n \rangle = \langle \psi_n | \nabla_R \psi_n \rangle^* + \langle \psi_n | \nabla_R \psi_n \rangle = 0.$$

Since $\langle \psi_n | \nabla_R \psi_n \rangle$ plus its complex conjugate is zero, it follows that

$$\langle \psi_n | \nabla_R \psi_n \rangle \quad \text{is imaginary,} \quad [10.51]$$

and hence, by Equation 10.48, $\gamma_n(t)$ is real. [Incidentally, if ψ_n itself is *real*, then so

[11] M. V. Berry, *Proc. R. Soc. Lond.* A **392**, 45 (1984), reprinted in Shapere and Wilczek, (footnote 9). It is astonishing, in retrospect, that such a fundamental result escaped notice for 60 years.

(obviously) is $\langle\psi_n|\nabla_R\psi_n\rangle$—this quantity is both real and imaginary, and it must therefore be *zero*. Evidently the geometric phase vanishes whenever the eigenfunctions (of $H(t)$) are real.]

2. Is Berry's phase measurable? We are accustomed to thinking that the phase of the wave function is arbitrary—physical quantities involve $|\Psi|^2$, and the phase factor cancels out. But $\gamma_n(T)$ *can* be measured, if (for example) we take a beam of particles (all in the state Ψ) and split it in two, so that one beam passes through an adiabatically changing potential, while the other does not. When the two beams are recombined, the total wave function has the form

$$\Psi = \frac{1}{2}\Psi_0 + \frac{1}{2}\Psi_0 e^{i\Gamma}, \qquad [10.52]$$

where Ψ_0 is the "direct" beam wave function, and Γ is the *extra* phase (in part dynamic, and in part geometric) acquired by the beam subjected to the varying H). In this case

$$|\Psi|^2 = \frac{1}{4}|\Psi_0|^2\left(1 + e^{i\Gamma}\right)\left(1 + e^{-i\Gamma}\right)$$

$$= \frac{1}{2}|\Psi_0|^2(1 + \cos\Gamma) = |\Psi_0|^2\cos^2(\Gamma/2). \qquad [10.53]$$

So by looking for points of constructive and destructive interference (where Γ is an even or odd multiple of π, respectively), one can easily measure Γ. (Berry, and other early writers, worried that the geometric phase might be swamped by a larger dynamic phase, but it has proved possible to arrange things so as to separate out the two contributions.)

3. Where does the derivation invoke the adiabatic hypothesis? At first glance, the argument going from Equation 10.40 to Equation 10.48 appears to have proved altogether *too* much. Why doesn't the derivation work *in reverse*, showing that as long as $\gamma_n(t)$ is given by Equation 10.48, the expression in Equation 10.40 satisfies the Schrödinger equation *exactly—whether or not the process is adiabatic*?(!) (This would, of course, be nonsense; it would imply that the adiabatic theorem is empty: No transitions *ever* occur, even if the change in the Hamiltonian is far from gradual.) The answer is that the step following Equation 10.43, in which we take the inner product, *cannot* in general be reversed: Although Equation 10.43 implies Equation 10.44, Equation 10.44 does *not* imply Equation 10.43. In fact, there is a serious fraud in the derivation, which I did not confess at the time because it somewhat spoils the beauty of the argument. The truth is that although Equation 10.44 is correct, Equation 10.43 is *not*.[12] For Equation 10.40 is only true in the extreme adiabatic limit—the

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[12]Indeed, if you take Equation 10.43 at face value, it can be solved directly for γ_n:

$$\frac{d\gamma_n}{dt} = i\frac{\partial}{\partial t}(\ln\psi_n) \Rightarrow \psi_n(x,t) = \phi_n(x)e^{-i\gamma_n(t)},$$

and hence (going back to Equation 10.40),

$$\Psi_n(x,t) = \phi_n(x)e^{-\frac{i}{\hbar}\int_0^t E_n(t')dt'}.$$

The geometric phase, in effect, *soaks up* the time dependence acquired by the eigenfunction $\psi_n(x,t)$ as a consequence of the change in H. But this is completely false, as we shall see in the examples.

exact solution would contain admixtures of other states:

$$\Psi_n(x,t) = \psi_n(x,t)e^{i\theta_n(t)}e^{i\gamma_n(t)} + \epsilon \sum_{m\neq n} c_m(t)\psi_m(x,t), \qquad [10.54]$$

where $\epsilon \equiv T_i/T_e$ characterizes the departure from adiabaticity (it goes to zero in the adiabatic limit). Inclusion of this term modifies Equation 10.43, to read

$$\frac{\partial \psi_n}{\partial t} + i\psi_n \frac{d\gamma_n}{dt} = -e^{-i\theta_n}e^{-i\gamma_n}\epsilon \sum_{m\neq n}\left[\left(\frac{i}{\hbar}c_m E_m + \frac{dc_m}{dt}\right)\psi_m + c_m\frac{\partial \psi_m}{\partial t}\right]. \qquad [10.55]$$

