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 you grab the support and shake it in a jerky manner the bob will swing around chaotically. But if you *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 of the external conditions* defines 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 a vibrating 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 *constant*, and only at the *end* of the calculation allow them to vary (slowly) with time. For example, the classical period of a pendulum of (fixed) length L is $2\pi\sqrt{L/g}$; if the length is now gradually *changing*, the period will presumably be $2\pi\sqrt{L(t)/g}$. A more subtle example occurred in our discussion of the hydrogen molecule ion (Section 7.3). We began

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

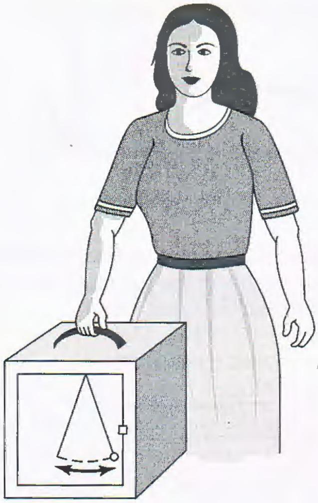

FIGURE 10.1: Adiabatic motion: If the case is transported very gradually, the pendulum inside keeps swinging with the same amplitude, in a plane parallel to the original one.

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 the Hamiltonian changes *gradually* from some initial form H^i to some final form H^f. The **adiabatic theorem** states that if the particle was initially in the nth eigenstate of H^i, it will be 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 10.2(a)):

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

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 10.2(b)):

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

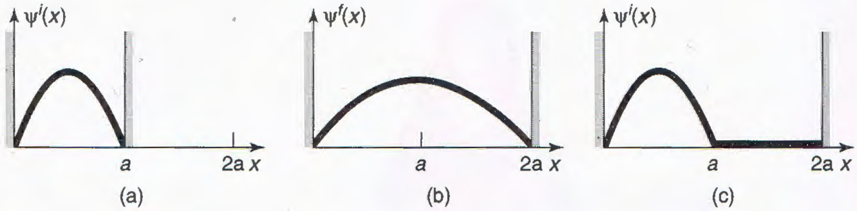

FIGURE 10.2: (a) Particle starts out in the ground state of the infinite square well. (b) If the wall moves *slowly*, the particle remains in the ground state. (c) If the wall moves *rapidly*, the particle is left (momentarily) in its initial state.

(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 *huge*. All we require is that it happen *slowly*. Energy is not conserved here: Whoever is moving the wall is extracting energy from the system, just like the piston on a slowly expanding cylinder of gas. By contrast, if the well expands *suddenly*, the resulting state is still $\psi^i(x)$ (Figure 10.2(c)), which is a complicated linear combination of eigenstates of the new Hamiltonian (Problem 2.38). In this case energy *is* conserved (at least, its *expectation value* is); as in the *free* expansion of a gas (into a vacuum) when the barrier is suddenly removed, no work is done.

$*\!*\!*$**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 (instantaneous) width of the well and $E_n^i \equiv n^2\pi^2\hbar^2/2ma^2$ is the nth allowed 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.

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

(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

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

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 $\exp(-i\alpha z^2) \cong 1$ 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

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

where $E_n(t) \equiv n^2\pi^2\hbar^2/2mw^2$ is the *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] If the Hamiltonian is *independent* of time, then a particle which starts out in the nth eigenstate,[4] ψ_n,

$$H\psi_n = E_n\psi_n, \tag{10.7}$$

[3]The 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*, Wiley, New York (1962), Vol. II, Chapter XVII, Section 12, J-T Hwang and Philip Pechukas, *J. Chem. Phys.* **67**, 4640, 1977, and Gasiorowicz, *Quantum Physics*, Wiley, New York (1974), Chapter 22, Problem 6. The argument given here follows B. H. Bransden and C. J. Joachain, *Introduction to Quantum Mechanics*, 2nd ed., Addison-Wesley, Boston, MA (2000), Section 9.4.

[4]I'll suppress the dependence on position (or spin, etc.); in this argument only the time dependence is at issue.

remains in the nth eigenstate, simply picking up a phase factor:

$$\Psi_n(t) = \psi_n e^{-iE_n t/\hbar}. \qquad [10.8]$$

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

$$H(t)\psi_n(t) = E_n(t)\psi_n(t), \qquad [10.9]$$

but they still constitute (at any particular instant) an orthonormal set

$$\langle \psi_n(t) | \psi_m(t) \rangle = \delta_{nm}, \qquad [10.10]$$

and they are complete, so the general solution to the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t) \qquad [10.11]$$

can be expressed as a linear combination of them:

$$\Psi(t) = \sum_n c_n(t)\psi_n(t)e^{i\theta_n(t)}, \qquad [10.12]$$

where

$$\theta_n(t) \equiv -\frac{1}{\hbar}\int_0^t E_n(t')\,dt' \qquad [10.13]$$

generalizes the "standard" phase factor to the case where E_n varies with time. (As usual, I could have included it in the coefficient $c_n(t)$, but it is convenient to factor out this portion of the time dependence, since it would be present even for a time-*in*dependent Hamiltonian.)

