When we studied cyclotron resonance, we found the Hamiltonian became

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

in the rotating frame,

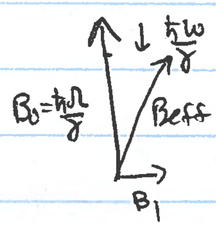
with $B_0 = \dfrac{\hbar\Omega}{\gamma}$ = stationary field

B_1 = rotating field at frequency ω.

So the spin sees a static field pointing in some direction which it precesses about.

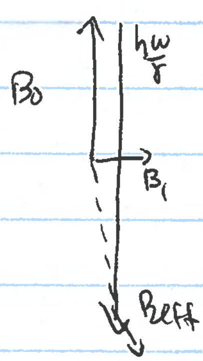
$$B_{eff} = \frac{\hbar(\Omega-\omega)}{\gamma}\,\hat{z} + B_1\,\hat{x}$$

Suppose we start with the spin up and $\omega \to 0$



as $\omega \to 0$ B_{eff} lies along $\hat{z}$ 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 $\omega \to \infty$

$\Rightarrow$ 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

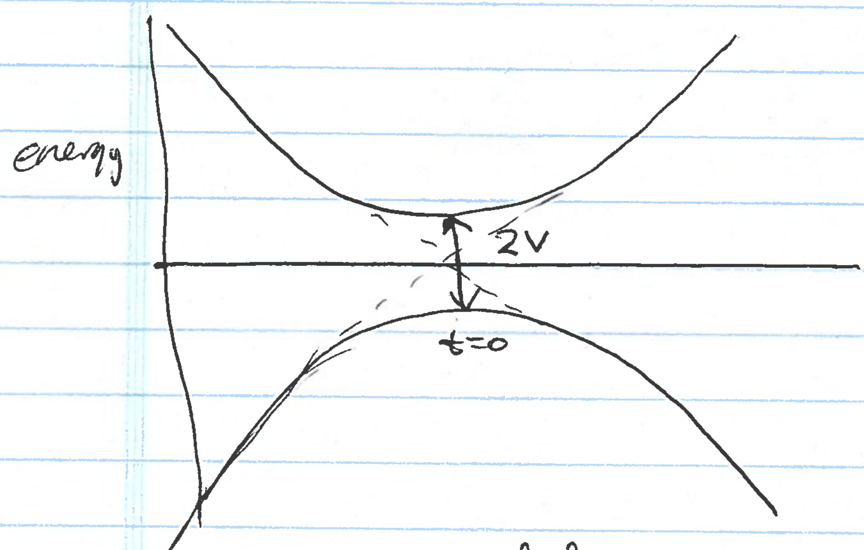
$$\hat{H}(t) = \begin{pmatrix} \delta t & V \\ V & -\delta t \end{pmatrix} = \delta t\, \sigma_z + V \sigma_x$$

and is time dependent.

The instantaneous energy eigenvalues are

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

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



dashed line for $V=0$.

avoided crossing

The eigenfunctions can always be written in the following form

$$|+\rangle = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \end{pmatrix} \qquad |-\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}$$

with θ 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

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

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

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

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

$$= 2\,\frac{\sqrt{(\delta t)^2+V^2} - \delta t}{V}\;\frac{1}{1 - \frac{\left(\sqrt{(\delta t)^2+V^2} - \delta t\right)^2}{V^2}}$$

$$= 2\,\frac{\sqrt{(\delta t)^2+V^2} - \delta t}{V}\;\frac{V^2}{V^2 - (\delta t)^2 - V^2 + 2\delta t\sqrt{(\delta t)^2+V^2} - (\delta t)^2}$$

$$= \frac{2V\left(\sqrt{(\delta t)^2+V^2} - \delta t\right)}{2\delta t\left(\sqrt{(\delta t)^2+V^2} - \delta t\right)} = \frac{V}{\delta t}$$

so we find $\boxed{\tan\theta = \frac{V}{\delta t}}$ Note $\theta=\pi$ at $t=-\infty$ runs down to 0 at $t=\infty$ $d\theta/dt<0$ as shown below.