Both terms on the left are first order in ϵ (if the Hamiltonian didn't change at *all*, both $\partial\psi_n/\partial t$ and γ_n would be zero), but *so are the first two terms on the right.* The *final* term is *second* order, so it can legitimately be ignored, but dropping the first two (as I did, implicitly, in my derivation of Equation 10.43), is illegal. For consistency (noting, while I'm at it, that γ_n is already first order, so $e^{i\gamma_n} \cong 1$ on the right), I *should* have written

$$\frac{\partial \psi_n}{\partial t} + i\psi_n \frac{d\gamma_n}{dt} = -e^{-i\theta_n}\epsilon \sum_{m\neq n}\left(\frac{i}{\hbar}c_m E_m + \frac{dc_m}{dt}\right)\psi_m, \qquad [10.56]$$

instead of Equation 10.43. Fortunately, the inner product (with ψ_n) kills the extra term, and that's how it comes about that Equation 10.44 is correct, even though Equation 10.43, from which it was obtained, was *not.* (See Problem 10.7.)

When the parameter space is three dimensional, $\mathbf{R} = (R_1, R_2, R_3)$, Berry's formula (Equation 10.49) is reminiscent of the expression for **magnetic flux** in terms of the vector potential $\mathbf{A}$. The flux, Φ, through a surface S bounded by a curve C (Figure 10.10), is

$$\Phi \equiv \int_S \mathbf{B}\cdot d\mathbf{a}. \qquad [10.57]$$

If we write the magnetic field in terms of the vector potential ($\mathbf{B} = \nabla \times \mathbf{A}$), and apply Stokes' theorem:

$$\Phi = \int_S (\nabla \times \mathbf{A})\cdot d\mathbf{a} = \oint_C \mathbf{A}\cdot d\mathbf{r}. \qquad [10.58]$$

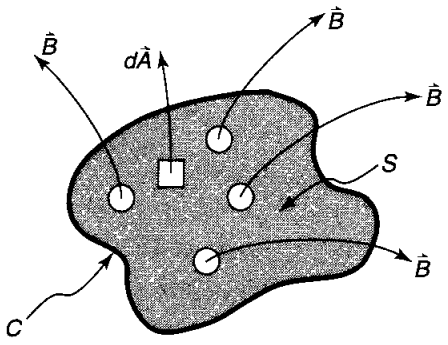

Figure 10.10: Magnetic flux through a surface S bounded by the closed curve C.

Thus Berry's phase can be thought of as the "flux" of a "magnetic field"

$$\text{"}\mathbf{B}\text{"} = i\nabla_R \times \langle \psi_n | \nabla_R \psi_n \rangle, \qquad [10.59]$$

through the (closed-loop) trajectory in parameter space. In the three-dimensional case, then, Berry's phase can be written as a surface integral,

$$\gamma_n(T) = i \int [\nabla_R \times \langle \psi_n | \nabla_R \psi_n \rangle] \cdot d\mathbf{a}. \qquad [10.60]$$

The magnetic analogy can be carried much further, but for our purposes Equation 10.60 is merely a convenient alternative expression for $\gamma_n(T)$.

***Problem 10.4**

(a) Use Equation 10.46 to calculate the geometric phase change when the infinite square well expands adiabatically from width w_1 to width w_2. Comment on this result.

(b) If the expansion occurs at a constant rate ($dw/dt = v$), what is the dynamic phase change for this process?

(c) If the well now contracts back to its original size, what is Berry's phase for the cycle?

Problem 10.5 The delta-function well (Equation 2.96) supports a single bound state (Equation 2.111). Calculate the geometric phase change when α gradually increases from α_1 to α_2. If the increase occurs at a constant rate ($d\alpha/dt = c$), what is the dynamic phase change for this process?

Problem 10.6 As I noted in the text (and Problems 10.4 and 10.5 confirm), if $\psi_n(x, t)$ is *real*, the geometric phase vanishes. You might try to beat this rap by tacking an unnecessary (but perfectly legal) phase factor onto the eigenfunctions: $\psi_n'(x, t) \equiv e^{i\phi_n}\psi_n(x, t)$, where $\phi_n(\mathbf{R})$ is an arbitrary (real) function. Try it. You'll get a nonzero geometric phase, all right, but note what happens when you put it back into Equation 10.40. And for a closed loop it gives *zero*. *Moral*: For nonzero Berry's phase, you need (1) more than one time-dependent parameter in the Hamiltonian, and (2) a Hamiltonian that yields nontrivially complex eigenfunctions.

