Physics 581: Open Quantum Systems

Lecture 3: Magnetic Resonance and Rabi flopping

All coherent spectroscopy has at its heart, spin magnetic resonance.
Father of the subject: I.I. Rabi, 1939 measured hyperfine structure & Lamb shift.

The problem of manipulating 2-levels of a quantum system:

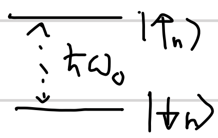
General form of the Hamiltonian, like any operator on $\mathbb{C}^2$

$$\hat{H} = A\hat{\mathbb{1}} + \vec{B}\cdot\hat{\vec{\sigma}} \equiv \text{spin-}\tfrac{1}{2} \text{ in a magnetic field}$$

"Zeeman" Hamiltonian (static $\vec{B}_0$): $\hat{H}_0 = -\hat{\vec{\mu}}\cdot\vec{B}_0$, $\quad \hat{\vec{\mu}} \equiv \gamma\vec{S}$, $\quad \gamma$: Gyromagnetic ration $= -2\mu_B$ (electron)

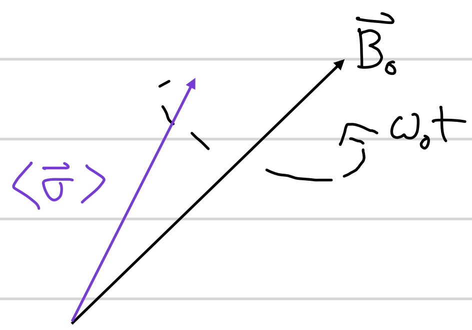
$$\Rightarrow \hat{H}_0 = \frac{\hbar\vec{\omega}_0}{2}\cdot\hat{\vec{\sigma}}, \quad \vec{\omega}_0 = -\gamma\vec{B}_0 \qquad \left(\omega_0 = |\gamma|\frac{B_0}{\hbar} = \frac{2\mu_B B_0}{\hbar} \text{ for electron}\right)$$

Eigenstates $|\uparrow_n\rangle, |\downarrow_n\rangle$: $\hat{H}_0|\updownarrow_n\rangle = \pm\frac{\hbar\omega_0}{2}|\updownarrow_n\rangle$



(Zeeman Splitting)

Unitary evolution: $U(t) = e^{-i\frac{\omega_0 t}{2}\hat{\sigma}_n} \equiv$ Larmor precession around $\vec{e}_n = \frac{\vec{B}_0}{|\vec{B}_0|}$.



Gyroscopic precession.

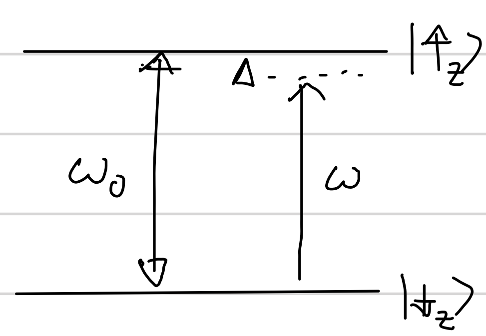
A spin in a magnetic field will precess and $\vec{B}_0$ at a rate $\omega_0 = |\gamma| B_0$. If the spin is aligned or anti-aligned it is in a "stationary state."

Magnetic Resonance

- Apply a strong magnetic field $\vec{B}_0$ along some axis: Defines the "quantization axis" z: $\quad \vec{B}_0 \equiv B_{\parallel}\, \vec{e}_z$

$$\hat{H}_0 = -\hat{\vec{\mu}} \cdot \vec{B}_0 = \frac{\hbar\omega_0}{2}\hat{\sigma}_z \qquad \omega_0 = |\gamma| B_0$$

- "Drive" the system with time dependent interaction, $\vec{B}_{int}(t)$, oscillating near resonance, $\quad \omega$ near ω_0



$$\hat{H}_{int}(t) = \hat{H}^{(+)} e^{-i\omega t} + \hat{H}^{(-)} e^{i\omega t}$$

Having decomposed the interaction Hamiltonian into its positive and negative frequency components. We recall, from time-dependent perturbation theory the the positive (negative) frequency components lead to absorption (emission).

From Fermi's Golden Rule: Rate of absorption $= \frac{2\pi}{\hbar^2} |\langle \uparrow_z | \hat{H}^{(+)} | \downarrow_z \rangle|^2 \mathcal{D}(\omega) \leftarrow$ Density of states at ω.

This is <u>not</u> the whole story. It is applicable for weak interaction and for

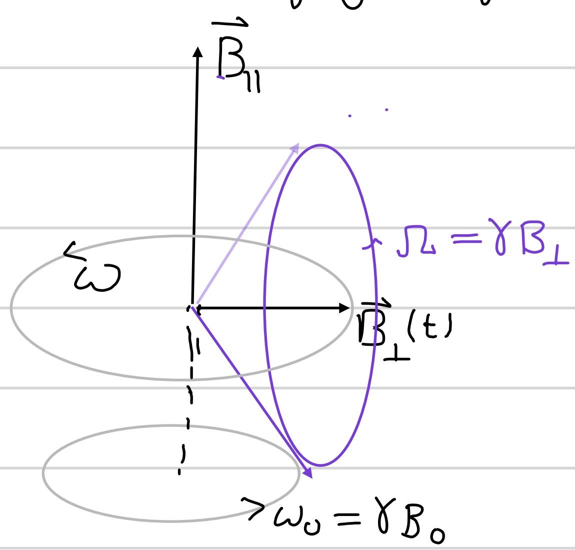
(i) Incoherent broad-band source (e.g. natural source of radiation)

and/or (ii) The final state has a "broad" linewidth

For an isolated two-level system, driven by a quasimonochromatic source, we need to go beyond time-dependent perturbation theory. There is new important physics — coherent unitary evolution!

