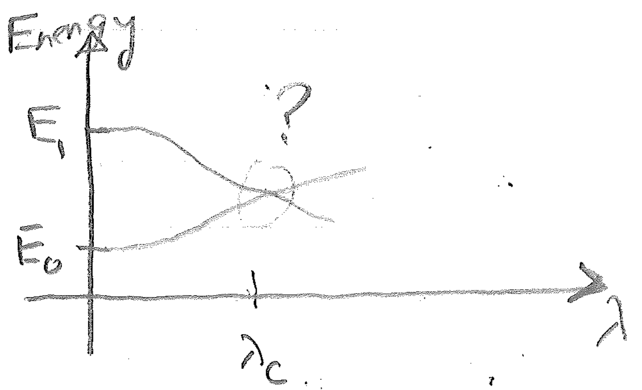
Lecture 6: Degeneracy and Avoided Crossings

An important paradigm in studying the energy spectrum of quantum systems is to see how spectrum varies as a function of some parameter λ

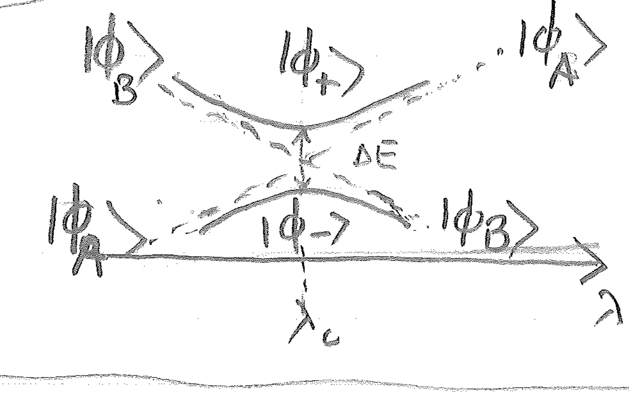
$$\hat{H}(\lambda)|\phi_n(\lambda)\rangle = E_n(\lambda)|\phi_n(\lambda)\rangle$$

Some parameter, such as an external field



We may run into a situation where two previously non-degenerate states are now made degenerate. Do they actually cross?

If $\langle\phi_0|\hat{H}(\lambda_c)|\phi_1\rangle \neq 0$ then from degenerate perturbation theory we know that the degeneracy is broken $\Rightarrow$ the crossing is avoided ("anti-crossing" or "avoided crossing")



Generic behavior @ anti-crossing

As a function of λ two states $|\phi_A\rangle, |\phi_B\rangle$ cross. Due to the interaction they "mix". Right at the crossing point the "character" of eigenstates is neither $|\phi_A\rangle$ nor $|\phi_B\rangle$ but the superposition:

$$|\phi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|\phi_A\rangle \pm e^{i\phi}|\phi_B\rangle\right)$$

the energy gap between $|\phi_+\rangle$ and $|\phi_-\rangle$ depends on a non-zero value for $\langle\phi_A(\lambda_c)|\hat{H}(\lambda_c)|\phi_B(\lambda_c)\rangle$

Two dimensional Hilbert space

The behavior of the crossing of two levels means we can focus our attention on a 2D Hilbert space. All such spaces are isomorphic. The most important example of a 2D Hilbert space is a spin-½ particle $\{|\uparrow\rangle, |\downarrow\rangle\}$. Thus all the important physics at an avoided crossing can be understood in terms of a spin-½ particle in a magnetic field

2D Hilbert space dynamics	$\Longleftrightarrow$	spin-½ particle in a B-field

General Hamiltonian:

Spin magnetic moment $\vec{\mu} = \underbrace{\gamma}_{\text{Gyro-magnetic moment}} \vec{S}$

Spin-$\frac{1}{2}$ $\quad \vec{S} = \frac{\hbar \vec{\sigma}}{2}$

Pauli matrices (representation in $\{|\Uparrow\rangle, |\Downarrow\rangle\}$)

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

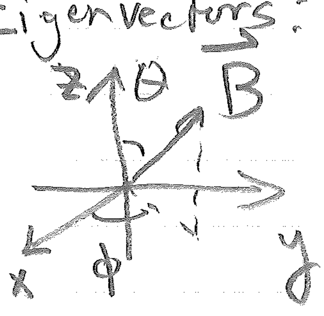
Magnetic interaction:

$$\hat{H} = -\hat{\vec{\mu}} \cdot \vec{B} = +\frac{\hbar \gamma \vec{B} \cdot \vec{\sigma}}{2} \equiv +\frac{\hbar \vec{\Omega}}{2} \cdot \vec{\sigma}$$