10.2.3 An Example

The classic example of Berry's phase is an electron at the origin, subjected to a magnetic field of constant magnitude but changing direction. Consider first the special case (analyzed in Section 10.1.3) in which **B**(t) precesses around at a constant angular

velocity ω, making a fixed angle α with the z-axis. The *exact* solution (for an electron that starts out with "spin up" along **B**) is given by Equation 10.33. In the adiabatic regime, $\omega \ll \omega_1$,

$$\lambda = \omega_1\sqrt{1 + 2\frac{\omega}{\omega_1}\cos\alpha + \left(\frac{\omega}{\omega_1}\right)^2} \cong \omega_1\left(1 + \frac{\omega}{\omega_1}\cos\alpha\right) = \omega_1 + \omega\cos\alpha, \quad [10.61]$$

and Equation 10.33 becomes

$$\chi(t) \cong e^{i\omega_1 t/2}e^{i(\omega\cos\alpha)t/2}e^{-i\omega t/2}\chi_+(t) + i\left[\frac{\omega}{\omega_1}\sin\alpha\sin\left(\frac{\omega_1 t}{2}\right)\right]e^{-i\omega t/2}\chi_-(t). \quad [10.62]$$

As $\omega/\omega_1 \to 0$ the second term drops out completely, and the result matches the expected adiabatic form (Equation 10.40). The dynamic phase is

$$\theta_+(t) = -\frac{1}{\hbar}\int_0^t E_+(t')\,dt' = \frac{\omega_1 t}{2} \quad [10.63]$$

(where $E_+ = -\hbar\omega_1/2$ is taken from Equation 10.29), so the geometric phase is

$$\gamma_+(t) = (\cos\alpha - 1)\frac{\omega t}{2}. \quad [10.64]$$

For a complete cycle $T = 2\pi/\omega$, and therefore Berry's phase is

$$\gamma_+(T) = \pi(\cos\alpha - 1). \quad [10.65]$$

Now consider the more general case, in which the tip of the magnetic field vector sweeps out an *arbitrary* closed curve on the surface of a sphere of radius $r = B_0$ (Figure 10.11). The eigenstate representing spin up along $\mathbf{B}(t)$ has the form (see Problem 4.31)

$$\chi_+ = \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{pmatrix}, \quad [10.66]$$

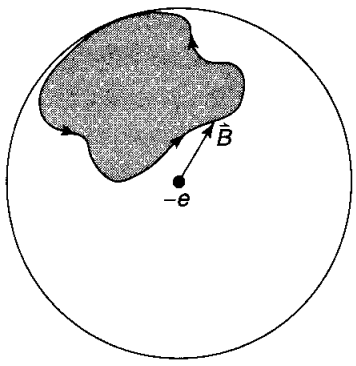

Figure 10.11: Magnetic field of constant magnitude but changing direction sweeps out a closed loop.

where θ and ϕ (the spherical coordinates of **B**) are now *both* functions of time. Looking up the gradient in spherical coordinates, we find

$$\nabla\chi_+ = \frac{\partial\chi_+}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial\chi_+}{\partial\theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial\chi_+}{\partial\phi}\hat{\phi}$$

$$= \frac{1}{r}\begin{pmatrix} -(1/2)\sin(\theta/2) \\ (1/2)e^{i\phi}\cos(\theta/2) \end{pmatrix}\hat{\theta} + \frac{1}{r\sin\theta}\begin{pmatrix} 0 \\ ie^{i\phi}\sin(\theta/2) \end{pmatrix}\hat{\phi}. \quad [10.67]$$

Hence

$$\langle\chi_+|\nabla\chi_+\rangle = \frac{1}{2r}\Big[-\sin(\theta/2)\cos(\theta/2)\,\hat{\theta} + \sin(\theta/2)\cos(\theta/2)\,\hat{\theta}$$

$$+ 2i\frac{\sin^2(\theta/2)}{\sin\theta}\hat{\phi}\Big] = i\frac{\sin^2(\theta/2)}{r\sin\theta}\hat{\phi}. \quad [10.68]$$

For Equation 10.60 we need the *curl* of this quantity:

$$\nabla\times\langle\chi_+|\nabla\chi_+\rangle = \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\left(\frac{i\sin^2(\theta/2)}{r\sin\theta}\right)\right]\hat{r} = \frac{i}{2r^2}\hat{r}. \quad [10.69]$$

According to Equation 10.60, then,

$$\gamma_+(T) = -\frac{1}{2}\int\frac{1}{r^2}\hat{r}\cdot d\mathbf{a}. \quad [10.70]$$

The integral is over the area on the sphere swept out by **B** in the course of the cycle, so $d\mathbf{a} = r^2\,d\Omega\,\hat{r}$, and hence

$$\gamma_+(T) = -\frac{1}{2}\int d\Omega = -\frac{1}{2}\Omega, \quad [10.71]$$

where Ω is the solid angle subtended at the origin. This is a delightfully simple result, and tantalizingly reminiscent of the classical problem with which we began the discussion (transport of a frictionless pendulum around a closed path on the surface of the earth). It says that if you take a magnet, and lead the electron's spin around adiabatically in an arbitrary closed path, the net (geometric) phase change will be minus one half the solid angle swept out by the magnetic field vector. In view of Equation 10.37, the general result is consistent with the special case Equation 10.65, as of course it *had* to be.

Problem 10.7 Consider, once again, the special case of the precessing field (Section 10.1.3).

(a) Use the eigenspinor (Equation 10.27) to determine $\langle\chi_+|(\partial\chi_+/\partial t)\rangle$, and put the result into Equation 10.44, for an alternative derivation of Equation 10.64.