Rabi-Oscillations

To drive the spin from $|\downarrow_z\rangle \Rightarrow |\uparrow_z\rangle$, the perturbing Hamiltonian must have off-diagonal matrix elements $\Rightarrow$ $\hat{H}_{int}$ must have term $\propto \hat{\sigma}_x$ and/or $\hat{\sigma}_y$ $\Rightarrow$ $\vec{B}_{int}(t)$ in x-y plane. To achieve resonance, consider the following geometry:



In the presence of the static field $\vec{B}_{\parallel}$, the spin precesses at freq $\omega_0 = \gamma B_{\parallel}$. By applying a transverse field that rotates in the x-y plane, we can achieve perfect resonance, flipping the spin from $|\downarrow_z\rangle$ to $|\uparrow_z\rangle$.

Mathematically, we seek the solution to the time-dependent Schrödinger equation:

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -\frac{i}{\hbar}\hat{H}(t)|\psi(t)\rangle, \quad \hat{H}(t) = \hat{H}_0 + \hat{H}_{int}(t),$$

$$\hat{H}_0 = -\hat{\vec{\mu}}\cdot\vec{B}_{\parallel} = \frac{\hbar\omega_0}{2}\hat{\sigma}_z, \quad \hat{H}_{int} = -\hat{\vec{\mu}}\cdot\vec{B}_{\perp}(t) = -\frac{\hbar\gamma B_x(t)}{2}\hat{\sigma}_x - \frac{\hbar\gamma B_y(t)}{2}\hat{\sigma}_y$$

Note: $[\hat{H}(t_1), \hat{H}(t_2)] \neq 0 \Rightarrow |\psi(t)\rangle = \mathcal{T}\left[e^{-\frac{i}{\hbar}\int_0^t \hat{H}(t')dt'}\right]$: Time-ordered exponential. No closed form solution

For the specific case of a rotating transverse field of constant amplitude:
$\vec{B}_{\perp}(t) = B_{\perp}\left(\cos(\omega t+\phi)\vec{e}_x + \sin(\omega t+\phi)\vec{e}_y\right) \Rightarrow$

$$\hat{H}_{int}(t) = \underbrace{-\frac{\hbar\gamma B_{\perp}}{2}}\left(\cos(\omega t+\phi)\hat{\sigma}_x + \sin(\omega t+\phi)\hat{\sigma}_y\right) = \frac{\hbar\Omega_{\perp}}{2}\left(e^{-i(\omega t+\phi)}\hat{\sigma}_+ + e^{i(\omega t+\phi)}\hat{\sigma}_-\right)$$

$\equiv \Omega$ the "Rabi frequency" $= -\gamma B_{\perp}$ (taking $\gamma < 0$)

From the geometrical picture, we see that if we go to a "rotating frame" co-rotating with the rotating field $\vec{B}_\perp(t)$, then in that frame, the Hamiltonian is static, and we can trivially integrate the Schrödinger equation.

Going to the rotating frame

We accomplish a frame transformation in quantum mechanics by making a unitary transformation. In the case of magnetic spin resonance, this is a physical rotation; in other cases (as we will see) the frame is abstract, and going to a rotating frame just means shifting the eigenvalues of the Hamiltonian, e.g. the familiar "interaction picture" in time-dependent perturbations.

Here, we move to rotating frame by rotation about the z-axis by angle ωt, where ω is the frequency of the rotating field $\vec{B}_\perp(t)$: $\hat{U}_{RF}(t) = e^{-i\frac{\omega t}{2}\hat{\sigma}_z}$

Observables in the rotating frame: $\hat{O}_{RF}(t) = \hat{U}^\dagger_{RF}(t)\,\underbrace{\hat{O}_S(t)}_{\text{Schröndinger Picture}}\,\hat{U}_{RF}(t)$

States in the rotating frame: $|\psi_{RF}(t)\rangle = \hat{U}^\dagger_{RF}(t)\,|\psi_S(t)\rangle$, so $\langle\psi_S(t)|\hat{O}_S(t)|\psi_S(t)\rangle = \langle\psi_{RF}(t)|\hat{O}_{RF}(t)|\psi_{RF}(t)\rangle$.

Schrödinger Eqn in the rotating frame:

$$\frac{\hbar}{-i}\frac{\partial}{\partial t}|\psi_{RF}(t)\rangle = \frac{\hbar}{-i}\frac{\partial}{\partial t}\left[\hat{U}^\dagger_{RF}(t)\,|\psi_S(t)\rangle\right] = \hat{U}^\dagger_{RF}\left[\frac{\hbar}{-i}\frac{\partial}{\partial t}|\psi_S(t)\rangle\right] + \left[\frac{\hbar}{-i}\frac{\partial \hat{U}^\dagger_{RF}}{\partial t}\right]|\psi_S(t)\rangle$$

$$\Rightarrow \frac{\hbar}{-i}\frac{\partial}{\partial t}|\psi_{RF}(t)\rangle = \left[\hat{U}^\dagger_{RF}\hat{H}_S(t) + \frac{\hbar}{-i}\frac{\partial \hat{U}^\dagger_{RF}}{\partial t}\right]|\psi_S\rangle = \underbrace{\left[\hat{U}^\dagger_{RF}\hat{H}_S\hat{U}_{RF} + \frac{\hbar}{-i}\frac{\partial \hat{U}^\dagger_{RF}}{\partial t}\hat{U}_{RF}\right]}_{\hat{H}_{RF}}|\psi_{RF}\rangle$$

$\Rightarrow$ New Hamiltonian in the rotating frame

$$\hat{H}_{RF} = \hat{U}^\dagger_{RF}\hat{H}_S\hat{U}_{RF} - \frac{\hbar\omega}{2}\hat{\sigma}_z\,, \qquad \hat{H}_S = \frac{\hbar\omega_0}{2}\hat{\sigma}_z + \hbar\Omega\left(e^{-i(\omega t+\phi)}\hat{\sigma}_+ + e^{i(\omega t+\phi)}\hat{\sigma}_-\right).$$

$$\Rightarrow \hat{H}_{RF} = -\hbar\frac{(\omega-\omega_0)}{2}\hat{\sigma}_z + \hbar\Omega\left(e^{-i(\omega t+\phi)}\hat{U}^\dagger_{RF}\hat{\sigma}_+\hat{U}_{RF} + e^{i(\omega t+\phi)}\hat{U}^\dagger_{RF}\hat{\sigma}_-\hat{U}_{RF}\right)$$

