Antiadiabatic Theorem for Crossing Levels

F. E. Low
Center for Theoretical Physics, Laboratory for Nuclear Science, and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 3 May 1989)

We consider in this Letter the time dependence of a system for which two levels (which are not, in general, decoupled) accidentally cross (or almost cross) for some value of the parameters of the Hamiltonian. We show that for a well-defined class of crossings or narrowly avoided crossings, in which the Hamiltonian changes slowly on its own scale, the system will behave oppositely to the usual adiabatic rule.

PACS numbers: 03.65.−w, 32.60.+i

We consider in this Letter the time dependence of a system for which two levels (which are not, in general, decoupled) accidentally cross (or almost cross) for some value of the parameters of the Hamiltonian. We show that for a well-defined class of crossings or narrowly avoided crossings the system will behave oppositely to the usual adiabatic rule.[1] That is, if the avoided crossing energy is called zero, the system will, with probability close to 1, jump from the state of positive energy to the one of negative energy. This has been known since 1932 for the Landau-Zener[2,3] process; we consider here a different situation, one in which θ and ϕ [as defined in Eq. (2) below] are slowly changing at the point of crossing.

To summarize the result, we characterize the two-state system by a Hamiltonian expressed in terms of an equivalent (negative) magnetic field (and unit magnetic moment):

$$H=\mathbf{B}(t)\cdot\boldsymbol{\sigma}\,, \tag{1}$$

with

$$\mathbf{B}(t)=B(\hat{\mathbf{i}}\sin\theta\cos\phi+\hat{\mathbf{j}}\sin\theta\sin\phi+\hat{\mathbf{k}}\cos\theta)\,, \tag{2}$$

where B, θ, and ϕ are functions of t and σ_x, σ_y, and σ_z are the usual Pauli matrices. Then our result holds provided

$$\left|\frac{dB}{dt}\right|\left[\left(\frac{d\theta}{dB}\right)^2+\sin^2\theta\left(\frac{d\phi}{dB}\right)^2\right]_{B=0}\ll 1\,. \tag{3}$$

The Landau-Zener case has

$$\mathbf{B}(t)=\hat{\mathbf{k}}B_0t/T+\hat{\mathbf{i}}B_x\,, \tag{4}$$

with B_0/T and B_z constant. The antiadiabatic behavior there results if

$$\frac{B_x^2}{|dB/dt|}\ll 1\,. \tag{5}$$

We discuss first the case where the energy eigenvalues $\pm|B|=\pm B$ go exactly through zero.

We choose as eigenfunctions of H

$$u_+=\begin{pmatrix}\cos(\theta/2)e^{-i\phi/2}\\ \sin(\theta/2)e^{i\phi/2}\end{pmatrix}\exp\left(-i\psi(t)+\frac{i}{2}\int_{\theta_0,\phi_0}^{\theta,\phi}\cos\theta\,d\phi\right), \tag{6a}$$

with eigenvalue B, and

$$u_-=\begin{pmatrix}\sin(\theta/2)e^{-i\phi/2}\\ -\cos(\theta/2)e^{i\phi/2}\end{pmatrix}\exp\left(i\psi(t)-\frac{i}{2}\int_{\theta_0,\phi_0}^{\theta,\phi}\cos\theta\,d\phi\right), \tag{6b}$$

with eigenvalue $-B$. Here

$$\psi(t)=\int_{t_0}^{t}dt'B(t') \tag{7}$$

and θ_0,ϕ_0 are the values of θ and ϕ at $t=t_0$, when the initial state is specified. The phases are chosen to make the self-coupling of u_+ and u_- in a time-dependent field vanish.