(b) Show that Equation 10.43 does *not* work, in this case. Use Equation 10.62 to determine c_- (in Equation 10.54). Confirm that the last term in Equation 10.55 is second order in ω (don't forget the $\epsilon = \omega/\omega_1$ out front). Show that $\gamma_+(t)$ (Equation 10.64) does satisfy the *corrected* version of Equation 10.43, Equation 10.56.

***Problem 10.8** Work out the analog to Equation 10.71 for a particle of spin 1. *Answer*: $-\Omega$ (for spin s the result is $-s\Omega/2$).

10.2.4 The Aharonov-Bohm Effect

In classical electrodynamics the potentials (φ and $\mathbf{A}$)[13] are not directly measurable—the physical quantities are the electric and magnetic fields:

$$\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}. \tag{10.72}$$

The fundamental laws of the theory (Maxwell's equations and the Lorentz force law) make no reference to potentials, which are (from a logical point of view) no more than convenient but dispensible scaffolding for getting a better purchase on the real structure (the fields). Indeed, you're perfectly free to *change* the potentials:

$$\varphi \to \varphi' = \varphi - \frac{\partial \Lambda}{\partial t}, \quad \mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\Lambda, \tag{10.73}$$

where Λ is an arbitrary function of position and time; this is called a gauge transformation, and it has no effect at all on the fields.

In quantum mechanics the potentials play a more significant role, for the Hamiltonian (Equation 4.201) is expressed in terms of φ and $\mathbf{A}$, not $\mathbf{E}$ and $\mathbf{B}$:

$$H = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)^2 + q\varphi. \tag{10.74}$$

Nevertheless, the theory is still invariant under gauge transformations (see Problem 4.53), and it was taken for granted until quite recently that there could be no electromagnetic influences in regions where $\mathbf{E}$ and $\mathbf{B}$ are zero—any more than there can be in the classical theory. But in 1959 Aharonov and Bohm[14] showed that the vector potential *can* affect the quantum behavior of a charged particle that never encounters an electromagnetic field. I'll work out a simple example first, then discuss the

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[13] I'm sorry, but we have reached a notational impasse: It is customary in quantum mechanics to use the letter V for *potential energy*, but in electrodynamics the same letter is reserved for the scalar potential. To avoid confusion I'll use φ for the scalar potential. See Problems 4.51, 4.52, and 4.53 for background on this material.

[14] Y. Aharonov and D. Bohm, *Phys. Rev.* **115**, 485 (1959). For a significant precursor, see W. Ehrenberg and R. E. Siday, *Proc. Phys. Soc. London* **B62**, 8 (1949).

Aharanov-Bohm effect itself, and finally indicate how it can be thought of as an example of Berry's phase.

Imagine a particle constrained to move in a circle of radius b (a bead on a wire ring, if you like). Along the axis runs a solenoid of radius $a < b$, carrying a magnetic field **B** (see Figure 10.12). If the solenoid is extremely long, the field inside is uniform, and the field outside is zero. But the vector potential outside the solenoid is *not* zero; in fact (adopting the convenient gauge condition $\nabla \cdot \mathbf{A} = 0$),[15]

$$\mathbf{A} = \frac{\Phi}{2\pi r}\hat{\phi}, \quad (r > a), \tag{10.75}$$

where $\Phi = \pi a^2 B$ is the **magnetic flux** through the solenoid. Meanwhile, the solenoid is uncharged, so the scalar potential φ is zero. In this case the Hamiltonian (Equation 10.74) becomes

$$H = \frac{1}{2m}\left[-\hbar^2\nabla^2 + q^2A^2 + 2i\hbar q\mathbf{A}\cdot\nabla\right]. \tag{10.76}$$

But the wave function depends only on the azimuthal angle ϕ, ($\theta = \pi/2$ and $r = b$) so $\nabla \to (\hat{\phi}/b)(d/d\phi)$, and the Schrödinger equation reads

$$\frac{1}{2m}\left[-\frac{\hbar^2}{b^2}\frac{d^2}{d\phi^2} + \left(\frac{q\Phi}{2\pi b}\right)^2 + i\frac{\hbar q\Phi}{\pi b^2}\frac{d}{d\phi}\right]\psi(\phi) = E\psi(\phi). \tag{10.77}$$

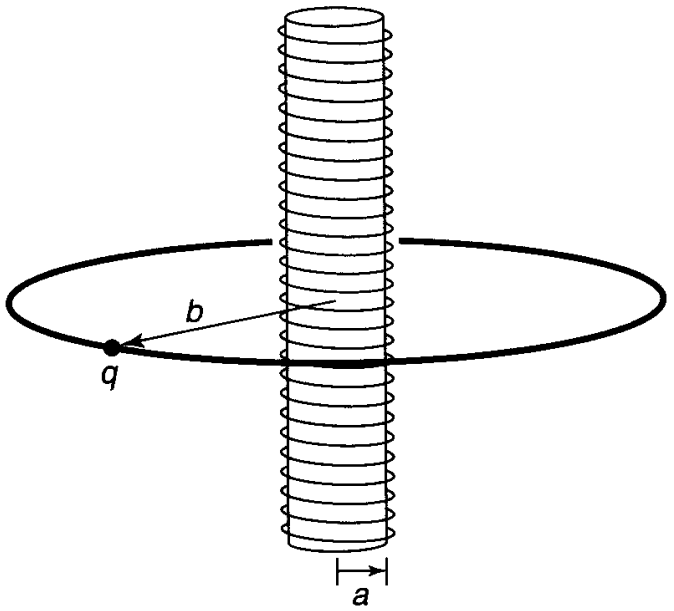

Figure 10.12: Charged bead on a circular ring through which a long solenoid passes.