I leave it as a simple exercise to show: $U_{RF}^{\dagger}\hat{\sigma}_{\pm}U_{RF} = e^{\pm i\omega t}\hat{\sigma}_{\pm}$

$$\Rightarrow \boxed{\hat{H}_{RF} = -\frac{\hbar\Delta}{2}\hat{\sigma}_z + \frac{\hbar\Omega}{2}\left(e^{-i\phi}\hat{\sigma}_+ + e^{+i\phi}\hat{\sigma}_-\right) = -\frac{\hbar\Delta}{2}\hat{\sigma}_z + \frac{\hbar\Omega}{2}\left(\cos\phi\,\hat{\sigma}_x + \sin\phi\,\hat{\sigma}_y\right)}$$

$\Delta = \omega - \omega_0$ (detuning), $\quad \Omega = \gamma B_\perp$ (Rabi frequency)

$\hat{H}_{RF}$ is time-independent as expected!

$$\hat{H}_{RF} = \frac{\hbar\vec{\Omega}_{tot}\cdot\hat{\vec{\sigma}}}{2}, \quad \vec{\Omega}_{tot} = -\Delta\vec{e}_z + \Omega\,\vec{e}_\perp(\phi) \quad (\vec{e}_\perp = \vec{e}_x\cos\phi + \vec{e}_y\sin\phi)$$

General solution: $|\psi_{RF}(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_{RF}t}|\psi_{RF}(0)\rangle = \hat{U}_{Rabi}(t)|\psi_{RF}(0)\rangle$

$\hat{U}_{Rabi} = e^{-i\frac{\vec{\Omega}_{tot}t}{2}\cdot\hat{\vec{\sigma}}}$: Rotation on the Bloch sphere

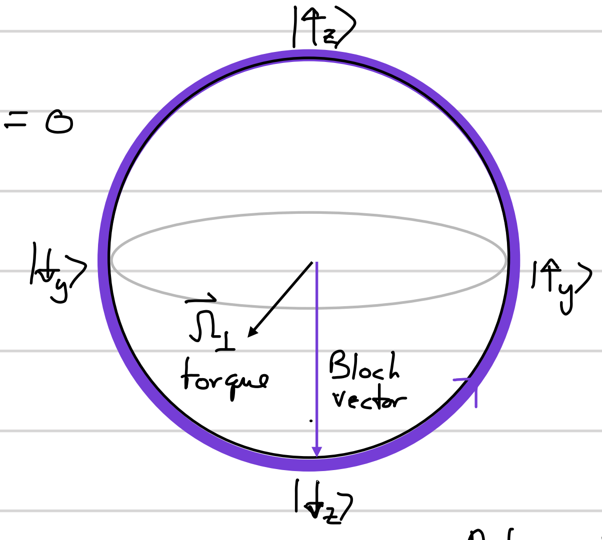
"Generalized Rabi frequency": $\Omega_{tot} = |\vec{\Omega}_{tot}| = \sqrt{\Omega^2 + \Delta^2}$

axis of rotation $\vec{e}_a = \frac{\vec{\Omega}_{tot}}{|\vec{\Omega}_{tot}|} = \frac{-\Delta}{\Omega_{tot}}\vec{e}_z + \frac{\Omega}{\Omega_{tot}}\vec{e}_\perp(\phi)$

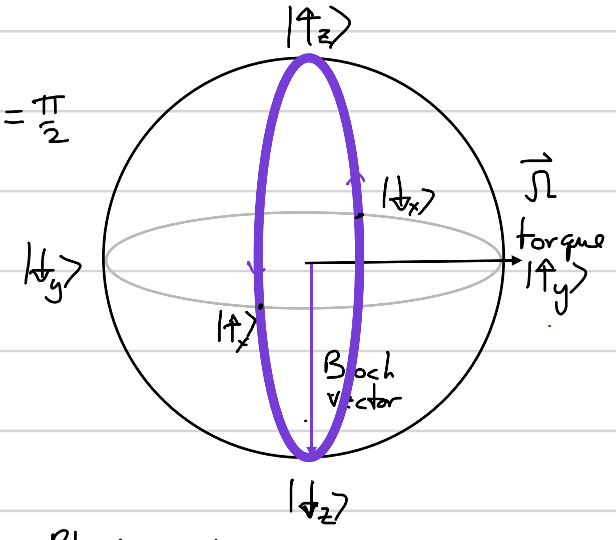
Consider the case $\Delta = 0$ (on resonance)

$$\hat{H}_{RF} = \frac{\hbar\Omega}{2}\vec{e}_\perp(\phi)\cdot\hat{\vec{\sigma}} = \frac{\hbar\Omega}{2}\left(\cos\phi\,\hat{\sigma}_x + \sin\phi\,\hat{\sigma}_y\right)$$

$\phi = 0$



$\phi = \frac{\pi}{2}$



Rabi rotations on Bloch sphere.

On resonance the Bloch vector precesses from north to south pole about an axis depending on ϕ.

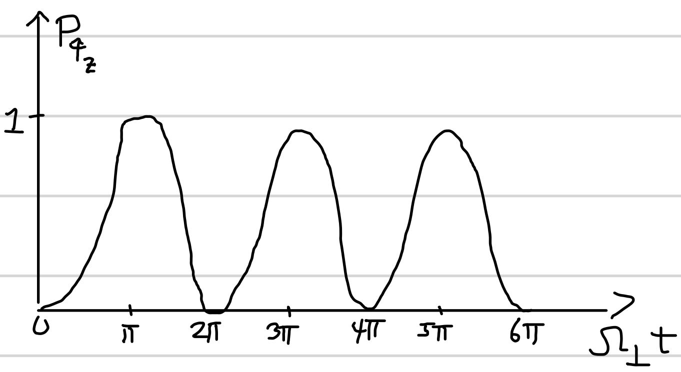
Written in terms of the Quantum evolution in the rotating frame: $|\psi_{RF}(t)\rangle = \hat{U}_{Rabi}\,|\downarrow_z\rangle$