"Larmor frequency" $\vec{\Omega} = \gamma \vec{B}$

Eigenvalues $\quad E_{\pm} = \pm \frac{\hbar}{2} |\vec{\Omega}| = \pm \frac{\hbar \gamma}{2} \sqrt{B_x^2 + B_y^2 + B_z^2}$

Eigenvectors: $\quad |\pm\rangle_n$ = spin-up/down along $\frac{\vec{B}}{|\vec{B}|} = \vec{n}$



$$|+\rangle_n = \cos\frac{\theta}{2} |\Uparrow\rangle + \sin\frac{\theta}{2} e^{+i\phi} |\Downarrow\rangle$$

$$|-\rangle_n = \sin\frac{\theta}{2} |\Uparrow\rangle - \cos\frac{\theta}{2} e^{+i\phi} |\Downarrow\rangle$$

$$\tan\theta = \frac{B_z}{\sqrt{B_x^2 + B_y^2}} \qquad \tan\phi = \frac{B_y}{B_x}$$

Example: $|+\rangle_z = |\Uparrow\rangle \qquad |-\rangle_z = |\Downarrow\rangle$

$$|+\rangle_x = \frac{1}{\sqrt{2}}(|\Uparrow\rangle + |\Downarrow\rangle), \quad |-\rangle_x = \frac{1}{\sqrt{2}}(|\Uparrow\rangle - |\Downarrow\rangle)$$

Avoided Crossing as Magnetic Resonance

Consider the following problem.

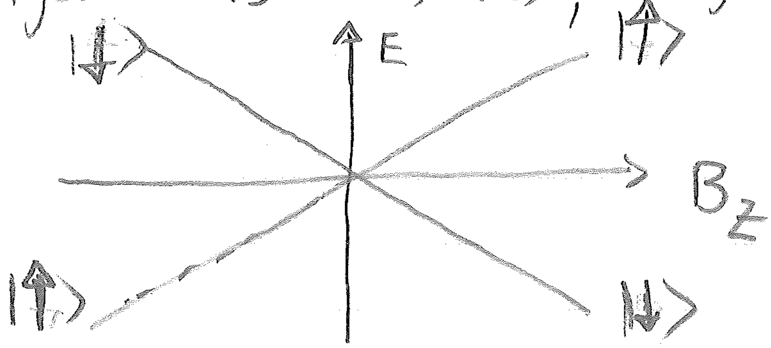
Let $\vec{B}_{total} = B_x \vec{e}_x + B_z \vec{e}_z$

Suppose B_x is fixed and we vary B_z

Consider first the case where $B_x = 0$

$$\Rightarrow \quad \hat{H} = +\frac{\hbar \gamma B_z}{2} \hat{\sigma}_z$$

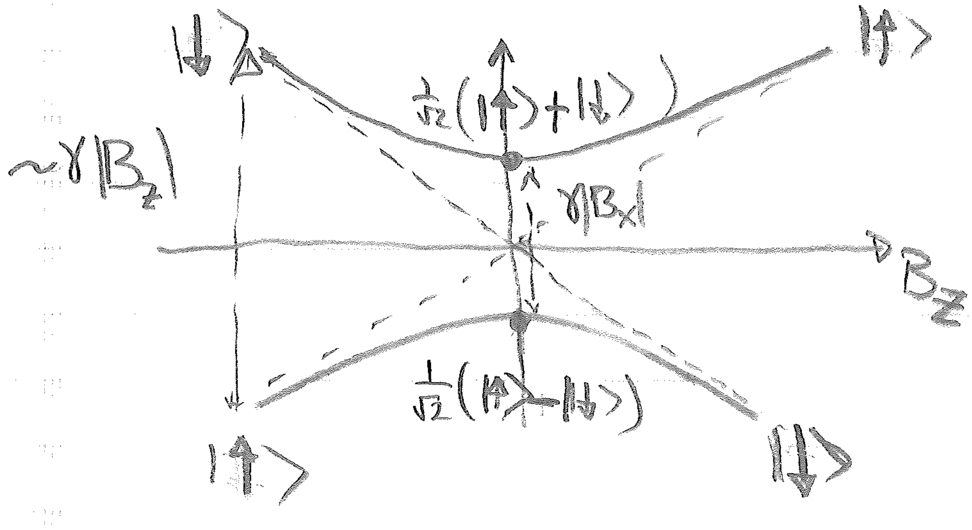
Eigenvectors $|\uparrow\rangle, |\downarrow\rangle$, Eigenvalues $\pm \frac{\hbar \gamma B_z}{2}$



