Phys 506 lecture 30: Landau-Zener tunneling

1 Introduction

When we studied magnetic resonance, we found the Hamiltonian became

$$\hat{H}_{\text{rot}} = -\hbar(\Omega - \omega)\hat{S}_z - \gamma B_1 \hat{S}_x$$

in the rotating frame, with $B_0 = \frac{\hbar\Omega}{\gamma}$ being the stationary field and B_1 the rotating field at frequency ω. Thus, the spin sees a static field pointing in some direction which it precesses about:

$$B_{\text{eff}} = \frac{\hbar(\Omega - \omega)}{\gamma}\hat{z} + B_1\hat{x}.$$

Suppose we start with the spin up and $\omega \to 0$. As $\omega \to 0$, B_{eff} lies along the $\hat{z}$ direction. As ω increases, B_{eff} rotates until it is in the $-\hat{z}$ direction. If the spin precesses about the B_{eff} axis as ω is slowly increased, it goes from spin up as $\omega \to 0$ to spin down as $\omega \to \infty$.

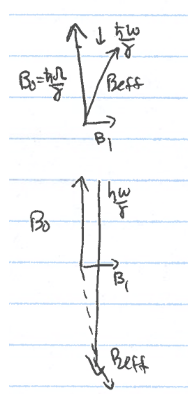


Figure 1: Schematic that shows how B_{eff} aligns along the positive z direction as $\omega to 0$ and the $-z$ direction as $\omega \to \infty$. Hence, if the spin precesses about B_{eff}, and we ramp ω from 0 to ∞, then the spin will start off precessing as a spin up particle, but will end as a s spin down particle. That is is flipped.

2 Landau-Zener problem

Hence, the spin can flip by ramping ω slowly. This type of flip of the spin is often studied as a 2×2 problem called the **Landau-Zener problem**. Here, the Hamiltonian is given by:

$$\hat{H}(t) = \begin{pmatrix} \delta t & V \\ V & -\delta t \end{pmatrix} = \delta t \sigma_z + V \sigma_x$$

and is time-dependent. The instantaneous energy eigenvalues are:

$$(\delta t - E)(-\delta t - E) - V^2 = 0$$

which simplifies to $E^2 = (\delta t)^2 + V^2$ or:

$$E_{\pm}(t) = \pm\sqrt{(\delta t)^2 + V^2}.$$

We can plot this as:

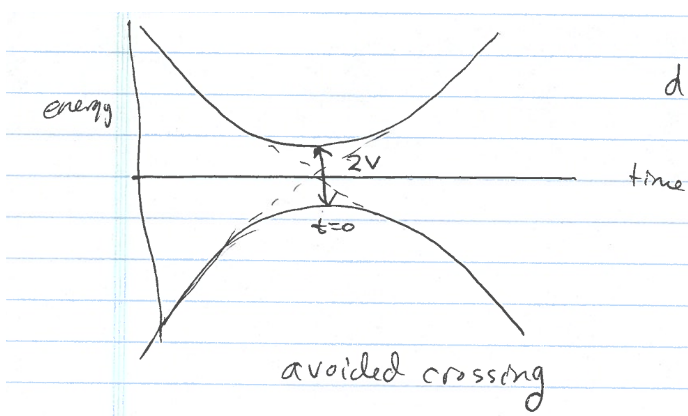


Figure 2:

where the dashed line is for $V = 0$. The eigenfunctions can always be written in the following form:

$$|+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} \quad \text{and} \quad |-\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix},$$

where θ is a function of time. These are the instantaneous eigenvectors. This form always holds since the states are orthonormal. To find $\theta(t)$, we force the eigenvalue equation to work:

$$\hat{H}(t)|+\rangle = E_+(t)|+\rangle,$$

which gives:

$$\delta t \cos\frac{\theta}{2} + V \sin\frac{\theta}{2} = \sqrt{(\delta t)^2 + V^2}\cos\frac{\theta}{2}.$$