$$\hat{U}_{Rabi} = e^{-i\vec{\Omega}_{tot}t\cdot\frac{\hat{\vec{\sigma}}}{2}} = \cos\left(\frac{\Omega_{tot}t}{2}\right)\hat{\mathbb{1}} - i\sin\left(\frac{\Omega_{tot}t}{2}\right)\vec{e}_a\cdot\hat{\vec{\sigma}}$$

$$= \cos\left(\frac{\Omega_{tot}t}{2}\right)\hat{\mathbb{1}} - i\sin\left(\frac{\Omega_{tot}t}{2}\right)\left[-\frac{\Delta}{\Omega_{tot}}\hat{\sigma}_z + \frac{\Omega}{\Omega_{tot}}\left(e^{-i\phi}\hat{\sigma}_+ + e^{+i\phi}\hat{\sigma}_-\right)\right]$$

On resonance $|\psi_{RF}(t)\rangle = \hat{U}_{Rabi}|\downarrow_z\rangle = \cos\left(\frac{\Omega_{tot}t}{2}\right)|\downarrow_z\rangle - i e^{-i\phi}\sin\left(\frac{\Omega_{tot}t}{2}\right)|\uparrow_z\rangle$

$$P_{\uparrow_z}(t) = |\langle\uparrow_z|\psi_{RF}(t)\rangle|^2 = \sin^2\left(\frac{\Omega t}{2}\right) = \frac{1+\cos(\Omega t)}{2}$$



Rabi flopping!
Population oscillates from $|\downarrow_z\rangle$ to $|\uparrow_z\rangle$.

Ex: "π-pulse", $\Omega_\perp t = \pi \Rightarrow |\psi_{RF}(\frac{\pi}{\Omega})\rangle = -ie^{-i\phi}|\uparrow_z\rangle \equiv |\uparrow_z\rangle$

A π-pulse flips spin-down to spin-up. It represents "perfect absorption". But this is not the full story. For suppose we stopped the pulse half-way, i.e. $\Omega t = \frac{\pi}{2}$.

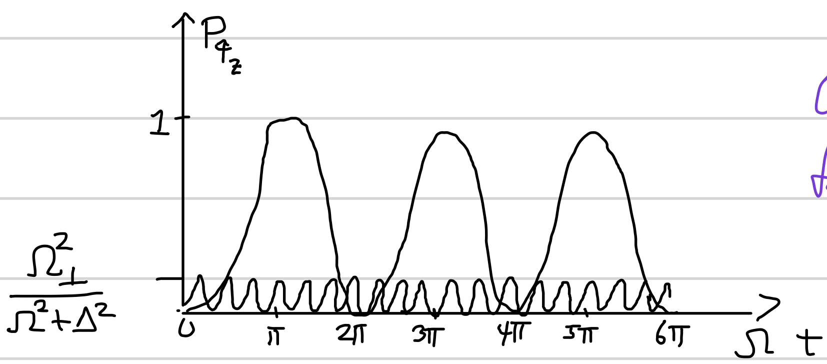
Ex: "$\frac{\pi}{2}$-pulse", $\Omega_\perp t = \frac{\pi}{2} \Rightarrow |\psi_{RF}(\frac{\pi}{2\Omega})\rangle = \frac{1}{\sqrt{2}}\left(|\downarrow_z\rangle - ie^{-i\phi}|\uparrow_z\rangle\right) = \frac{-ie^{-i\phi}}{\sqrt{2}}\left(|\uparrow_z\rangle + ie^{i\phi}|\downarrow_z\rangle\right)$

⇒ A $\frac{\pi}{2}$-pulse of magnetic energy acting on $|\downarrow_z\rangle$ creates a 50-50 superposition of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$ which a phase between them that depends on the phase of the applied oscillator. An important point is that the evolution is coherent. That is, at all stages of the evolution, the spin is in a coherent superposition of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$. Stopping the coherent evolution half wave from spin-up to spin down leaves the system in a 50-50 superposition

Note: For a 2π-pulse, $|\psi(\frac{2\pi}{\Omega})\rangle = -|\downarrow_z\rangle$. The accumulation of the phase -1 has no physical effect on a spin-½ state. But it reflects the difference between SU(2) rotations and SO(3) rotations in Euclidean 3D space.

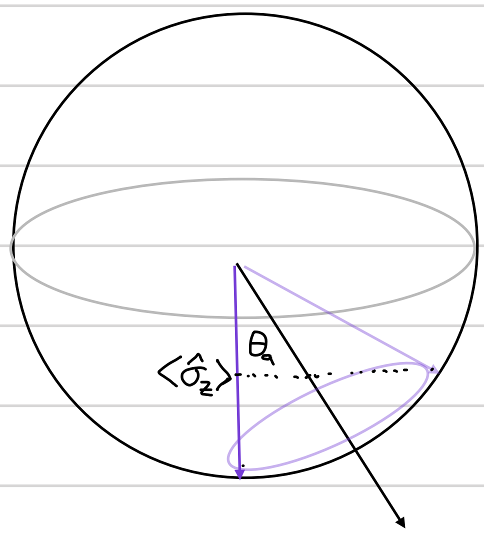
General Rabi Solution: $|\psi_{RF}(t)\rangle = \hat{U}_{Rabi}|\psi(0)\rangle$, with $|\psi(0)\rangle = |\downarrow_z\rangle$

$$\boxed{\begin{aligned} \Rightarrow |\psi_{RF}(t)\rangle &= \left[\cos\left(\frac{\Omega_{tot}t}{2}\right) + i\frac{\Delta}{\Omega_{tot}}\sin\left(\frac{\Omega_{tot}t}{2}\right)\right]|\downarrow_z\rangle + \left[-ie^{-i\phi}\frac{\Omega}{\Omega_{tot}}\sin\left(\frac{\Omega_{tot}t}{2}\right)\right]|\uparrow_z\rangle \\ P_{\uparrow_z}(t) = |\langle\uparrow_z|\psi_{RF}(t)\rangle|^2 &= \frac{\Omega^2}{\Omega_{tot}^2}\sin^2\left(\frac{\Omega_{tot}t}{2}\right) = \frac{\Omega^2}{\Omega^2+\Delta^2}\sin^2\left(\frac{\Omega_{tot}t}{2}\right) \end{aligned}}$$