Cross @ $B_z = 0$

Now include $B_x \neq 0$. For $|B_z| \gg |B_x|$ the eigenstates are approximately $|\uparrow\rangle, |\downarrow\rangle$,

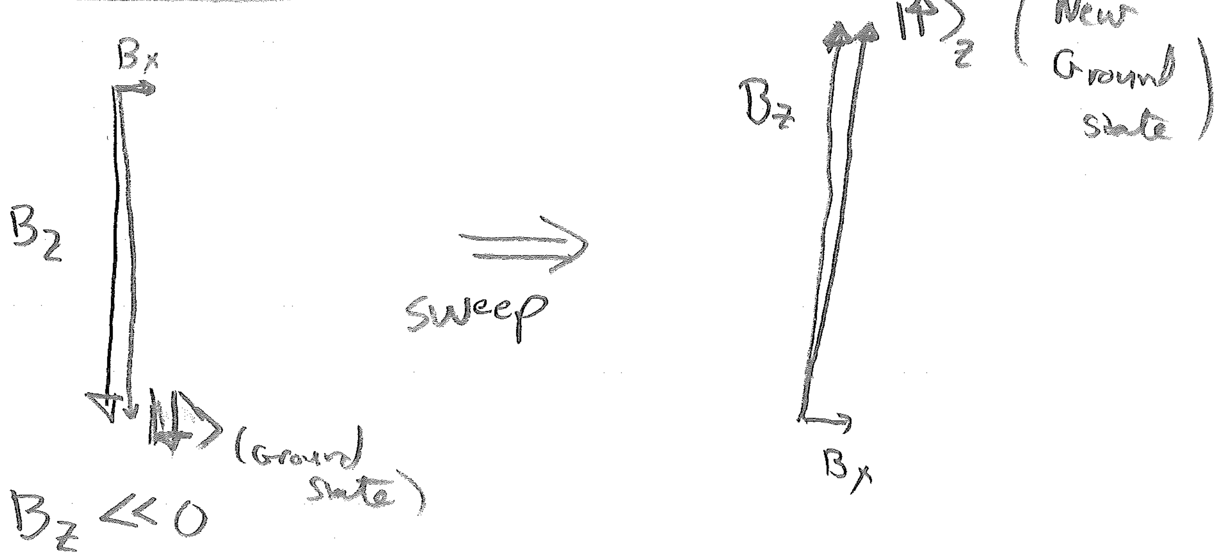
But @ $B_z = 0$, eigenstates at $|\pm\rangle = \frac{|\uparrow\rangle \pm |\downarrow\rangle}{\sqrt{2}}$



At degeneracy state states "mix" to form superposition of "bare states"

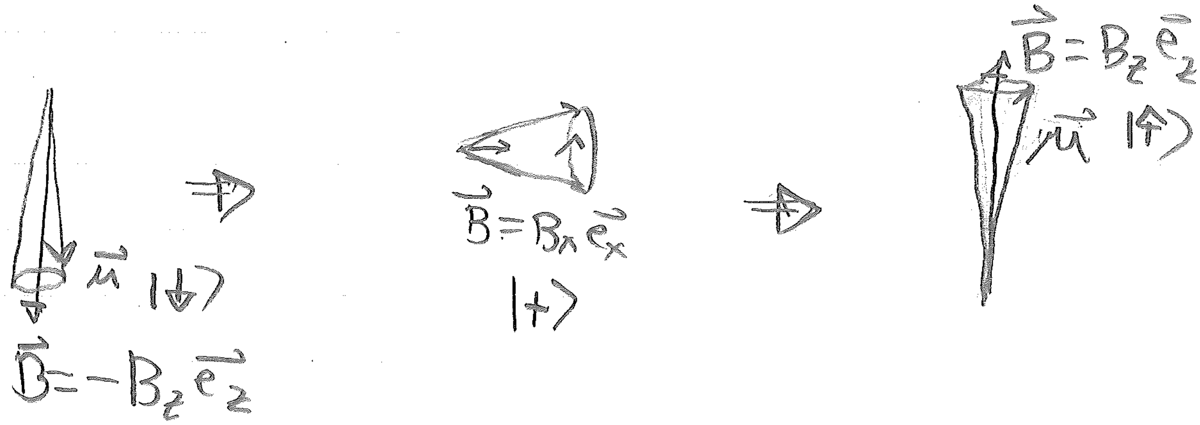
Note: The "nature" of the eigenstate flips as we move through the avoided crossing

Geometric picture:



Adiabatic evolution:

If we change $B_z(t)$ (as function of time) we can adiabatically bring the spin from $|\Downarrow\rangle$ to $|\Uparrow\rangle$