Substituting Equation 10.12 into Equation 10.11 we obtain

$$i\hbar \sum_n \left[\dot{c}_n\psi_n + c_n\dot{\psi}_n + ic_n\psi_n\dot{\theta}_n\right]e^{i\theta_n} = \sum_n c_n(H\psi_n)e^{i\theta_n} \qquad [10.14]$$

(I use a dot to denote the time derivative). In view of Equations 10.9 and 10.13 the last two terms cancel, leaving

$$\sum_n \dot{c}_n\psi_n e^{i\theta_n} = -\sum_n c_n\dot{\psi}_n e^{i\theta_n}. \qquad [10.15]$$

Taking the inner product with ψ_m, and invoking the orthonormality of the instantaneous eigenfunctions (Equation 10.10),

$$\sum_n \dot{c}_n\delta_{mn}e^{i\theta_n} = -\sum_n c_n\langle \psi_m | \dot{\psi}_n \rangle e^{i\theta_n},$$

or

$$\dot{c}_m(t) = -\sum_n c_n \langle \psi_m | \dot{\psi}_n \rangle e^{i(\theta_n - \theta_m)}. \tag{10.16}$$

Now, differentiating Equation 10.9 with respect to time yields

$$\dot{H}\psi_n + H\dot{\psi}_n = \dot{E}_n\psi_n + E_n\dot{\psi}_n,$$

and hence (again taking the inner product with ψ_m)

$$\langle \psi_m | \dot{H} | \psi_n \rangle + \langle \psi_m | H | \dot{\psi}_n \rangle = \dot{E}_n \delta_{mn} + E_n \langle \psi_m | \dot{\psi}_n \rangle. \tag{10.17}$$

Exploiting the hermiticity of H to write $\langle \psi_m | H | \dot{\psi}_n \rangle = E_m \langle \psi_m | \dot{\psi}_n \rangle$, it follows that for $n \neq m$

$$\langle \psi_m | \dot{H} | \psi_n \rangle = (E_n - E_m) \langle \psi_m | \dot{\psi}_n \rangle. \tag{10.18}$$

Putting this into Equation 10.16 (and assuming, remember, that the energies are nondegenerate) we conclude that

$$\dot{c}_m(t) = -c_m \langle \psi_m | \dot{\psi}_m \rangle - \sum_{n \neq m} c_n \frac{\langle \psi_m | \dot{H} | \psi_n \rangle}{E_n - E_m} e^{(-i/\hbar)\int_0^t [E_n(t') - E_m(t')]dt'}. \tag{10.19}$$

This result is *exact*. Now comes the adiabatic approximation: Assume that $\dot{H}$ is extremely small, and drop the second term,[5] leaving

$$\dot{c}_m(t) = -c_m \langle \psi_m | \dot{\psi}_m \rangle, \tag{10.20}$$

with the solution

$$c_m(t) = c_m(0) e^{i\gamma_m(t)}, \tag{10.21}$$

where[6]

$$\gamma_m(t) \equiv i \int_0^t \left\langle \psi_m(t') \middle| \frac{\partial}{\partial t'} \psi_m(t') \right\rangle dt'. \tag{10.22}$$

In particular, if the particle starts out in the nth eigenstate (which is to say, if $c_n(0) = 1$, and $c_m(0) = 0$ for $m \neq n$), then (Equation 10.12)

$$\boxed{\Psi_n(t) = e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t),} \tag{10.23}$$

so it remains in the nth eigenstate (of the evolving Hamiltonian), picking up only a couple of phase factors. QED

[5] Rigorous justification of this step is not trivial. See A. C. Aguiar Pinto *et al.*, *Am. J. Phys.* **68**, 955 (2000).

[6] Notice that γ is *real*, since the normalization of ψ_m entails $(d/dt)\langle \psi_m | \psi_m \rangle = \langle \psi_m | \dot{\psi}_m \rangle + \langle \dot{\psi}_m | \psi_m \rangle = 2\mathrm{Re}\left(\langle \psi_m | \dot{\psi}_m \rangle\right) = 0$.

Example 10.1 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 10.3):

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

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

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

The normalized eigenspinors of $H(t)$ are

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

and

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

they represent spin up and spin down, respectively, *along the instantaneous direction of* $\mathbf{B}(t)$ (see Problem 4.30). The corresponding eigenvalues are

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

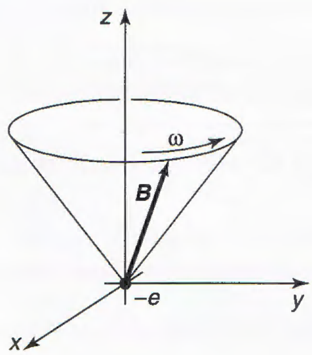

FIGURE 10.3: Magnetic field sweeps around in a cone, at angular velocity ω (Equation 10.24).

Suppose the electron starts out with spin up, along $\mathbf{B}(0)$:[7]

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

The exact solution to the time-dependent Schrödinger equation is (Problem 10.2):

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

where

$$\lambda \equiv \sqrt{\omega^2 + \omega_1^2 - 2\omega\omega_1\cos\alpha}. \tag{10.32}$$

Or, expressing it as a linear combination of χ_+ and χ_-:

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

Evidently the (exact) probability of a transition to spin down (along the current direction of $\mathbf{B}$) is

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

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

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

as advertised. The magnetic field leads the electron around by its nose, with the spin always pointing in the direction of $\mathbf{B}$. 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 10.4).

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[7]This is essentially the same as Problem 9.20, except that now the electron starts out with spin up along $\mathbf{B}$, whereas in Equation 9.20(d) it started out with spin up along z.