Off resonance, there is never unit probability for the spin to go from $\downarrow_z \Rightarrow \uparrow_z$.
The probability amplitude also oscillates faster @ $\Omega_{tot} = \sqrt{\Omega^2+\Delta^2}$

Off-Resonance Bloch Sphere Picture



$\vec{\Omega}_{tot} = -\Delta\vec{e}_z + \Omega\,\vec{e}_\perp$

The angle the torque axis with the $-z$ axis $\tan\theta_a = \frac{\Omega}{-\Delta}$

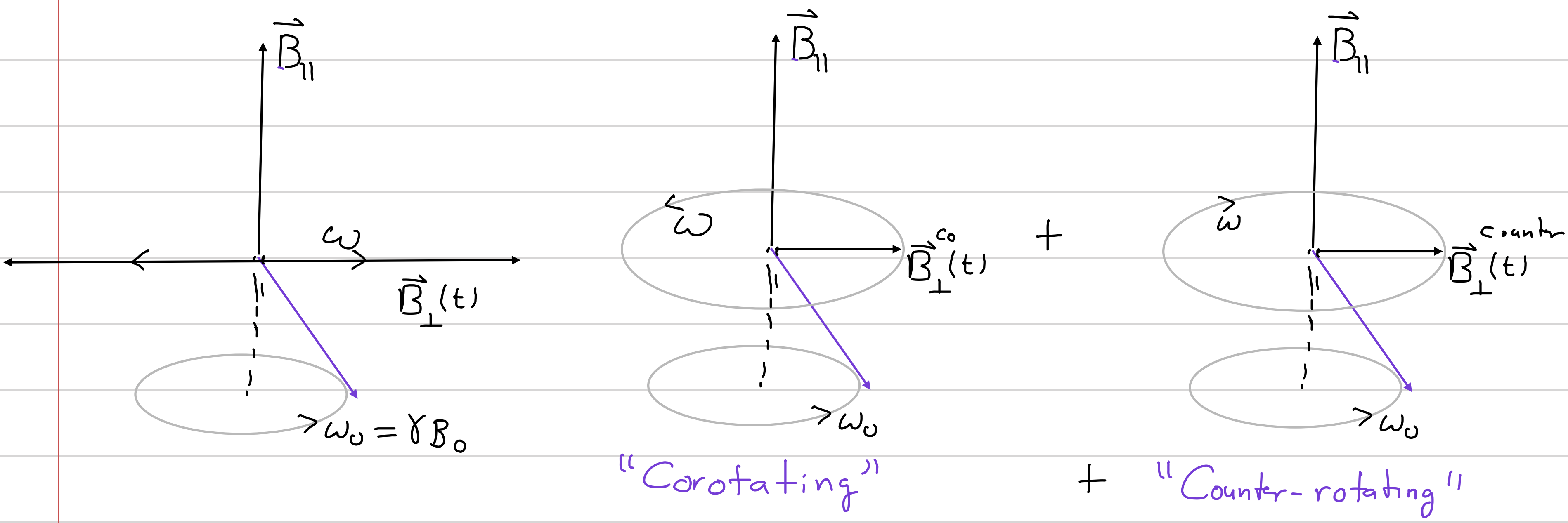
$$\begin{aligned} \Rightarrow \langle\hat{\sigma}_z\rangle^{max} &= -\cos 2\theta_a = 2\sin^2\theta_a - 1 \\ &= 2\frac{\Omega^2}{\Omega^2+\Delta^2} - 1 = P_{\uparrow_z} - P_{\downarrow_z} \\ &= 2P_{\uparrow_z} - 1 \Rightarrow P_{\uparrow_z} = \frac{\Omega_\perp^2}{\Omega_\perp^2+\Delta^2} \end{aligned}$$

✓

Rotating wave approximation (RWA)

Suppose that instead of rotating transverse field, we had a linearly oscillating field along a transverse axis, say the x-axis

$$B_x\cos(\omega t)\,\vec{e}_x = \underbrace{\frac{B_x}{2}\left[\cos\omega t\,\vec{e}_x + \sin\omega t\,\vec{e}_y\right]}_{\text{Right hand circulating}} + \underbrace{\frac{B_x}{2}\left[\cos\omega t\,\vec{e}_x - \sin\omega t\,\vec{e}_y\right]}_{\text{Left hand circulating}}$$



The linearly oscillating field decomposes into "co-rotating" and "counter-rotating" terms. Only the co-rotating term in near resonance. When $|\omega - \omega_0| << \omega_0$ and $\Omega << \omega_0$, the counter rotating term oscillates so fast in the rotating frame, that " net effect on the Bloch vector is negligible. This is known as the rotating wave approximation (RWA).

Formally, consider the interaction Hamiltonian in the Schrödinger picture

$$\hat{H}_{int}^{(S)} = -\vec{\mu}\cdot\vec{e}_x B_x \cos\omega t = -\frac{\hbar\gamma}{2} B_x \cos\omega t\, \hat{\sigma}_x = -\frac{\hbar\gamma B_x}{4}\left(e^{-i\omega t} + e^{+i\omega t}\right)\left(\hat{\sigma}_+ + \hat{\sigma}_-\right)$$