Simplifying, we obtain:

$$\tan\frac{\theta}{2} = \frac{\sqrt{(\delta t)^2 + V^2} - \delta t}{V}.$$

Using the trig identity

$$\tan\theta = \tan\left(\frac{\theta}{2} + \frac{\theta}{2}\right) = \frac{\tan\frac{\theta}{2} + \tan\frac{\theta}{2}}{1 - \tan^2\frac{\theta}{2}},$$

We get:

$$\begin{aligned}
\tan\theta &= \frac{2\sqrt{(\delta t)^2 + V^2} - \delta t}{V} \frac{1}{1 - \frac{\left(\sqrt{(\delta t)^2 + V^2} - \delta t\right)^2}{V^2}} \\
&= \frac{2\sqrt{(\delta t)^2 + V^2} - \delta t}{V} \cdot \frac{V^2}{V^2 - ((\delta t)^2 + V^2) - \delta t^2 + 2\delta t\sqrt{(\delta t)^2 + V^2}} \\
&= \frac{2V\sqrt{(\delta t)^2 + V^2} - \delta t}{2\delta t(\sqrt{(\delta t)^2 + V^2} - \delta t)} = \frac{V}{\delta t}
\end{aligned}$$

Thus, we get:

$$\boxed{\tan\theta = \frac{V}{\delta t}.}$$

Note that $\theta = \pi$ at $t \to -\infty$ and runs down to 0 at $t \to \infty$. We also have that $\frac{d\theta}{dt} < 0$ as shown below.

3 Solution for small δ

Now, recall our first attempt at time-dependent problems, in which we started with:

$$|\psi(t)\rangle = \sum_n c_n(t)|n(t)\rangle$$
$$\hat{H}(t)|n(t)\rangle = E_n(t)|n(t)\rangle.$$

And hence, we get the time-dependent Schrödinger equation becomes:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \sum_n \left(i\hbar\frac{dc_n(t)}{dt}|n(t)\rangle + i\hbar c_n(t)\frac{\partial|n(t)\rangle}{\partial t}\right) = \hat{H}(t)|\psi(t)\rangle = \sum_n c_n(t)E_n(t)|n(t)\rangle$$

Let:

$$c_n(t) = \alpha_n(t)\exp\left[-\frac{i}{\hbar}\int^t E_n(t')\,dt'\right].$$

The phase in the exponential is called the dynamical phase. Then, taking the derivative, we find:

$$i\hbar \frac{d}{dt} c_n(t) = i\hbar \frac{d}{dt} \alpha_n(t) e^{-\frac{i}{\hbar}\int^t E_n(t')\,dt'} + \alpha_n(t) e^{-\frac{i}{\hbar}\int^t E_n(t')\,dt'} E_n(t)$$

and we get:

$$i\hbar \sum_n \left[\frac{d}{dt} \alpha_n(t) e^{-\frac{i}{\hbar}\int^t E_n(t')\,dt'} |n(t)\rangle + \alpha_n(t) e^{-\frac{i}{\hbar}\int^t E_n(t')\,dt'} \frac{\partial |n(t)\rangle}{\partial t} \right] = 0.$$

Multiplying by $\langle m(t)| \exp(\frac{i}{\hbar} \int^t E_m(t')dt')$, we obtain:

$$\frac{d}{dt} \alpha_m(t) = -\sum_{n \neq m} \alpha_n(t) e^{-\frac{i}{\hbar}\int^t \left(E_n(t') - E_m(t')\right) dt'} \frac{\langle m(t)| \frac{\partial}{\partial t} |n(t)\rangle}{i\hbar}.$$

For us, we assume the system starts in the lowest energy state $|-\rangle$. If the ramping $\delta \to 0$ in time is slow, the state essentially remains in $|-\rangle$ with the probability of it being in $|+\rangle$ being very small. Hence, $\alpha_-(t) \sim 1$ and $\alpha_+(-\infty) = 0$. The above equation gives (after integrating):

$$\alpha_+(\infty) = -\int_{-\infty}^{\infty} dt\, \alpha_-(t) e^{\frac{i}{\hbar}\int^t (E_-(t') - E_+(t'))dt'} \langle +| \frac{\partial}{\partial t} |-\rangle$$