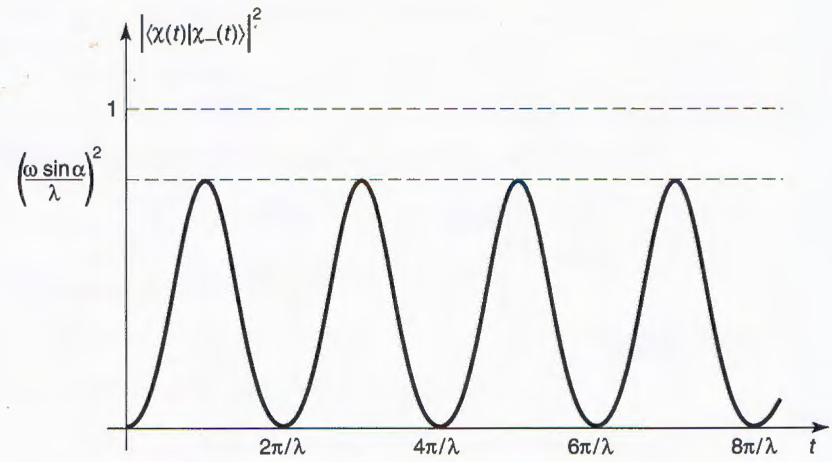

FIGURE 10.4: Plot of the transition probability, Equation 10.34, in the *non*adiabatic regime ($\omega \gg \omega_1$).

∗∗**Problem 10.2** Check that Equation 10.31 satisfies the time-dependent Schrödinger equation for the Hamiltonian in Equation 10.25. Also confirm Equation 10.33, and show that the sum of the squares of the coefficients is 1, as required for normalization.

10.2 BERRY'S PHASE

10.2.1 Nonholonomic Processes

Let's go back 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 10.5). For the moment, pretend the earth is not rotating. Very gently (that is, *adiabatically*), I carry it down the longitude line passing through Portland, to the equator. At this point it is swinging north-south. Now I carry it (still swinging north-south) part way around the equator. And finally, I take it back up to the North Pole, along the new longitude line.

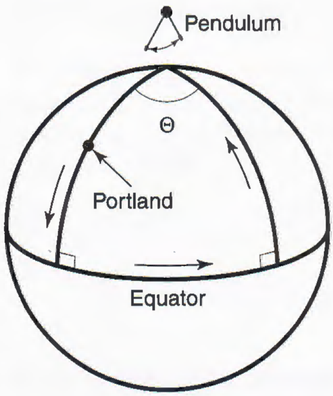

FIGURE 10.5: Itinerary for adiabatic transport of a pendulum on the surface of the earth.

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.

As it happens, 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

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

This is a particularly nice way to express the answer, because it turns out to be independent of the *shape* of the path (Figure 10.6).[8]

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*

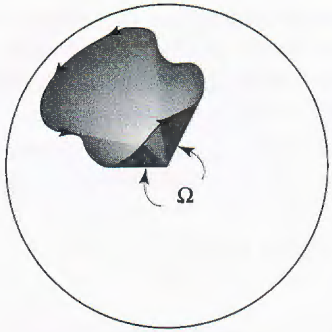

FIGURE 10.6: Arbitrary path on the surface of a sphere, subtending a solid angle Ω.

[8]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.

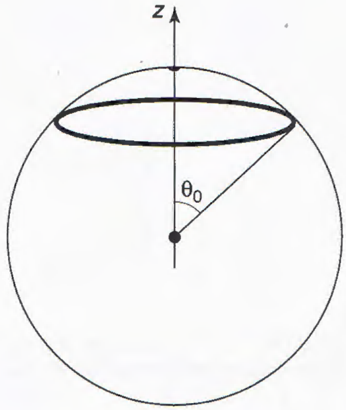

FIGURE 10.7: Path of a Foucault pendulum, in the course of one day.

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 10.7) 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,[9] 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 parameters of 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.[10] 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?

[9]See, for example, Jerry B. Marion and Stephen T. Thornton, *Classical Dynamics of Particles and Systems*, 4th ed., Saunders, Fort Worth, TX (1995), Example 10.5. Geographers measure latitude (λ) up from the equator, rather than down from the pole, so $\cos\theta_0 = \sin\lambda$.

[10]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*, World Scientific, Singapore (1989).

10.2.2 Geometric Phase

In Section 10.1.2 I showed that a particle which starts out in the nth eigenstate of $H(0)$ remains, under adiabatic conditions, in the nth eigenstate of $H(t)$, picking up only a time-dependent phase factor. Specifically, its wave function is (Equation 10.23)

$$\Psi_n(t) = e^{i[\theta_n(t)+\gamma_n(t)]}\psi_n(t), \tag{10.38}$$

where

$$\theta_n(t) \equiv -\frac{1}{\hbar}\int_0^t E_n(t')\,dt' \tag{10.39}$$

is the **dynamic phase** (generalizing the usual factor $\exp(-iE_nt/\hbar)$ to the case where E_n is a function of time), and

$$\gamma_n(t) \equiv i\int_0^t \left\langle \psi_n(t') \middle| \frac{\partial}{\partial t'}\psi_n(t')\right\rangle dt' \tag{10.40}$$

is the so-called **geometric phase**.