Transforming to the rotating frame

$$\hat{H}_{int}^{(RF)} = -\frac{\hbar\gamma B_x}{4}\left(e^{-i\omega t} + e^{+i\omega t}\right)\left(\hat{\sigma}_+ e^{+i\omega t} + \hat{\sigma}_- e^{-i\omega t}\right)$$

$$= \underbrace{-\frac{\hbar\gamma B}{4}\left(\hat{\sigma}_+ + \hat{\sigma}_-\right)}_{\text{Co-rotating terms}} \underbrace{-\frac{\hbar\gamma B_x}{4}\left(e^{+2i\omega t}\hat{\sigma}_+ + e^{-2i\omega t}\hat{\sigma}_-\right)}_{\text{Counter-rotating terms}} \approx \frac{\hbar\Omega}{4}\left(\hat{\sigma}_+ + \hat{\sigma}_-\right)$$

$$\Omega = -\gamma B_x$$

The counter-rotating terms oscillate like 2ω, whereas the characteristic dynamics of the Bloch vector is at rates $\Omega, \Delta \Rightarrow$ Rapid oscillations average to zero. This can be made more rigorous using the "method of averages"

Different Representations

When examining the problem of Rabi oscillations, there are a number of different representations we use:

- **Probability amplitudes**

In the rotating frame $|\psi_{RF}\rangle = c_{\uparrow_z}|\uparrow_z\rangle + c_{\downarrow_z}|\downarrow_z\rangle$

$$\hat{H}_{RF} = -\frac{\hbar\Delta}{2}\hat{\sigma}_z + \frac{\hbar\Omega}{2}\hat{\sigma}_x \quad \text{(choosing drive phase } \phi = 0\text{)}$$

$\Rightarrow$ Matrix representation

$$\underbrace{\frac{d}{dt}\begin{bmatrix} c_\uparrow \\ c_\downarrow \end{bmatrix}}_{|\psi_{RF}\rangle} = \underbrace{\frac{-i}{2}\begin{bmatrix} -\Delta & \Omega_\perp \\ \Omega_\perp & \Delta \end{bmatrix}}_{-\frac{i}{\hbar}\hat{H}_{RF}} \underbrace{\begin{bmatrix} c_\uparrow \\ c_\downarrow \end{bmatrix}}_{|\psi_{RF}\rangle} \Rightarrow \begin{aligned} \dot{c}_\uparrow &= \tfrac{i}{2}\Delta c_\uparrow - \tfrac{i}{2}\Omega c_\downarrow \\ \dot{c}_\downarrow &= -\tfrac{i}{2}\Delta c_\downarrow - \tfrac{i}{2}\Omega c_\uparrow \end{aligned}$$

On resonance: $\dot{c}_\uparrow = -i\frac{\Omega}{2}c_\downarrow$, $\dot{c}_\downarrow = i\frac{\Omega}{2}c_\uparrow \Rightarrow \ddot{c}_\uparrow = -\frac{\Omega^2}{4}c_\uparrow$ (SHO diff 'eqn)

$$\Rightarrow c_\uparrow(t) = c_\uparrow(0)\cos\left(\frac{\Omega t}{2}\right) + \frac{2}{\Omega}\dot{c}_\uparrow(0)\sin\left(\frac{\Omega t}{2}\right) = c_\uparrow(0)\cos\left(\frac{\Omega t}{2}\right) - i c_\downarrow(0)\sin\left(\frac{\Omega t}{2}\right)$$

with $c_\uparrow(0) = 0$, $c_\downarrow(0) = 1 \Rightarrow c_\uparrow(t) = -i\sin\left(\frac{\Omega t}{2}\right)$, $P_\uparrow(t) = \sin^2\left(\frac{\Omega t}{2}\right)$ ✓

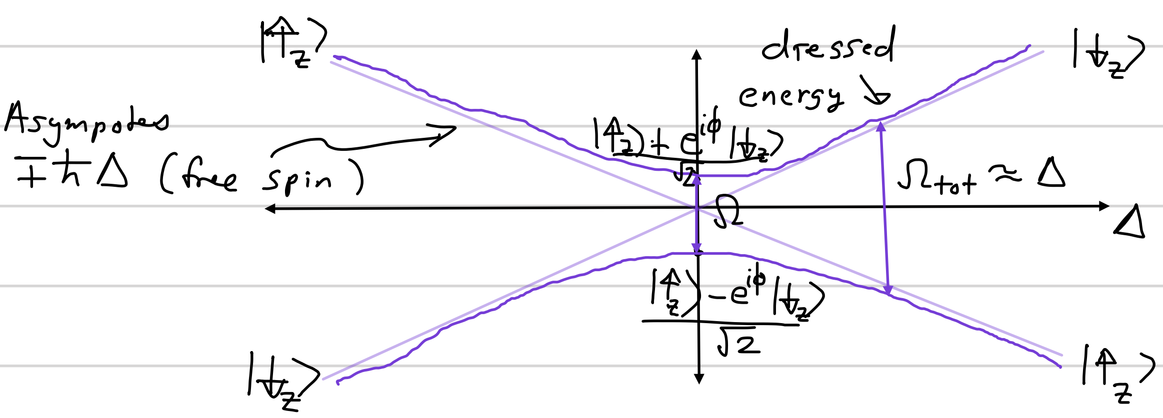
General Case: Consider eigenvectors and eigenvalues of the Hamiltonian

$$\hat{H}_{RF} = \frac{\hbar\vec{\Omega}_{tot}}{2}\cdot\hat{\vec{\sigma}} = \frac{\hbar\Omega_{tot}}{2}\vec{e}_a\cdot\hat{\vec{\sigma}}, \quad \text{where } \Omega_{tot} = \sqrt{\Omega_\perp^2 + \Delta^2},$$

$$\vec{e}_a = \frac{\vec{\Omega}_{tot}}{\Omega_{tot}} = \frac{\Omega}{\Omega_{tot}}\vec{e}_\perp + \frac{-\Delta}{\Omega_{tot}}\vec{e}_z = \sin\theta(\cos\phi\,\vec{e}_x + \sin\phi\,\vec{e}_y) + \cos\theta\,\vec{e}_z \quad \left(\tan\theta = \frac{\Omega}{-\Delta}\right)$$

$$\Rightarrow \text{Eigenvalues: } E_\pm = \pm\frac{\hbar\Omega_{tot}}{2} = \pm\frac{\hbar}{2}\sqrt{\Omega^2+\Delta^2}$$