This is a linear differential equation with constant coefficients:

$$\frac{d^2\psi}{d\phi^2} - 2i\beta\frac{d\psi}{d\phi} + \epsilon\psi = 0, \tag{10.78}$$

[15]See, for instance, D. J. Griffiths, *Introduction to Electrodynamics*, 2nd ed. (Englewood Cliffs, NJ: Prentice Hall, 1989), Equation 5.65.

where

$$\beta \equiv \frac{q\Phi}{2\pi\hbar} \quad \text{and} \quad \epsilon \equiv \frac{2mb^2E}{\hbar^2} - \beta^2. \tag{10.79}$$

Solutions are of the form

$$\psi = Ae^{i\lambda\phi}, \tag{10.80}$$

with

$$\lambda = \beta \pm \sqrt{\beta^2 + \epsilon} = \beta \pm \frac{b}{\hbar}\sqrt{2mE}. \tag{10.81}$$

Continuity of $\psi(\phi)$, at $\phi = 2\pi$, requires that λ be an *integer*:

$$\beta \pm \frac{b}{\hbar}\sqrt{2mE} = n, \tag{10.82}$$

and it follows that

$$E_n = \frac{\hbar^2}{2mb^2}\left(n - \frac{q\Phi}{2\pi\hbar}\right)^2, \quad (n = 0, \pm 1, \pm 2, \ldots). \tag{10.83}$$

The solenoid lifts the twofold degeneracy of the bead on a ring (Problem 2.43): Positive n, representing a particle traveling in the *same* direction as the current in the solenoid, has a somewhat *lower* energy (assuming q is positive) than negative n, describing a particle traveling in the *opposite* direction. And, more important, the allowed energies clearly depend on the field inside the solenoid, *even though the field at the location of the particle is zero.*[16]

More generally, suppose a particle is moving through a region where **B** is zero (so $\nabla \times \mathbf{A} = 0$), but **A** itself is *not*. (I'll assume that **A** is static, although the method can be generalized to time-dependent potentials.) The (time-dependent) Schrödinger equation,

$$\left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)^2 + V\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t}, \tag{10.84}$$

with potential energy V—which may or may not include an electrical contribution $q\varphi$—can be simplified by writing

$$\Psi = e^{ig}\Psi', \tag{10.85}$$

where

$$g(\mathbf{r}) \equiv \frac{q}{\hbar}\int_{\mathcal{O}}^{\mathbf{r}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}', \tag{10.86}$$

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[16]It is a peculiar property of **superconducting** rings that the enclosed flux is *quantized*: $\Phi = (2\pi\hbar/q)n'$, where n' is an integer. In this case the effect is undetectable, since $E_n = (\hbar^2/2mb^2)(n + n')^2$, and $(n + n')$ is just another integer. (Incidentally, the charge q here turns out to be *twice* the charge of an electron; the superconducting electrons are locked together in pairs.) However, **flux quantization** is enforced by the *superconductor* (which induces circulating currents to make up the difference), not by the solenoid or the electromagnetic field, and it does not occur in the example considered here.

and $\mathcal{O}$ is some (arbitrarily chosen) reference point. Note that this definition makes sense *only* when $\nabla \times \mathbf{A} = 0$ throughout the region in question—otherwise the line integral depends entirely on the *path* taken from $\mathcal{O}$ to $\mathbf{r}$, and hence does not define a function of $\mathbf{r}$. In terms of Ψ', the gradient of Ψ is

$$\nabla\Psi = e^{ig}(i\nabla g)\Psi' + e^{ig}(\nabla\Psi');$$

but $\nabla g = (q/\hbar)\mathbf{A}$, so

$$\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)\Psi = \frac{\hbar}{i}e^{ig}\nabla\Psi', \qquad [10.87]$$

and it follows that

$$\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)^2\Psi = -\hbar^2 e^{ig}\nabla^2\Psi'. \qquad [10.88]$$

Putting this into Equation 10.84, and canceling the common factor of e^{ig}, we are left with

$$-\frac{\hbar^2}{2m}\nabla^2\Psi' + V\Psi' = i\hbar\frac{\partial\Psi'}{\partial t}. \qquad [10.89]$$

Evidently Ψ' satisfies the Schrödinger equation *without* $\mathbf{A}$. If we can solve Equation 10.89, correcting for the presence of a (curl-free) vector potential is trivial: You just tack on the phase factor e^{ig}.