Now $\psi_n(t)$ 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 expanding square well.) Thus

$$\frac{\partial\psi_n}{\partial t} = \frac{\partial\psi_n}{\partial R}\frac{dR}{dt}, \tag{10.41}$$

so

$$\gamma_n(t) = i\int_0^t \left\langle \psi_n \middle| \frac{\partial\psi_n}{\partial R}\right\rangle \frac{dR}{dt'}\,dt' = i\int_{R_i}^{R_f} \left\langle \psi_n \middle| \frac{\partial\psi_n}{\partial R}\right\rangle dR, \tag{10.42}$$

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*!

However, I assumed (in Equation 10.41) 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

$$\frac{\partial\psi_n}{\partial t} = \frac{\partial\psi_n}{\partial R_1}\frac{dR_1}{dt} + \frac{\partial\psi_n}{\partial R_2}\frac{dR_2}{dt} + \cdots + \frac{\partial\psi_n}{\partial R_N}\frac{dR_N}{dt} = (\nabla_R\psi_n)\cdot\frac{d\mathbf{R}}{dt}, \tag{10.43}$$

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

$$\gamma_n(t) = i\int_{\mathbf{R}_i}^{\mathbf{R}_f} \langle\psi_n|\nabla_R\psi_n\rangle\cdot d\mathbf{R}, \tag{10.44}$$

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

$$\boxed{\gamma_n(T) = i \oint \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\mathbf{R}.} \quad [10.45]$$

This is a *line* integral around a closed loop in parameter-space, and it is *not*, in general, zero. Equation 10.45 was first obtained by Michael 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.

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. For this reason, most people assumed until recently that the geometric phase was of no conceivable physical significance—after all, the phase of $\psi_n(t)$ itself is arbitrary. It was Berry's insight that if you carry the Hamiltonian around a closed *loop*, bringing it back to its original form, the relative phase at the beginning and the end of the process is *not* arbitrary, and can actually be measured.

For example, suppose 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

$$\Psi = \frac{1}{2}\Psi_0 + \frac{1}{2}\Psi_0 e^{i\Gamma}, \quad [10.46]$$

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

$$\begin{aligned}|\Psi|^2 &= \frac{1}{4}|\Psi_0|^2\left(1+e^{i\Gamma}\right)\left(1+e^{-i\Gamma}\right)\\ &= \frac{1}{2}|\Psi_0|^2(1+\cos\Gamma) = |\Psi_0|^2\cos^2(\Gamma/2).\end{aligned} \quad [10.47]$$

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

[11]M. V. Berry, *Proc. R. Soc. Lond.* A **392**, 45 (1984), reprinted in Wilczek and Shapere (footnote 10). It is astonishing, in retrospect, that this result escaped notice for sixty years.

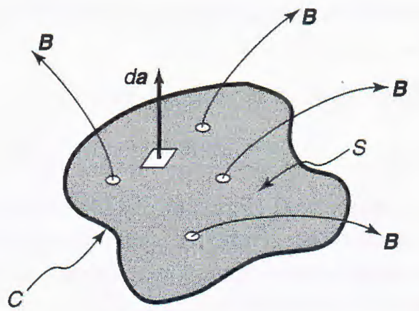

FIGURE 10.8: Magnetic flux through a surface S bounded by the closed curve C.

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.)

When the parameter space is three dimensional, $\mathbf{R} = (R_1, R_2, R_3)$, Berry's formula (Equation 10.45) is reminiscent of the expression for **magnetic flux** in terms of the vector potential **A**. The flux, Φ, through a surface S bounded by a curve C (Figure 10.8), is

$$\Phi \equiv \int_S \mathbf{B} \cdot d\mathbf{a}. \qquad [10.48]$$

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

$$\Phi = \int_S (\nabla \times \mathbf{A}) \cdot d\mathbf{a} = \oint_C \mathbf{A} \cdot d\mathbf{r}. \qquad [10.49]$$

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

$$\text{“}\mathbf{B}\text{”} = i\nabla_R \times \langle \psi_n | \nabla_R \psi_n \rangle, \qquad [10.50]$$

through the (closed loop) trajectory in parameter-space. To put it the other way around, in the three-dimensional case Berry's phase can be written as a surface integral,

$$\gamma_n(T) = i \int [\nabla_R \times \langle \psi_n | \nabla_R \psi_n \rangle] \cdot d\mathbf{a}. \qquad [10.51]$$

The magnetic analogy can be carried much further, but for our purposes Equation 10.51 is merely a convenient alternative expression for $\gamma_n(T)$.

∗Problem 10.3

(a) Use Equation 10.42 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 10.4 The delta function well (Equation 2.114) supports a single bound state (Equation 2.129). 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 10.5 Show that if $\psi_n(t)$ is *real*, the geometric phase vanishes. (Problems 10.3 and 10.4 are examples of this.) You might try to beat the rap by tacking an unnecessary (but perfectly legal) phase factor onto the eigenfunctions: $\psi_n'(t) \equiv e^{i\phi_n}\psi_n(t)$, 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 10.23. And for a *closed* loop it gives *zero*. *Moral:* For nonzero Berry's phase, you need (i) more than one time-dependent parameter in the Hamiltonian, and (ii) a Hamiltonian that yields nontrivially complex eigenfunctions.