Eigenvectors $|+\rangle = \cos\frac{\theta}{2}|\uparrow_z\rangle + e^{i\phi}\sin\frac{\theta}{2}|\downarrow_z\rangle$, $|-\rangle = \sin\frac{\theta}{2}|\uparrow_z\rangle - e^{i\phi}\cos\frac{\theta}{2}|\downarrow_z\rangle$ "Dressed States"



Generic Avoided crossing

- Dynamical of the Bloch vector $\Rightarrow$

Define $\vec{Q} = \langle \hat{\vec{\sigma}} \rangle = (u, v, w)$ (in rotating frame)

Heisenberg equations of motion $\frac{d\hat{\vec{\sigma}}}{dt} = -\frac{i}{\hbar}[\hat{\vec{\sigma}}, \hat{H}_{RF}] \Rightarrow \frac{d}{dt}\vec{Q} = \vec{\Omega}_{tot} \times \vec{Q}$

$$\Rightarrow \frac{d}{dt}\begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} 0 & -\Delta & 0 \\ +\Delta & 0 & -\Omega \\ 0 & \Omega & 0 \end{bmatrix}\begin{bmatrix} u \\ v \\ w \end{bmatrix}$$

$\frac{d}{dt}u = -\Delta v$, $\frac{d}{dt}v = +\Delta u - \Omega w$, $\frac{d}{dt}w = \Omega v$ "Bloch equations"

<u>Connection to absorption & emission of light by a two level atom</u>

Our initial motivation to study two-level quantum systems was to study absorption and emission of light by atoms close to resonance.

The field drives transitions between two levels $|g\rangle$ ($\equiv |\downarrow_z\rangle$) and $|e\rangle$ ($\equiv |\uparrow_z\rangle$).

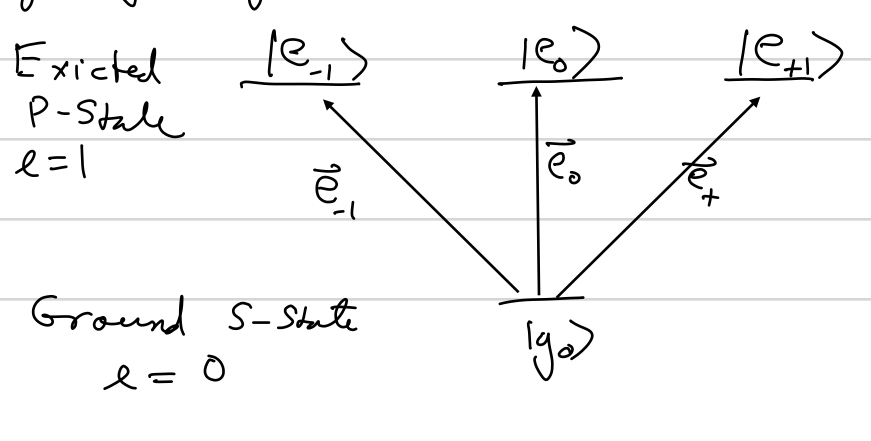
We take here a monochromatic, oscillating at frequency ω_L, w/ polarization $\vec{\epsilon}$. At the position of the atom

$$\vec{E}(\vec{R},t) = \mathrm{Re}\left(\vec{\epsilon}\, E_0\, e^{i\phi(\vec{R})} e^{-i\omega_L t}\right) = \frac{1}{2}\vec{\epsilon}\, E_0\, e^{i\phi(R)} e^{-i\omega_L t} + \text{c.c.}$$

The total Hamiltonian $\hat{H}(t) = \underbrace{\hat{H}_A}_{\text{Atomic Hamiltonian}} + \underbrace{\hat{H}_{AL}(t)}_{\text{Atom-light interaction}}$

In the electric dipole approximation $\hat{H}_{AL}(t) = -\hat{\vec{d}} \cdot \vec{E}(\vec{R},t)$

For concreteness, consider a dipole-allowed $S \to P$ transition ingoring any electron or nuclear spin



According to the electric dipole selection rules $\Delta m_\ell = 0, \pm 1$, with the transition driven b $\vec{\epsilon} = \vec{e}_0, \vec{e}_{\pm 1}$

$\vec{e}_0 = \vec{e}_z$, $\vec{e}_{\pm 1} = \frac{\vec{e}_x \pm i\vec{e}_y}{\sqrt{2}}$

The dipole operator has only off-diagonal elements between excited and ground state because of parity symmetry. In this subspace

$$\hat{\vec{d}} = \langle e|d|g\rangle \left(|e_{+1}\rangle\langle g|\,\vec{e}^{\,*}_{+1} + |e_0\rangle\langle g|\,\vec{e}^{\,*}_0 + |e_{-1}\rangle\langle g|\,\vec{e}^{\,*}_{-1} \right) + h.c.$$

Since $\vec{e}^{\,*}_0 = \vec{e}_0$, $\vec{e}^{\,*}_{\pm 1} = \vec{e}_{\mp 1}$

$$\hat{\vec{d}} = \langle e|d|g\rangle \Big[\left(|e_{+1}\rangle\langle g| + |g\rangle\langle e_{-1}| \right) \vec{e}^{\,*}_{+1} + \left(|e_0\rangle\langle g| + |g\rangle\langle e_0| \right) \vec{e}_0 + \left(|e_{-1}\rangle\langle g| + |g\rangle\langle e_{-1}| \right) \vec{e}^{\,*}_{-1} \Big]$$

Here $\langle e|d|g\rangle$ is the "dipole matrix element," which is the same for all three sublevels (Note, more generally, including fine or hyperfine structure, there would be a "reduced matrix element" and Clebsch-Gordan coeff.)
We will denote $d_{eg} \equiv \langle e|d|g\rangle$
Let us take the laser to be linearly polarized along $\vec{e}_0$

$$\Rightarrow -\hat{\vec{d}} \cdot \vec{E}_L(\vec{R},t) = -d_{eg} E_0 \left(|e_0\rangle\langle g| + |g\rangle\langle e_0| \right) \left(\frac{e^{-i\phi_L(\vec{R})} e^{-i\omega_L t} + e^{+i\phi_L(\vec{R})} e^{+i\omega_L t}}{2} \right)$$