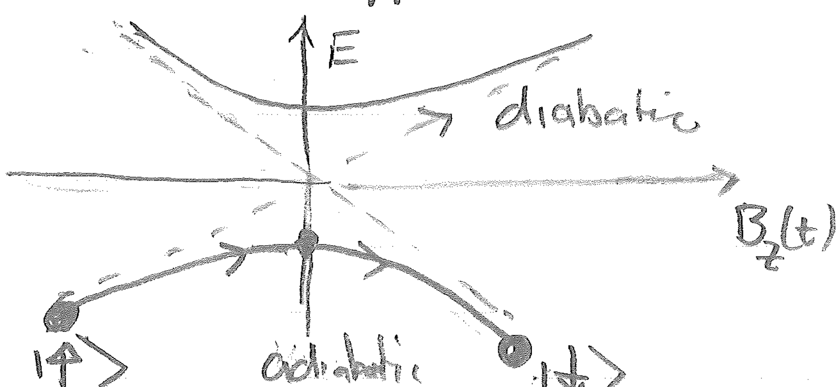


"Adiabatic following of Larmor precession"

Quantum mechanically:

Adiabatic theorem: Given $\hat{H}(\lambda(t))$. If $\lambda(t)$ changes "slowly enough", then if the system starts in an eigenstate is stays in that instantaneous eigenstate:

$$\text{If } |\psi(0)\rangle = |\phi_n(\lambda(0))\rangle \Rightarrow |\psi(t)\rangle \approx |\phi_n(\lambda(t))\rangle$$



If the change is made too quickly, we can apply the "sudden approximation", in which case the state does not change $\Rightarrow$ "diabatic"

Using the Larmor precession picture we see the critical condition is that the rate of change of $\vec{B}$ be slow compared to the rate at which the magnetic moment presesses

$$\frac{\frac{d}{dt}|\vec{B}|}{|\vec{B}|} \ll \gamma|\vec{B}|$$

Since $|\vec{B}|$ is smallest @ $B_z = 0$, we require

$$\frac{\left|\frac{dB_z}{dt}\right|_{B_z=0}}{|B_x|} \ll \gamma |B_x|$$

or $\boxed{\left|\frac{d\,\gamma B_z}{dt}\right|_{B_z=0} \ll \left(\gamma |B_x|\right)^2}$ Condition for Adiabaticity

<u>Mapping of two-state system to spin-1/2</u>

Let us consider a Hamiltonian operator restricted to ~~a~~ the subspace spanned by two orthogonal states $|\phi_a\rangle$ and $|\phi_b\rangle$. In this basis $\hat{H}$ is a 2X2 matrix:

$$\hat{H} \doteq \begin{bmatrix} E_a^{(0)} & H_{ab} \\ H_{ab}^{*} & E_b^{(0)} \end{bmatrix}$$

$$= \frac{E_a^{(0)}+E_b^{(0)}}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{E_a^{(0)}-E_b^{(0)}}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$+ \mathrm{Re}(H_{ab})\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \mathrm{Im}(H_{ab})\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

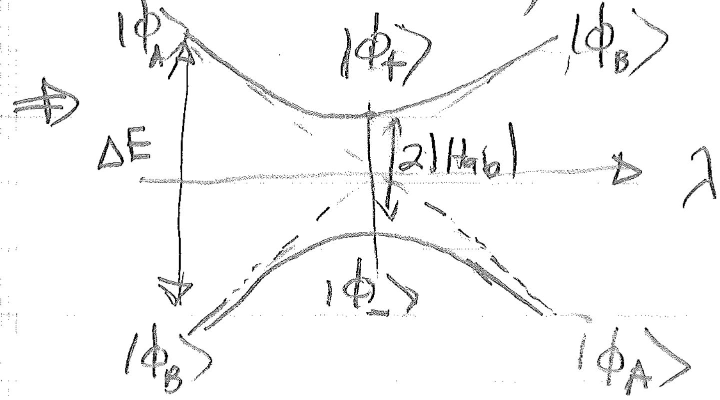
$\Rightarrow \quad \hat{H} = E\,\hat{\mathbb{1}} + \frac{\hbar\vec{\Omega}\cdot\vec{\sigma}}{2}$ where (next page)

$$\bar{E} = (E_a + E_b)/2$$

$$\hbar\Omega_z = E_a^{(0)} - E_b^{(0)}$$

$$\hbar\Omega_x = 2\,\mathrm{Re}(H_{ab}), \quad \hbar\Omega_z = 2\,\mathrm{Im}(H_{ab})$$