Example 10.2 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 Example 10.1) in which $\mathbf{B}(t)$ 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 $\mathbf{B}$) is given by Equation 10.33. In the adiabatic regime, $\omega \ll \omega_1$,

$$\lambda = \omega_1\sqrt{1 - 2\frac{\omega}{\omega_1}\cos\alpha + \left(\frac{\omega}{\omega_1}\right)^2} \cong \omega_1\left(1 - \frac{\omega}{\omega_1}\cos\alpha\right) = \omega_1 - \omega\cos\alpha, \quad [10.52]$$

and Equation 10.33 becomes

$$\chi(t) \cong e^{-i\omega_1 t/2}e^{i(\omega\cos\alpha)t/2}e^{-i\omega t/2}\chi_+(t) + i\left[\frac{\omega}{\omega_1}\sin\alpha\sin\left(\frac{\omega_1 t}{2}\right)\right]e^{+i\omega t/2}\chi_-(t). \quad [10.53]$$

As $\omega/\omega_1 \to 0$ the second term drops out completely, and the result matches the expected adiabatic form (Equation 10.23). The dynamic phase is

$$\theta_+(t) = -\frac{1}{\hbar}\int_0^t E_+(t')\,dt' = -\frac{\omega_1 t}{2}, \quad [10.54]$$

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

$$\gamma_+(t) = (\cos\alpha - 1)\frac{\omega t}{2}. \qquad [10.55]$$

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

$$\gamma_+(T) = \pi(\cos\alpha - 1). \qquad [10.56]$$

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 10.9). The eigenstate representing spin up along $\mathbf{B}(t)$ has the form (see Problem 4.30):

$$\chi_+ = \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{pmatrix}, \qquad [10.57]$$

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

$$\begin{aligned} \nabla\chi_+ &= \frac{\partial\chi_+}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial\chi_+}{\partial\theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial\chi_+}{\partial\phi}\hat{\phi} \\ &= \frac{1}{r}\begin{pmatrix} -(1/2)\sin(\theta/2) \\ (1/2)e^{i\phi}\cos(\theta/2) \end{pmatrix}\hat{\theta} + \frac{1}{r\sin\theta}\begin{pmatrix} 0 \\ ie^{i\phi}\sin(\theta/2) \end{pmatrix}\hat{\phi}. \end{aligned} \qquad [10.58]$$

Hence

$$\begin{aligned} \langle\chi_+|\nabla\chi_+\rangle &= \frac{1}{2r}\left[-\sin(\theta/2)\cos(\theta/2)\,\hat{\theta} + \sin(\theta/2)\cos(\theta/2)\,\hat{\theta} + 2i\frac{\sin^2(\theta/2)}{\sin\theta}\hat{\phi}\right] \\ &= i\frac{\sin^2(\theta/2)}{r\sin\theta}\hat{\phi}. \end{aligned} \qquad [10.59]$$

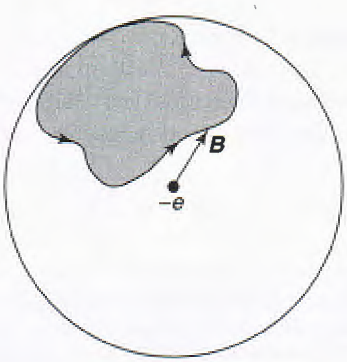

FIGURE 10.9: Magnetic field of constant magnitude but changing direction sweeps out a closed loop.

For Equation 10.51 we need the *curl* of this quantity:

$$\nabla \times \langle \chi_+ | \nabla \chi_+ \rangle = \frac{1}{r \sin\theta} \frac{\partial}{\partial \theta} \left[\sin\theta \left(\frac{i \sin^2(\theta/2)}{r \sin\theta} \right) \right] \hat{r} = \frac{i}{2r^2} \hat{r}. \qquad [10.60]$$

According to Equation 10.51, then,

$$\gamma_+(T) = -\frac{1}{2} \int \frac{1}{r^2} \hat{r} \cdot d\mathbf{a}. \qquad [10.61]$$

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 we conclude that

$$\gamma_+(T) = -\frac{1}{2} \int d\Omega = -\frac{1}{2} \Omega, \qquad [10.62]$$

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, this general result is consistent with the special case (Equation 10.56), as of course it *had* to be.

*****Problem 10.6** Work out the analog to Equation 10.62 for a particle of spin 1. *Answer:* $-\Omega$. (Incidentally, for spin s the result is $-s\Omega$.)

10.2.3 The Aharonov-Bohm Effect

In classical electrodynamics the potentials (φ and $\mathbf{A}$)[12] are not directly measurable—the *physical* quantities are the electric and magnetic *fields*:

$$\mathbf{E} = -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}. \qquad [10.63]$$

[12] It is customary in quantum mechanics to use the letter V for *potential energy*, but in electrodynamics the same letter is ordinarily reserved for the scalar potential. To avoid confusion I use φ for the scalar potential. See Problems 4.59, 4.60, and 4.61 for background to this section.

The fundamental laws (Maxwell's equations and the Lorentz force rule) make no reference to potentials, which are (from a logical point of view) no more than convenient but dispensable theoretical constructs. Indeed, you can with impunity *change* the potentials:

$$\varphi \to \varphi' = \varphi - \frac{\partial \Lambda}{\partial t}, \quad \mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\Lambda, \qquad [10.64]$$

where Λ is any function of position and time; this is called a **gauge transformation**, and it has no effect on the fields (as you can easily check using Equation 10.63).