Aharonov and Bohm proposed an experiment in which a beam of electrons is split in two, and passed either side of a long solenoid, before being recombined (Figure 10.13). The beams are kept well away from the solenoid itself, so they encounter only regions where $\mathbf{B} = 0$. But $\mathbf{A}$, which is given by Equation 10.75, is *not* zero, and (assuming V is the same on both sides), the two beams arrive with *different phases*:

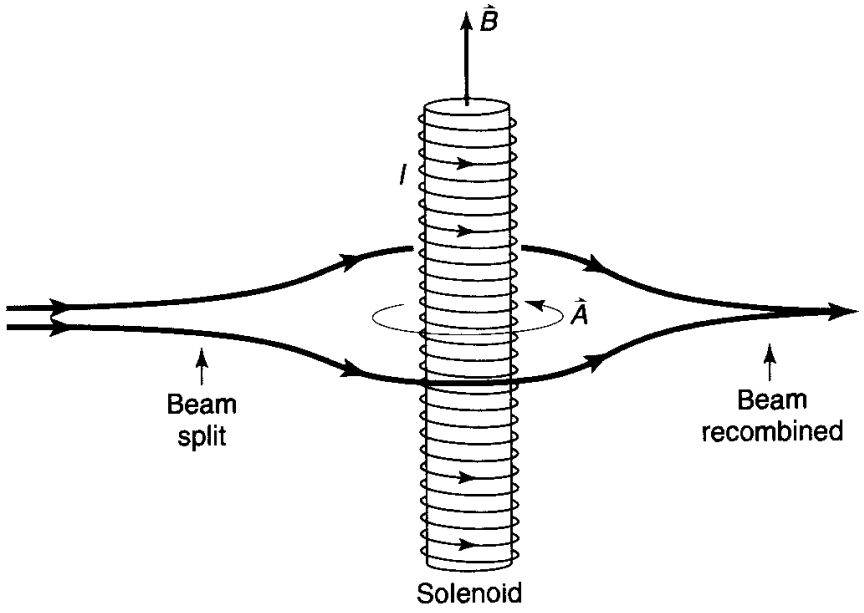

Figure 10.13: The Aharonov-Bohm effect: electron beam splits, with half passing either side of a long solenoid.

$$g = \frac{q}{\hbar}\int \mathbf{A}\cdot d\mathbf{r} = \frac{q\Phi}{2\pi\hbar}\int \left(\frac{1}{r}\hat{\phi}\right)\cdot(r\hat{\phi}\,d\phi) = \pm\frac{q\Phi}{2\hbar}. \qquad [10.90]$$

The plus sign applies to the electrons traveling in the same direction as **A**—which is to say, in the same direction as the current in the solenoid. The beams arrive *out of phase* by an amount proportional to the magnetic flux their paths encircle:

$$\text{phase difference} = \frac{q\Phi}{\hbar}. \qquad [10.91]$$

This phase shift leads to measurable interference (as in Equation 10.53), and has been confirmed experimentally by Chambers and others.[17]

The Aharonov-Bohm effect can be regarded as an example of geometric phase, as Berry himself noted in his first paper. Suppose the charged particle is confined to a box (which is centered at point **R** outside the solenoid) by a potential $V(\mathbf{r}-\mathbf{R})$—see Figure 10.14. (In a moment we're going to transport the box around the solenoid, so **R** will become a function of time, but for now it is just some fixed vector.) The eigenfunctions of the Hamiltonian are determined by

$$\left\{\frac{1}{2m}\left[\frac{\hbar}{i}\nabla - q\mathbf{A}(\mathbf{r})\right]^2 + V(\mathbf{r}-\mathbf{R})\right\}\psi_n = E_n\psi_n. \qquad [10.92]$$

We have already learned how to solve equations of this form:

$$\psi_n = e^{ig}\psi_n', \qquad [10.93]$$

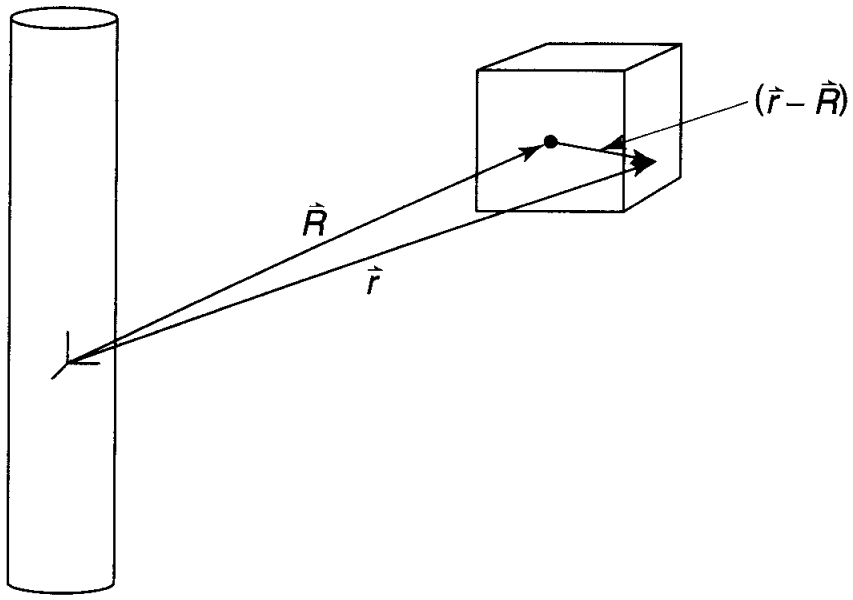

Figure 10.14: Particle confined to a box, by a potential $V(\mathbf{r}-\mathbf{R})$.