The Schrödinger equation for an arbitrary state $\chi=a_+u_++a_-u_-$ is

$$\dot a_++\exp\left(2i\psi(t)-i\int\cos\theta\,d\phi\right)\left(v_+,\frac{\partial v_-}{\partial t}\right)a_-=0 \tag{8a}$$

and

$$\dot a_-+\exp\left(-2i\psi(t)+i\int\cos\theta\,d\phi\right)\left(v_-,\frac{\partial v_+}{\partial t}\right)a_+=0\,, \tag{8b}$$

where the $v_\pm$ are the $u_\pm$ with the explicit factors

$$\exp\left[\pm\left(i\psi(t)-\frac{i}{2}\int_{\theta_0,\phi_0}^{\theta,\phi}\cos\theta\,d\phi\right)\right]$$

removed.

We wish to study the time dependence of $a_\pm$ for the case where the time dependence of H is very slow on the scale of H itself. That is, we assume $dt=Td\lambda$, where the time T is large on an appropriate scale (to be discussed below). B, θ, and ϕ are ordinary functions of λ which may change substantially as λ goes from λ_0 to λ_f. The conditions of the usual adiabatic theorem are violated, however, in that $B(\lambda)$ goes through zero between λ_0 and λ_f. We choose the point $\lambda=0$ to be the zero of $B(\lambda)$. For λ not too far from zero we will have

$$B=B_0(\lambda+\alpha\lambda^2+\cdots) \tag{9}$$

and

$$\psi=TB_0\left[\left(\frac{\lambda^2}{2}+\frac{\alpha\lambda^3}{3}+\cdots\right)-\text{const}\right]. \tag{10}$$

In terms of λ, Eq. (8b) for a_- becomes

$$\frac{da_-}{d\lambda}+\exp\left(-2i\psi(t)+i\int\cos\theta\, d\phi\right)\left(v_-,\frac{\partial v_+}{\partial\lambda}\right)a_+=0. \tag{11}$$

Assuming smooth behavior of θ and ϕ near $\lambda=0$, $a_+(\lambda_0)=1$, and $a_-(\lambda_0)=0$ we find, setting $a_+=1$ in Eq. (11),

$$a_-(\lambda)\sim-\int_{\lambda_0}^{\lambda}\exp\left[-2iB_0T\left(\frac{\lambda^2}{2}\right)\right]d\lambda\left[\exp\left(i\int\cos\theta\, d\phi\right)\left(v_-,\frac{\partial v_+}{\partial\lambda}\right)\right]_{\lambda=0}e^{i\Phi_0}, \tag{12}$$

$$\sim(1-i)\left(\frac{\pi}{2B_0T}\right)^{1/2}e^{i\Phi_0}\left[\exp\left(i\int\cos\theta\, d\phi\right)\left(v_-,\frac{\partial v_+}{\partial\lambda}\right)\right]_{\lambda=0}, \tag{13}$$

where Φ_0 is a constant phase.

Thus, for large B_0T, the transition amplitude from u_+ to u_- goes like $1/(B_0T)^{1/2}$. Note that the adiabatically forbidden transition amplitude with an energy gap ΔB would go like $1/\Delta BT$. Note also, however, that in our case it is positive to positive energy that is forbidden. In the energy-gap case it is positive to negative energy that would be forbidden; here, the latter is enforced.

The bracketed expression in Eq. (13) is

$$\exp\left(i\int\cos\theta\, d\phi\right)\left(v_-,\frac{\partial v_+}{\partial\lambda}\right)=-\frac{1}{2}\exp\left(i\int\cos\theta\, d\phi\right)\left(\frac{d\theta}{d\lambda}+i\sin\theta\frac{d\phi}{d\lambda}\right), \tag{14}$$

and can be shown to be rotationally invariant (for θ and ϕ real polar angles of a magnetic field) as must be the case.