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

$$H = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)^2 + q\varphi. \qquad [10.65]$$

Nevertheless, the theory is still invariant under gauge transformations (see Problem 4.61), and for a long time it was taken for granted 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[13] showed that the vector potential *can* affect the quantum behavior of a charged particle, even when it is moving through a region in which the field itself is zero. I'll work out a simple example first, then discuss the Aharonov-Bohm effect, and finally indicate how it all relates to 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 steady electric current I (see Figure 10.10). If the solenoid is extremely long, the magnetic field inside it 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 $\nabla \cdot \mathbf{A} = 0$),[14]

$$\mathbf{A} = \frac{\Phi}{2\pi r}\hat{\phi}, \quad (r > a), \qquad [10.66]$$

where $\Phi = \pi a^2 B$ is the **magnetic flux** through the solenoid. Meanwhile, the solenoid itself is uncharged, so the scalar potential φ is zero. In this case the Hamiltonian (Equation 10.65) becomes

$$H = \frac{1}{2m}\left[-\hbar^2\nabla^2 + q^2A^2 + 2i\hbar q\mathbf{A}\cdot\nabla\right]. \qquad [10.67]$$

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[13] 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).

[14] See, for instance, D. J. Griffiths, *Introduction to Electrodynamics*, 3rd ed., Prentice Hall, Upper Saddle River, NJ (1999), Equation 5.71.

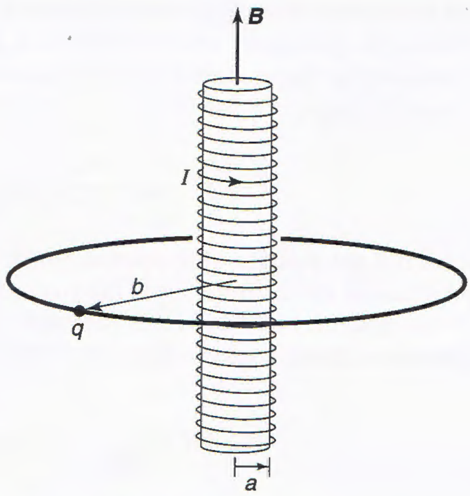

FIGURE 10.10: Charged bead on a circular ring through which a long solenoid passes.

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

$$\frac{1}{2m}\left[-\frac{\hbar^2}{b^2}\frac{d^2}{d\phi^2} + \left(\frac{q\Phi}{2\pi b}\right)^2 + i\frac{\hbar q\Phi}{\pi b^2}\frac{d}{d\phi}\right]\psi(\phi) = E\psi(\phi). \tag{10.68}$$

This is a linear differential equation with constant coefficients:

$$\frac{d^2\psi}{d\phi^2} - 2i\beta\frac{d\psi}{d\phi} + \epsilon\psi = 0, \tag{10.69}$$

where

$$\beta \equiv \frac{q\Phi}{2\pi\hbar} \quad \text{and} \quad \epsilon \equiv \frac{2mb^2E}{\hbar^2} - \beta^2. \tag{10.70}$$

Solutions are of the form

$$\psi = Ae^{i\lambda\phi}, \tag{10.71}$$

with

$$\lambda = \beta \pm \sqrt{\beta^2 + \epsilon} = \beta \pm \frac{b}{\hbar}\sqrt{2mE}. \tag{10.72}$$

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

$$\beta \pm \frac{b}{\hbar}\sqrt{2mE} = n, \tag{10.73}$$

and it follows that

$$E_n = \frac{\hbar^2}{2mb^2}\left(n - \frac{q\Phi}{2\pi\hbar}\right)^2, \quad (n = 0, \pm 1, \pm 2, \ldots). \qquad [10.74]$$

The solenoid lifts the two-fold degeneracy of the bead-on-a-ring (Problem 2.46): 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. 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*![15]

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

$$\left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)^2 + V\right]\Psi = i\hbar\frac{\partial \Psi}{\partial t}, \qquad [10.75]$$

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

$$\Psi = e^{ig}\Psi', \qquad [10.76]$$

where

$$g(\mathbf{r}) \equiv \frac{q}{\hbar}\int_{\mathcal{O}}^{\mathbf{r}} \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}', \qquad [10.77]$$

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 would depend on the *path* taken from $\mathcal{O}$ to $\mathbf{r}$, and hence would 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

$$\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)\Psi = \frac{\hbar}{i}e^{ig}\nabla\Psi', \qquad [10.78]$$

[15]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 that 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 (nonsuperconducting) example considered here.

and it follows that

$$\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)^2 \Psi = -\hbar^2 e^{ig}\nabla^2\Psi'. \qquad [10.79]$$

Putting this into Equation 10.75, and cancelling the common factor e^{ig}, we are left with

$$-\frac{\hbar^2}{2m}\nabla^2\Psi' + V\Psi' = i\hbar\frac{\partial\Psi'}{\partial t}. \qquad [10.80]$$

Evidently Ψ' satisfies the Schrödinger equation *without* **A**. If we can solve Equation 10.80, correcting for the presence of a (curl-free) vector potential will be trivial: 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 10.11). The beams are kept well away from the solenoid itself, so they encounter only regions where $\mathbf{B} = 0$. But **A**, which is given by Equation 10.66, is *not* zero, and (assuming V is the same on both sides), the two beams arrive with *different phases*:

$$g = \frac{q}{\hbar}\int \mathbf{A}\cdot d\mathbf{r} = \frac{q\Phi}{2\pi\hbar}\int\left(\frac{1}{r}\hat{\phi}\right)\cdot(r\hat{\phi}\,d\phi) = \pm\frac{q\Phi}{2\hbar}. \qquad [10.81]$$