[17] R. G. Chambers, *Phys. Rev. Lett.* **5**, 3 (1960).

where[18]

$$g \equiv \frac{q}{\hbar}\int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}' \qquad [10.94]$$

and ψ' satisfies the same eigenvalue equation, only with $\mathbf{A} \to 0$:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}-\mathbf{R})\right]\psi_n' = E_n\psi_n'. \qquad [10.95]$$

Notice that ψ_n' is a function only of the combination $(\mathbf{r}-\mathbf{R})$, not (like ψ_n) of $\mathbf{r}$ and $\mathbf{R}$ separately.

Now let's carry the box around the solenoid (in this case the process doesn't even have to be adiabatic). To determine Berry's phase, we must first evaluate the quantity $\langle\psi_n|\nabla_R\psi_n\rangle$. Noting that

$$\nabla_R\psi_n = \nabla_R\left[e^{ig}\psi_n'(\mathbf{r}-\mathbf{R})\right] = -i\frac{q}{\hbar}\mathbf{A}(\mathbf{R})e^{ig}\psi_n'(\mathbf{r}-\mathbf{R}) + e^{ig}\nabla_R\psi_n'(\mathbf{r}-\mathbf{R}),$$

we find

$$\begin{aligned}&\langle\psi_n|\nabla_R\psi_n\rangle\\ &= \int e^{-ig}[\psi_n'(\mathbf{r}-\mathbf{R})]^* e^{ig}\left[-i\frac{q}{\hbar}\mathbf{A}(\mathbf{R})\psi_n'(\mathbf{r}-\mathbf{R}) + \nabla_R\psi_n'(\mathbf{r}-\mathbf{R})\right]d^3\mathbf{r}\\ &= -i\frac{q}{\hbar}\mathbf{A}(\mathbf{R}) - \int[\psi_n'(\mathbf{r}-\mathbf{R})]^*\nabla\psi_n'(\mathbf{r}-\mathbf{R})\,d^3\mathbf{r}. \qquad [10.96]\end{aligned}$$

The ∇ with no subscript denotes the gradient with respect to $\mathbf{r}$, and I used the fact that $\nabla_R = -\nabla$, when acting on a function of $(\mathbf{r}-\mathbf{R})$. But the last integral is $i/\hbar$ times the expectation value of momentum, in an eigenstate of the Hamiltonian $-(\hbar^2/2m)\nabla^2 + V$, which we know from Section 2.1 is *zero*. So

$$\langle\psi_n|\nabla_R\psi_n\rangle = -i\frac{q}{\hbar}\mathbf{A}(\mathbf{R}). \qquad [10.97]$$

Putting this into Berry's formula (Equation 10.49), we conclude that

$$\gamma_n(T) = \frac{q}{\hbar}\oint\mathbf{A}(\mathbf{R})\cdot d\mathbf{R} = \frac{q}{\hbar}\int(\nabla\times\mathbf{A})\cdot d\mathbf{a} = \frac{q\Phi}{\hbar}, \qquad [10.98]$$

which neatly confirms the Aharonov-Bohm result (Equation 10.91), and reveals that the Aharonov-Bohm effect is a particular instance of geometric phase.[19]

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[18] It is convenient to set the reference point $\mathcal{O}$ at the center of the box, for this guarantees that we recover the original phase convention for ψ_n when we complete the journey around the solenoid. If you use a fixed point in space, for example, you'll have to readjust the phase "by hand", at the far end; this leads to exactly the same answer, but it's a crude way to do it. In general, when choosing the phase convention for the eigenfunctions in Equation 10.39, you want to make sure that $\psi_n(x, T) = \psi_n(x, 0)$ so that no spurious phase changes are introduced.

[19] Incidentally, in this case the analogy between Berry's phase and magnetic flux (Equation 10.59) becomes *almost* an identity: "$\mathbf{B}$" = $(q/\hbar)\mathbf{B}$.

What are we to make of the Aharonov-Bohm effect? Evidently our classical preconceptions are simply *mistaken*: There *can* be electromagnetic effects in regions where the fields are zero. Note, however, that this does not make **A** itself measurable—only the enclosed *flux* comes into the final answer, and the theory remains gauge invariant.

Problem 10.9

(a) Derive Equation 10.76, from Equation 10.74.

(b) Derive Equation 10.88, starting with Equation 10.87.