The transition probability is

$$p=|a_-|^2=\frac{\pi}{4B_0T}\left[\left(\frac{d\theta}{d\lambda}\right)^2+\sin^2\theta\left(\frac{d\phi}{d\lambda}\right)^2\right]_{\lambda=0}, \tag{15}$$

or, expressed in terms of B and dB/dt,[4]

$$p=\frac{\pi}{4}\left\{\left|\frac{dB}{dt}\right|\left[\left(\frac{d\theta}{dB}\right)^2+\sin^2\theta\left(\frac{d\phi}{dB}\right)^2\right]\right\}_{B=0}. \tag{16}$$

Several comments can be made: Evidently, any coupling of v_- and v_+ requires that θ or ϕ be changing as B goes through zero. This is clearly a requirement for the case of an actual magnetic field, since the wave functions $v_\pm$ depend only on the field direction. For a more general system which can be reduced to a two-state problem, the effective two-state Hamiltonian will, for small λ, contain terms of order λ^2 arising from virtual transitions out of the two states in question. It follows that the coefficients $d\theta/dB$ and $d\phi/dB$ in Eq. (16) also depend on the spectrum of and matrix elements to higher states to which the two states are coupled.

We are now in a position to characterize the well-defined class of crossings referred to in the abstract. First, the probability p must be small compared to 1 in order to set $a_+=1$ in going from Eq. (11) to Eq. (12). Second, the λ^3 term in ψ in Eq. (10) will be negligible in the important range of integration provided

$$\frac{d^2B}{dt^2}\Big/\left(\frac{dB}{dt}\right)^{3/2}\Bigg|_{B=0}$$

is also small compared to 1. The first of these conditions is clearly required for the antiadiabatic behavior to hold. The second is required for the explicit formula Eq. (16) for the small violation of antiadiabaticity to hold as well.

The system we have considered is unrealistic, in that two levels will rarely exactly cross. In particular, if two levels do cross for a given set of internal parameters —magnitudes and direction of electric and magnetic fields, for example—then a small change in *one* of the parameters—for example, the relative angle of the two fields—will not, in general, allow a new choice of the other parameters that will maintain the crossing. (However, see below for an interesting exception.) We should then consider the case of levels that almost cross, and show that our result holds there as well.

If the equivalent magnetic field does not go through zero, $B(t)$ cannot change sign, so that the vector $\mathbf{B}$ must change sign by the transformation $\theta\to\theta'=\pi-\theta$ and $\phi\to\phi'=\phi+\pi$. The state of the system will go from energy $|B|$ to energy $-|B|$ if the time during which θ and ϕ make this change is short enough so that the *sudden* approximation holds. This follows since the wave function

$$v_+=\begin{pmatrix}\cos(\theta/2)e^{-i\phi/2}\\ \sin(\theta/2)e^{i\phi/2}\end{pmatrix}$$

is in fact the wave function of a state of energy $-|B|$ after the change of θ and ϕ. That is, in terms of the new angles of the field, to within a phase,

$$v_+ = \begin{pmatrix} \sin(\theta'/2)e^{-i\phi'/2} \\ -\cos(\theta'/2)e^{i\phi'/2} \end{pmatrix},$$

the eigenfunction with energy $-|B|$. This can also be seen more simply be noting that as $\theta,\phi \to \theta',\phi'$, $H \to -H$ and $\chi \to \chi$.

For the above considerations to hold the residual energy gap must be small enough. The following criteria determine how small. We assume the following:

(1) The true energies are well approximated by a linear time dependence from t_0 to a time $t_a < 0$ before the avoided crossing, and from a time $t_b \sim |t_a|$ until t_f after the avoided crossing; thus, if $B_\perp$ is the actual minimum energy gap, we must have $B_0|t_a|/T \gg B_\perp$, or $B_0\lambda_a \sim B_0\lambda_b \gg B_\perp$.

(2) The transition amplitude from t_0 to t_a and t_b to t_f must be approximately given by our formula (13); thus, as $t \to t_a$ from below, or t_b from above, $d\theta/d\lambda + i\sin\theta\, d\phi/d\lambda$ must seem to approach a limit of order unity.

(3) There is violation of the sudden approximation; $|t_a - t_b|\lambda_a B_0$ must be much smaller than our calculated transition amplitude, $1/(B_0T)^{1/2}$.

All of these criteria are met by the following relation between the three independent small numbers of our model:

$$1/B_0T \gg \lambda_a^{4/3} \sim \lambda_b^{4/3} \gg (B_\perp/B_0)^{4/3}. \qquad (17)$$

Note that the Landau-Zener[2,3] formula holds for a process that does not satisfy these inequalities, since there the derivative $d\theta/d\lambda$ does not approach order unity for any value of t_a or t_b.