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

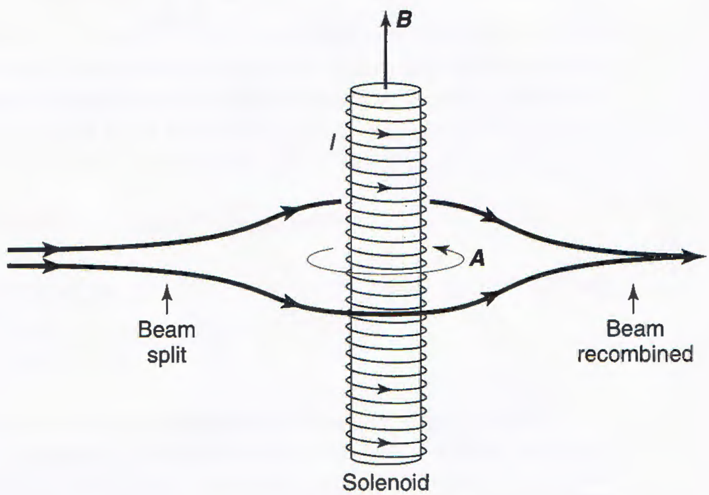

FIGURE 10.11: The Aharonov-Bohm effect: The electron beam splits, with half passing either side of a long solenoid.

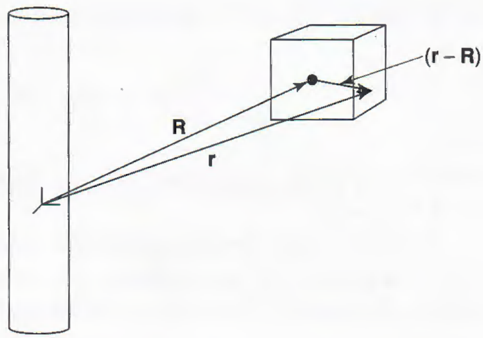

FIGURE 10.12: Particle confined to a box, by a potential $V(\mathbf{r} - \mathbf{R})$.

of phase by an amount proportional to the magnetic flux their paths encircle:

$$\text{phase difference} = \frac{q\Phi}{\hbar}. \tag{10.82}$$

This phase shift leads to measurable interference (Equation 10.47), which has been confirmed experimentally by Chambers and others.[16]

As Berry pointed out in his first paper on the subject, the Aharonov-Bohm effect can be regarded as an example of geometric phase. Suppose the charged particle is confined to a box (which is centered at point $\mathbf{R}$ outside the solenoid) by a potential $V(\mathbf{r} - \mathbf{R})$—see Figure 10.12. (In a moment we're going to transport the box around the solenoid, so $\mathbf{R}$ will become a function of time, but for now it is just some fixed vector.) The eigenfunctions of the Hamiltonian are determined by

$$\left\{\frac{1}{2m}\left[\frac{\hbar}{i}\nabla - q\mathbf{A}(\mathbf{r})\right]^2 + V(\mathbf{r} - \mathbf{R})\right\}\psi_n = E_n\psi_n. \tag{10.83}$$

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

$$\psi_n = e^{ig}\psi_n', \tag{10.84}$$

where[17]

$$g \equiv \frac{q}{\hbar}\int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}', \tag{10.85}$$

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

[17] 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 when we complete the journey around the solenoid. If you use a point in fixed *space*, for example, you'll have to readjust the phase "by hand," at the far end, because the path will have wrapped around the solenoid, circling regions where the curl of $\mathbf{A}$ does not vanish. 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 10.9, you want to make sure that $\psi_n(x, T) = \psi_n(x, 0)$, so that no spurious phase changes are introduced.

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

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}-\mathbf{R})\right]\psi_n' = E_n\psi_n'. \qquad [10.86]$$

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

Now let's carry the box around the solenoid (in this application 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

$$\begin{aligned}\langle\psi_n|\nabla_R\psi_n\rangle \\ &= \int e^{-ig}[\psi_n'(\mathbf{r}-\mathbf{R})]^* e^{ig}\left[-i\frac{q}{\hbar}\mathbf{A}(\mathbf{R})\psi_n'(\mathbf{r}-\mathbf{R}) + \nabla_R\psi_n'(\mathbf{r}-\mathbf{R})\right]d^3\mathbf{r} \\ &= -i\frac{q}{\hbar}\mathbf{A}(\mathbf{R}) - \int[\psi_n'(\mathbf{r}-\mathbf{R})]^*\nabla\psi_n'(\mathbf{r}-\mathbf{R})\,d^3\mathbf{r}. \qquad [10.87]\end{aligned}$$

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

$$\langle\psi_n|\nabla_R\psi_n\rangle = -i\frac{q}{\hbar}\mathbf{A}(\mathbf{R}). \qquad [10.88]$$

Putting this into Berry's formula (Equation 10.45), we conclude that

$$\gamma_n(T) = \frac{q}{\hbar}\oint\mathbf{A}(\mathbf{R})\cdot d\mathbf{R} = \frac{q}{\hbar}\int(\nabla\times\mathbf{A})\cdot d\mathbf{a} = \frac{q\Phi}{\hbar}, \qquad [10.89]$$

which neatly confirms the Aharonov-Bohm result (Equation 10.82), and reveals that the Aharonov-Bohm effect is a particular instance of geometric phase.[18]

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 $\mathbf{A}$ itself

[18] Incidentally, in this case the analogy between Berry's phase and magnetic flux (Equation 10.50) is *almost* an identity: "$\mathbf{B}$" $= (q/\hbar)\mathbf{B}$.

measurable—only the enclosed *flux* comes into the final answer, and the theory remains gauge invariant.