$\Rightarrow$



$$|\phi_\pm\rangle = \frac{|\phi_A\rangle \pm e^{i\varphi}|\phi_B\rangle}{\sqrt{2}}$$

$$\varphi = \tan^{-1}\left(\frac{\mathrm{Im}(H_{ab})}{\mathrm{Re}(H_{ab})}\right)$$

Adiabatic Transfer

We mentioned the "adiabatic theorem" of quantum mechanics. Formally, we want to solve the "initial value problem" of time-evolution by the Schrödinger eq.

$$\frac{\partial}{\partial t}|\Psi(t)\rangle = -\frac{i}{\hbar}\hat{H}[\lambda(t)]\,|\Psi(t)\rangle$$

$$\text{with} \quad |\Psi(0)\rangle = |\phi_a(\lambda(0))\rangle$$

In other words, $\hat{H}$ is a function of time through the time-dependent change in the parameter, $\lambda(t)$. At $t=0$ the state is an eigenstate of the initial Hamiltonian. We then want to find the state at a later time.

(Next Page)

According to the adiabatic theorem

$$|\psi(t)\rangle \approx |\phi_a(\lambda(t))\rangle$$

if for the nearest level b

$$\left| \frac{\langle \phi_b | \frac{\partial \hat{H}}{\partial t} | \phi_a \rangle}{(E_a - E_b)} \right| \ll \frac{|E_a - E_b|}{\hbar}$$

transition rate

energy gap/$\hbar$

Consider again the problem of spin in a B-field

$$\hat{H} = \gamma \hbar (B_x \hat{\sigma}_x + B_z(t) \hat{\sigma}_z)$$

Minimum gap when $B_z(t_c) = 0$

There $E_a - E_b = \hbar \gamma |B_x|$

Condition for adiabaticity:

$$\left| \frac{\partial}{\partial t} \gamma B_z(t_c) \right| \ll |\gamma B_x|^2$$

Just as before

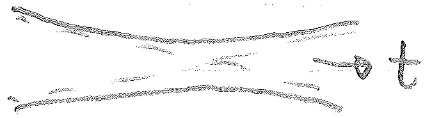
Connecting this to an arbitrary 2-state crossing, the condition for adiabaticity

$$\frac{1}{\hbar}\frac{\partial}{\partial t}\left(E_a^{(0)}(t_c) - E_b^{(0)}(t_c)\right) << |2 H_{ab}|^2$$

Define <u>adiabaticity parameter</u>

$$\boxed{A \equiv \frac{|2 H_{ab}|^2}{\frac{1}{\hbar}\left|\frac{d}{dt}E_a^{(0)} - \frac{d}{dt}E_b^{(0)}\right|} >> 1}$$

The parameter, A, depends on the strength of the coupling between $|\phi_a^{(0)}\rangle$ and $|\phi_b^{(0)}\rangle$ and the difference in the derivatives of the (bare) energy levels w.r.t. time



easilly adiabatic

tough to stay adiabatic

Landau and Zener studied the probability to stay adiabatic as we move through the crossing under a special case $\Rightarrow$ Landau-Zener Crossing

Landau-Zener

Consider a spin with B_x constant
$B_z = \alpha t$ (linear sweep)

At time $t \to -\infty$ $|\psi\rangle \to |\downarrow\rangle$

The diabatic "transfer probability"

$$P_{diab} = |C_\downarrow(+\infty)|^2$$

Solution: Zener, Proc. Roy. Soc. London A.
vol 37, page 396 (193)

$$|C_\uparrow(t)|^2 = A e^{-\frac{\pi}{2}A} \left| D_{iA+1}\left(\sqrt{\alpha}\, t\, e^{\frac{i3\pi}{4}}\right)\right|^2$$

Parabolic cylindrical fnct

$$A = \frac{(\gamma B_x)^2}{\gamma\alpha} = \frac{|\langle\downarrow| H |\uparrow\rangle|^2}{\left|\frac{1}{\hbar}\frac{d}{dt}\left(E_\uparrow^{(0)} - E_\downarrow^{(0)}\right)\right|}$$

In the limit $t \to \infty$

$$\boxed{P_{diab} = e^{-2\pi A}}$$

We see that if $2\pi A \gg 1$, it is exponentially unlikely for the system to cross diabatically.

Landau was the first to study this.
The dynamics near the crossing between two-levels is know as "Landau-Zener crossing".

Since the probability to go from one level to the other is exponentially small when $2\pi A \gg 1$, such dynamics are known as

"<u>Landau-Zener tunnelling</u>"