We consider as an example the $n=2$ states of a spinless, nonrelativistic hydrogen atom in electric and magnetic fields, **E** and **B**, making an angle θ with each other. We pick **E** in the z direction, quantize along the z axis, and for simplicity choose **B** in the x-z plane.

The Hamiltonian is then (with E and B in appropriate units; i.e., if $\boldsymbol{\epsilon}$ and $\boldsymbol{\beta}$ are the actual magnetic fields, then $\mathbf{E} = p\boldsymbol{\epsilon}$ and $\mathbf{B} = \mu\boldsymbol{\beta}$, where p is the $n=2$, S-P dipole matrix element and μ is the Bohr magneton)

$$H = \begin{pmatrix} 0 & E & 0 & 0 \\ E & 0 & B_x/\sqrt{2} & B_x/\sqrt{2} \\ 0 & B_x/\sqrt{2} & B_z & 0 \\ 0 & B_x/\sqrt{2} & 0 & -B_z \end{pmatrix}, \qquad (18)$$

with eigenvalues W such that

$$2W^2 = B^2 + E^2 \pm [(B^2 - E^2)^2 + 4E^2B_x^2]^{1/2}. \qquad (19)$$

This level crossing occurs at $B = E$ and $B_x = B\sin\theta = 0$. With $B = E$, $W = \pm E[\cos(\theta/2) \pm \sin(\theta/2)]$, where the two $\pm$ signs are, of course, independent. We would then choose

$$\lambda = 2\sin(\theta/2) \approx \theta \qquad (20)$$

for θ not too large.

The crossing is avoided if $B = E(1+\delta)$ and $\theta \geq \theta_0$.[5] The residual gap, $B_\perp$, is given by

$$B_\perp \simeq E(\delta^2 + \sin^2\theta_0)^{1/2}, \qquad (21)$$

and B_0 by

$$B_0 = E. \qquad (22)$$

The conditions (17) become, with $\theta = t/T$,

$$(\delta^2 + \sin^2\theta_0)^{2/3} \ll \theta_a^{4/3} \ll \frac{1}{ET} \simeq \frac{1}{E}\frac{d\theta}{dt} \ll 1. \qquad (23)$$

The transition amplitude is then given by Eq. (13) with $\int \cos\theta\, d\phi = 0$ and

$$(v_-, \partial v_+/\partial\theta)|_{\theta=\theta_a \approx 0} = -\tfrac{1}{4}.$$

I would like to thank Dan Kleppner, Mike Kash, Bob Silbey, and Michael Berry for helpful discussions. This work was supported in part by funds provided by the U.S. Department of Energy under Contract No. DE-AC02-76ER03069.

[1]See, for example, L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1949), pp. 207–210.

[2]L. D. Landau, Phys. Z. Sowjetunion **2**, 46 (1932).

[3]C. Zener, Proc. Roy. Soc. London A **137**, 696 (1932).

[4]An exact solution of Eq. (8) for $B(t)$ and $\theta(t)$ both linear functions of t and ϕ constant has been obtained by M. Berry (private communication). With $a_+(-\infty) = 1$ and $a_-(-\infty) = 0$, he obtains $|a_+(\infty)|^2 = e^{-p}$ and $|a_-(\infty)|^2 = 1 - e^{-p}$, with p given by Eq. (16).

[5]The following example of a level crossing which will not be avoided was pointed out to me by R. Silbey. In the system described by Eq. (19), two levels go through zero simultaneously for $\theta = \pi/2$ and any E, B, and ϕ. It turns out for this case that the coefficient $(v_-, \partial v_+/\partial\lambda)$ goes to zero as W goes through zero. The transition amplitude a_- goes like $1/B_0T$ [instead of $1/(B_0T)^{1/2}$], with a coefficient which depends on the behavior of the field configuration for $|\lambda| \sim 1$.