We define the <u>Rabi frequency</u> associated with this electric-dipole coupling

$$\hbar\Omega \equiv -d_{eg} E_0$$

In terms of the Pauli operators for this pseudospin

$$\hat{H}_{AL}(t) = \frac{\hbar\Omega}{2} \left(\hat{\sigma}_+ + \hat{\sigma}_- \right) \left(e^{i\phi(\vec{R})} e^{-i\omega_L t} + e^{-i\phi(\vec{R})} e^{+i\omega_L t} \right)$$

The atom Hamiltonian $\hat{H}_A = E_{e_0} |e_0\rangle\langle e_0| + E_{g_0} |g_0\rangle\langle g_0| = \frac{E_{e_0} + E_{g_0}}{2} \hat{\mathbb{1}} + \frac{\hbar\omega_{eg}}{2} \hat{\sigma}_z$
where $\hbar\omega_{eg} = E_{e_0} - E_{g_0}$ is the Bohr freq. (resonance frequency)
We can neglect the identity term, which is equivalent to taking the ground state energy half-way between E_{e_0} and E_{g_0}

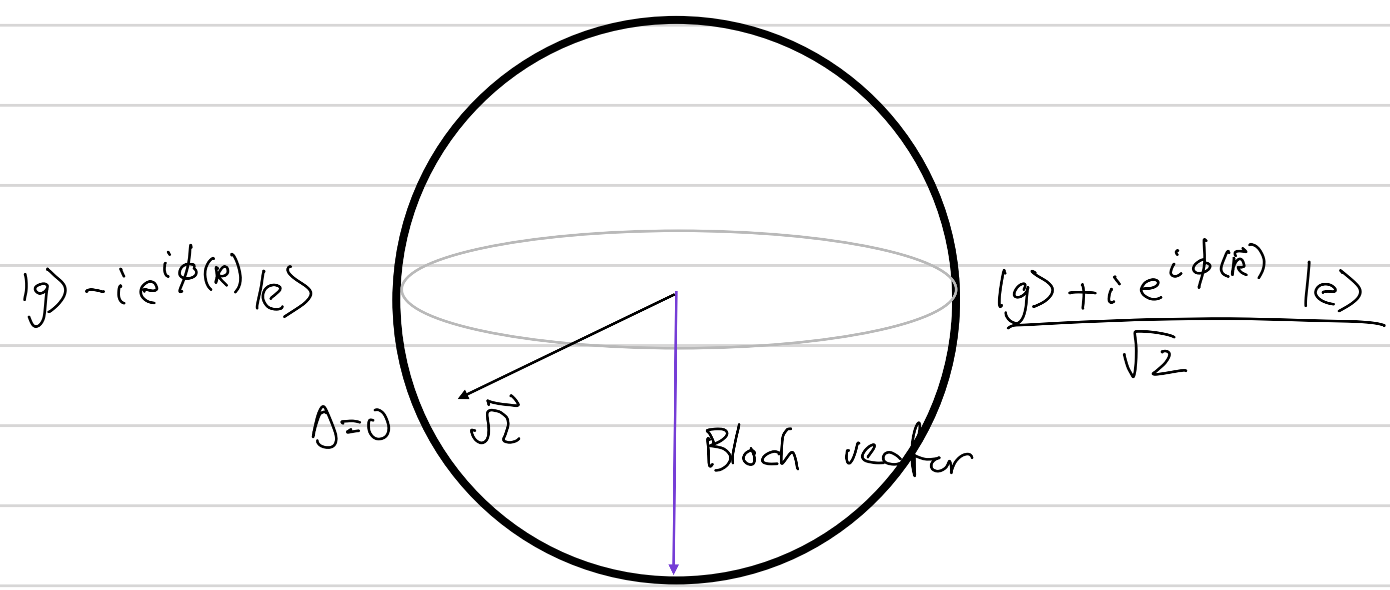
Going to the rotating frame the interact Ham

$$\hat{H} = -\frac{\hbar\Delta}{2}\hat{\sigma}_z + \frac{\hbar\Omega}{2}\left(\hat{\sigma}_+ e^{+i\omega_L t} + \hat{\sigma}_- e^{-i\omega_L t}\right)\left(e^{i\phi_L(\vec{R})} e^{-i\omega_L t} + e^{-i\phi(\vec{R})} e^{+i\omega_L t}\right)$$

Making the RWA, dropping rapidly oscillating terms

$$\Rightarrow \boxed{\begin{aligned} &\hat{H} = -\frac{\hbar\Delta}{2}\hat{\sigma}_z + \frac{\hbar\Omega}{2}\left(\cos\phi(\vec{R})\,\hat{\sigma}_x - \sin(\phi(\vec{R}))\,\hat{\sigma}_y\right) \quad \left(\text{Note phase has opposite sign}\right) \\ &\Delta = \omega_L - \omega_{eg}, \quad \Omega = -\frac{d_{eg}E_0}{\hbar} = -\frac{\langle e|\vec{d}\cdot\vec{\epsilon}|g\rangle E_0}{\hbar}, \quad \phi_L(\vec{R}) = \vec{k}_L\cdot\vec{R} - \phi_0 \end{aligned}}$$

The coherent interaction between the two-level atom and the laser field leads to Rabi flopping.



A $\frac{\pi}{2}$-pulse will create a 50-50 superposition of $|g\rangle$ and $|e\rangle$

Note: We the polarization is circular, we have the following terms

$$\hat{H}_{AL} = \Big(\langle e_{+1}|\vec{d}\cdot\vec{\epsilon}_+|g_0\rangle \underbrace{|e_{+1}\rangle\langle g_0|}_{\text{Absorb } \vec{e}_+} + \langle g_0|\vec{d}\cdot\vec{\epsilon}_+|e_-\rangle \underbrace{|g_0\rangle\langle e_-|}_{\text{Emit } \vec{e}_-}\Big)\frac{E_0}{2}e^{-i\omega_L t} + h.c.$$

In the RWA the second, counter-rotating term is negligible. Only for a true spin ½ particle can we avoid the RWA.