FURTHER PROBLEMS FOR CHAPTER 10

* * ***Problem 10.10** Suppose the one-dimensional harmonic oscillator (mass m, frequency ω) is subjected to a driving force of the form $F(t) = m\omega^2 f(t)$, where $f(t)$ is some specified function [I have factored out $m\omega^2$ for notational convenience; notice that $f(t)$ has the dimensions of *length*]. The Hamiltonian is

$$H(t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 - m\omega^2 x f(t). \qquad [10.99]$$

Assume that the force was first turned on at time $t = 0$: $f(t) = 0$ for $t \leq 0$. This system can be solved exactly, both in classical mechanics and in quantum mechanics.[20]

(a) Determine the *classical* position of the oscillator, assuming it started out at rest at the origin [$x_c(0) = \dot{x}_c(0) = 0$]. *Answer*:

$$x_c(t) = \omega \int_0^t f(t') \sin[\omega(t - t')]\, dt'. \qquad [10.100]$$

(b) Show that the solution to the (time-dependent) Schrödinger equation for this oscillator, assuming it started out in the nth state of the *undriven* oscillator [$\Psi(x, 0) = \psi_n(x)$, where $\psi_n(x)$ is given by Equation 2.50], can be written as

$$\Psi(x, t) = \psi_n(x - x_c) e^{\frac{i}{\hbar}\left[-(n+\frac{1}{2})\hbar\omega t + m\dot{x}_c(x - \frac{x_c}{2}) + \frac{m\omega^2}{2}\int_0^t f(t')x_c(t')dt'\right]}. \qquad [10.101]$$

(c) Show that the eigenfunctions and eigenvalues of $H(t)$ are

$$\psi_n(x, t) = \psi_n(x - f); \quad E_n(t) = \left(n + \frac{1}{2}\right)\hbar\omega - \frac{1}{2}m\omega^2 f^2. \qquad [10.102]$$

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[20] See Y. Nogami, *Am. J. Phys.* **59**, 64 (1991) and references therein.

(d) Show that in the adiabatic approximation the classical position (Equation 10.100) reduces to $x_c(t) \cong f(t)$. *Hint*: Use the integration-by-parts trick of Section 10.1.2. State the precise criterion—analogous to Equation 10.15—for adiabaticity.

(e) Confirm the adiabatic theorem for this example, by using the results in (c) and (d) to show that

$$\Psi(x,t) \cong \psi_n(x,t)e^{i\theta_n(t)}e^{i\gamma_n(t)}. \qquad [10.103]$$

Check that the dynamic phase has the correct form (Equation 10.41). Is the geometric phase what you would expect?

***Problem 10.11** In time-dependent perturbation theory, we used the completeness of the unperturbed eigenfunctions (of H_0) to expand $\Psi(x,t)$ (see Equation 9.81). But we could as well use the instantaneous eigenfunctions of $H(t)$ (Equation 10.39), since they, too, are complete:

$$\Psi(x,t) = \sum_n c_n(t)\psi_n(x,t)e^{i\theta_n}, \qquad [10.104]$$

where $\theta_n(t)$ is given by Equation 10.41. We can use this expansion to develop an **adiabatic series**, whose leading term is the adiabatic approximation itself and whose successive terms represent the *departure* from perfect adiabaticity.

(a) Insert Equation 10.104 into the (time-dependent) Schrödinger equation, and obtain the following formula for the coefficients:

$$\dot{c}_m = -\sum_n \langle\psi_m|\frac{\partial\psi_n}{\partial t}\rangle c_n e^{i(\theta_n-\theta_m)}. \qquad [10.105]$$

(b) Suppose the system starts out in the N^{th} state; in the adiabatic approximation, it *remains* in the N^{th} state, picking up (at most) a time-dependent geometric phase (compare Equations 10.40 and 10.104):

$$c_n(t) = \delta_{nN}e^{i\gamma_N(t)}. \qquad [10.106]$$

Substitute this into the right side of Equation 10.105, and obtain the "first correction" to adiabaticity:

$$c_m(t) = c_m(0) - \int_0^t \langle\psi_m|\frac{\partial\psi_N}{\partial t'}\rangle e^{i\gamma_N}e^{i(\theta_N-\theta_m)}\,dt'. \qquad [10.107]$$

This enables us to calculate transition probabilities in the *nearly* adiabatic regime. To develop the "second correction," we would insert Equation 10.107 on the right side of Equation 10.105, and so on.

(c) As an example, apply Equation 10.107 to the driven-oscillator (Problem 10.10). Show that (in the near-adiabatic approximation) transitions are possible only to the two immediately adjacent levels, for which

$$c_{N+1}(t) = i\sqrt{\frac{m\omega}{2\hbar}}\sqrt{N+1}\int_0^t \dot{f}(t')e^{i\omega t'}\,dt',$$

$$c_{N-1}(t) = i\sqrt{\frac{m\omega}{2\hbar}}\sqrt{N}\int_0^t \dot{f}(t')e^{-i\omega t'}\,dt'.$$

(The transition *probabilities* are the absolute squares of these, of course.)