Since $\langle -| \frac{\partial}{\partial t} |-\rangle = 0$ as we now show:

$$\frac{\partial}{\partial t}|+\rangle = -\frac{d\theta}{dt}\frac{1}{2}\begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix} = -\frac{1}{2}\frac{d\theta}{dt}|-\rangle$$

$$\frac{\partial}{\partial t}|-\rangle = \frac{d\theta}{dt}\frac{1}{2}\begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} = \frac{1}{2}\frac{d\theta}{dt}|+\rangle.$$

Thus:

$$\begin{cases} \langle -|\frac{\partial}{\partial t}|-\rangle = \langle +|\frac{\partial}{\partial t}|+\rangle = 0 \\ \langle +|\frac{\partial}{\partial t}|-\rangle = \frac{1}{2}\frac{d\theta}{dt} \\ \langle -|\frac{\partial}{\partial t}|+\rangle = -\frac{1}{2}\frac{d\theta}{dt}. \end{cases}$$

Therefore:

$$\alpha_+(\infty) \sim -\frac{1}{2}\int_{-\infty}^{\infty} dt \frac{d\theta}{dt} e^{\frac{2i}{\hbar}\int^t \sqrt{(\delta t')^2 + V^2}dt'}.$$

Now recall the equation $\tan\theta(t) = \frac{V}{\delta t}$ and rearrange it to get $\sec^2\theta \frac{d\theta}{dt} = -\frac{V}{(\delta t^2)}$ and solve for $d\theta/dt$ to get:

$$\frac{d\theta}{dt} = -\frac{V}{\delta t^2}\frac{1}{1 + \left(\frac{V}{\delta t}\right)^2} = -\frac{V\delta}{(\delta t)^2 + V^2}$$

Plugging this for our formula for $a_+(\infty)$, we get:

$$\boxed{\alpha_+(\infty) \sim \frac{1}{2}\int_0^{\infty} dt \frac{V\delta}{(\delta t)^2 + V^2} e^{\frac{2i}{\hbar}\int^t \sqrt{(\delta t')^2 + V^2}dt'}}.$$

One can evaluate this using complex analysis to give:

$$\alpha_+(\infty) \sim \frac{\pi}{3} e^{-\pi V^2/\delta}$$

or:

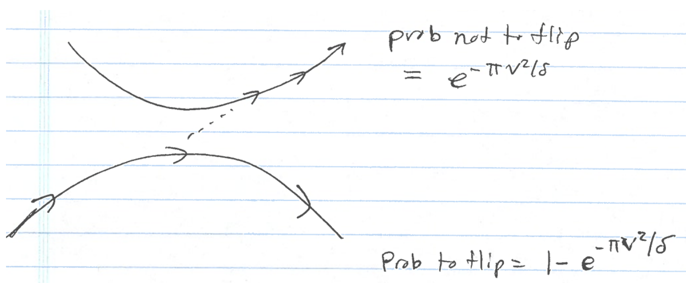
$$P(t) = |\alpha_+(\infty)|^2 = \frac{\pi^2}{9} e^{-\pi V^2/\delta}$$

Note however that this result is only approximate. The correct answer, worked out by Zener using parabolic cylinder functions which solve Weber's equation, yields:

$$P(t) = e^{-\pi V^2/\delta}$$

4 Summary of the results

This holds for all δ, not just in the limit $\delta \to 0$. So as δ is made large, the probability to *not* flip the spin grows. Further note that this is a *nonperturbative* result in δ, so regular time-dependent perturbation theory will not work well. This is essentially because the time-dependent piece of $H(t)$ varies from very large to very small and is not always small. In pictures we have:



For the adiabatic limit, $\delta \to 0$ and we always flip. For the diabatic limit, $\delta \to \infty$ and we never flip. The true case is somewhere in between.

One can also solve the problem numerically, but it has a number of challenges. One needs to evolve over an infinite time range, and the result has significant oscillations that are very slow to damp. Using a combination of ideas can allow you to get accurate results.