Recall our first attempt at time-dependent problems

$$|\psi(t)\rangle = \sum_n c_n(t)\,|n(t)\rangle$$

$$\hat{H}(t)\,|n(t)\rangle = E_n(t)\,|n(t)\rangle$$

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \sum_n\left(i\hbar\frac{\partial}{\partial t}c_n(t)\,|n(t)\rangle + i\hbar\, c_n(t)\frac{\partial}{\partial t}|n(t)\rangle\right)$$

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

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

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

and we get

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

multiply by $\langle m(t)|$ to get

$$\boxed{\frac{d}{dt}\alpha_m(t) = -\sum_n \alpha_n(t)\,e^{-\frac{i}{\hbar}\int^t (E_n(t')-E_m(t'))dt'}\langle m(t)|\frac{\partial}{\partial t}|n(t)\rangle}$$

For us, we imagine we start in the lowest energy state $|-\rangle$. If $\delta \to 0$ the ramping in time is very slow. Then one expects that the state essentially remains in $|-\rangle$ with the probability of $|+\rangle$ being small.

So $\alpha_-(t) \sim 1$ and $\alpha_+(-\infty) = 0$

The above equation then gives (after integrating)

$$\alpha_+(\infty) = -\int_{-\infty}^{+\infty} dt \, \underbrace{\alpha_-(t)}_{\sim 1} \, e^{-\frac{i}{\hbar}\int^t (E_-(t') - E_+(t'))dt'} \langle +|\frac{\partial}{\partial t}|-\rangle$$

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

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

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

so $\langle +|\frac{\partial}{\partial t}|+\rangle = \langle -|\frac{\partial}{\partial t}|-\rangle = 0$

$\langle +|\frac{\partial}{\partial t}|-\rangle = \frac{1}{2}\frac{d\theta}{dt}$ $\quad \langle -|\frac{\partial}{\partial t}|+\rangle = -\frac{1}{2}\frac{d\theta}{dt}$

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

But $\tan\theta(t) = \frac{V}{\delta t} \Rightarrow \sec^2\theta \frac{d\theta}{dt} = -\frac{V}{\delta t^2}$

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

So we get

$$\boxed{\alpha_+(\infty) \cong \frac{1}{2}\int_{-\infty}^{+\infty} dt \, \frac{V\delta}{(\delta t)^2+V^2} \, e^{\frac{2i}{\hbar}\int^t \sqrt{(\delta t')^2+V^2}\, dt'}}$$

One can evaluate this using complex analysis to give

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

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

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

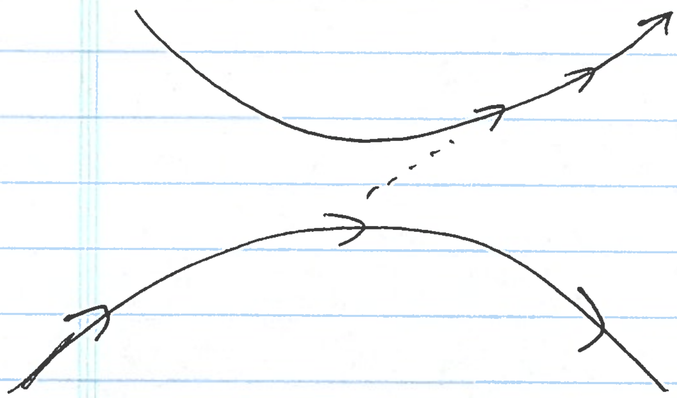
$$\boxed{P(+) = e^{-\pi V^2/\delta}}$$

which holds for all δ, not just the limit $\delta \to 0$.

So as δ is made large, the probability to <u>not</u> flip the spin grows.

Note, this is a <u>nonperturbative</u> 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



prob not to flip $= e^{-\pi V^2/\delta}$

Prob to flip $= 1 - e^{-\pi V^2/\delta}$

For adiabatic limit, $\delta \to 0$ and we always flip

For diabatic limit, $\delta \to \infty$ and we never flip.

True case is somewhere in between.