Problem 10.7

(a) Derive Equation 10.67 from Equation 10.65.

(b) Derive Equation 10.79, starting with Equation 10.78.

FURTHER PROBLEMS FOR CHAPTER 10

* * ***Problem 10.8** A particle starts out in the ground state of the infinite square well (on the interval $0 \leq x \leq a$). Now a wall is slowly erected, slightly off-center:[19]

$$V(x) = f(t)\delta\left(x - \frac{a}{2} - \epsilon\right),$$

where $f(t)$ rises gradually from 0 to ∞. According to the adiabatic theorem, the particle will remain in the ground state of the evolving Hamiltonian.

(a) Find (and sketch) the ground state at $t \to \infty$. *Hint:* This should be the ground state of the infinite square well with an impenetrable barrier at $a/2 + \epsilon$. Note that the particle is confined to the (slightly) larger left "half" of the well.

(b) Find the (transcendental) equation for the ground state of the Hamiltonian at time t. *Answer:*

$$z \sin z = T[\cos z - \cos(z\delta)],$$

where $z \equiv ka$, $T \equiv maf(t)/\hbar^2$, $\delta \equiv 2\epsilon/a$, and $k \equiv \sqrt{2mE}/\hbar$.

(c) Setting $\delta = 0$, solve graphically for z, and show that the smallest z goes from π to 2π as T goes from 0 to ∞. Explain this result.

(d) Now set $\delta = 0.01$ and solve numerically for z, using $T = 0, 1, 5, 20, 100,$ and 1000.

(e) Find the probability P_r that the particle is in the right "half" of the well, as a function of z and δ. *Answer:* $P_r = 1/[1 + (I_+/I_-)]$, where $I_\pm \equiv \left[1 \pm \delta - (1/z)\sin\left(z(1 \pm \delta)\right)\right]\sin^2[z(1 \mp \delta)/2]$. Evaluate this expression numerically for the T's in part (d). Comment on your results.

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[19] Julio Gea-Banacloche, *Am. J. Phys.* **70**, 307 (2002) uses a rectangular barrier; the delta-function version was suggested by M. Lakner and J. Peternelj, *Am. J. Phys.* **71**, 519 (2003).

(f) Plot the ground state wave function for those same values of T and δ. Note how it gets squeezed into the left half of the well, as the barrier grows.[20]

*****Problem 10.9** 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; $f(t)$ has the dimensions of *length*). The Hamiltonian is

$$H(t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 - m\omega^2 x f(t). \qquad [10.90]$$

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.[21]

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

$$x_c(t) = \omega \int_0^t f(t')\sin[\omega(t - t')]\,dt'. \qquad [10.91]$$

(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 2.61), can be written as

$$\Psi(x, t) = \psi_n(x - x_c)e^{\frac{i}{\hbar}\left[-(n+\frac{1}{2})\hbar\omega t + m\dot{x}_c(x - \frac{x_c}{2}) + \frac{m\omega^2}{2}\int_0^t f(t')x_c(t')dt'\right]}. \qquad [10.92]$$

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

$$\psi_n(x, t) = \psi_n(x - f); \quad E_n(t) = \left(n + \frac{1}{2}\right)\hbar\omega - \frac{1}{2}m\omega^2 f^2. \qquad [10.93]$$

(d) Show that in the adiabatic approximation the classical position (Equation 10.91) reduces to $x_c(t) \cong f(t)$. State the precise criterion for adiabaticity, in this context, as a constraint on the time derivative of f. *Hint:* Write $\sin[\omega(t - t')]$ as $(1/\omega)(d/dt')\cos[\omega(t - t')]$ and use integration by parts.

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[20] Gea-Banacloche (footnote 19) discusses the evolution of the wave function *without* assuming the adiabatic theorem, and confirms these results in the adiabatic limit.

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

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

$$\Psi(x, t) \cong \psi_n(x, t) e^{i\theta_n(t)} e^{i\gamma_n(t)}. \tag{10.94}$$

Check that the dynamic phase has the correct form (Equation 10.39). Is the geometric phase what you would expect?

Problem 10.10 The adiabatic approximation can be regarded as the first term in an **adiabatic series** for the coefficients $c_m(t)$ in Equation 10.12. Suppose the system starts out in the nth state; in the adiabatic approximation, it *remains* in the nth state, picking up only a time-dependent geometric phase factor (Equation 10.21):

$$c_m(t) = \delta_{mn} e^{i\gamma_n(t)}.$$

(a) Substitute this into the right side of Equation 10.16 to obtain the "first correction" to adiabaticity:

$$c_m(t) = c_m(0) - \int_0^t \left\langle \psi_m(t') \middle| \frac{\partial}{\partial t'} \psi_n(t') \right\rangle e^{i\gamma_n(t')} e^{i(\theta_n(t') - \theta_m(t'))}\, dt'. \tag{10.95}$$

This enables us to calculate transition probabilities in the *nearly* adiabatic regime. To develop the "second correction," we would insert Equation 10.95 on the right side of Equation 10.16, and so on.

(b) As an example, apply Equation 10.95 to the driven oscillator (Problem 10.9). Show that (in the near-adiabatic approximation) transitions are possible only to the two immediately adjacent levels, for which

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

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

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