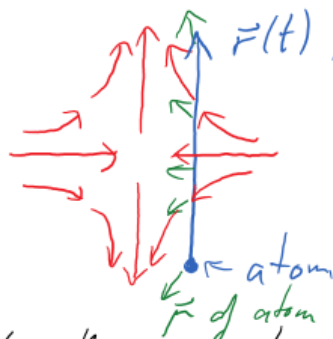


Lecture 4 - Magnetic Resonance, the Quantum Way

An analogous adiabatic following is also what we count on in magnetic trapping.

Take a quadrupole magnetic trap:



At the location of atom,
B-field is $\vec{B}(\vec{r}(t)) \equiv \vec{B}_0(t)$

We want the magnetic moment of the atom to follow tightly the local magnetic field direction. Otherwise it would no longer be trapped.

So we need that the rate of change of the direction of \vec{B} , $\dot{\theta} \approx \frac{\dot{B}}{B} = \frac{B'v}{B} = \frac{v}{r}$ is much smaller than the precession period

$$\Omega_L = \gamma B = \gamma B' r$$

$$\Rightarrow \frac{v}{r} \ll \gamma B' r \Rightarrow r = \sqrt{\frac{v}{\gamma B'}} \text{ is the}$$

radius of the "Majorana hole" within which the particles will be lost from the trap.

Solutions: 1. Plug the hole! Ketterle et al. PRL 75, 3969 (1995)

Enables \Rightarrow BEC 2. TOP trap: Rotate the magnetic field zero rapidly on a large circle.
Cornell group, PRL 74, 3352 (1995)

Quantized spin in a magnetic field:

$$\hat{H} = -\hat{\vec{\mu}} \cdot \vec{B} = -\gamma \hat{L}_z B_0$$

\hat{L}_z is the operator associated with angular momentum along z .

Heisenberg equations of motion

$$\frac{d}{dt} \hat{O} = \frac{i}{\hbar} [\hat{H}, \hat{O}] + \frac{\partial \hat{O}}{\partial t}$$

$$\Rightarrow \frac{d}{dt} \hat{\mu}_k = \frac{i\gamma}{\hbar} [\hat{H}, \hat{L}_k]$$

using $[\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k$ we see

$$\frac{d}{dt} \hat{\mu}_k = \gamma \hat{\vec{\mu}} \times \vec{B} \quad \text{exact!}$$

and in particular

$$\frac{d}{dt} \langle \hat{\mu}_k \rangle = \gamma \langle \hat{\vec{\mu}} \rangle \times \vec{B} \quad \text{also valid for expectation values}$$

\Rightarrow Same equation of motion as for a classical magnetic moment for any value of angular momentum!

Comments:

- this is valid for any angular momentum operator, so also for spin $\frac{1}{2}$!
 - and therefore for any two-level system that can be mapped onto spin precession
 - valid for the case of several angular momenta within an atom coupled to a total angular momentum \vec{F} (as long as \vec{B} is not large enough to "break" the coupling).
 - valid also for a system of N two-level systems symmetrically coupled to an external field. In this case, we have an effective angular momentum $\vec{L} = \frac{N}{2}$
- Spin precession \rightarrow Dicke superradiance
constructive interference
of N "aligned" particles.

Two-level system, spin $\frac{1}{2}$

$$\begin{array}{lll}
 \text{---} |e\rangle & \text{---} |\uparrow\rangle & \text{---} m = +\frac{1}{2} \\
 \text{---} |g\rangle & \text{---} |\downarrow\rangle & \text{---} m = -\frac{1}{2}
 \end{array}$$

$$\langle p_z \rangle = \frac{\gamma \hbar}{2} (P_{\downarrow} - P_{\uparrow}) = \frac{\gamma \hbar}{2} (2P_e - 1)$$

Lecture 4 - Magnetic Resonance, the Quantum Way

Start at $t=0$ with $P_g(t=0) = 1$.

$$P_e(t) = \frac{1}{\hbar\gamma} \underbrace{\langle \mu_z \rangle}_{\text{use classical solution}} + \frac{1}{2}$$

$$= \frac{1}{2} - \frac{1}{2} \left(1 - 2 \frac{\omega_R^2}{\Omega_R^2} \sin^2\left(\frac{\Omega_R t}{2}\right) \right)$$

$$P_e(t) = \frac{\omega_R^2}{\Omega_R^2} \sin^2\left(\frac{\Omega_R t}{2}\right)$$

Rabi transition probability

Spin $\frac{1}{2}$ Hamiltonian

$$|e\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |g\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\vec{B}_0 = B_0 \hat{z}$$

$$H_0 = -\vec{\mu} \cdot \vec{B} = -\gamma \hat{S}_z B_0$$

$$= \frac{\hbar\omega_0}{2} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\sigma_z \text{ Pauli matrix}}$$

\Rightarrow Eigenstates are $|e\rangle, |g\rangle$, with eigenenergies $\pm \frac{\hbar\omega_0}{2}$

Lecture 4 - Magnetic Resonance, the Quantum Way

Take a spin initially aligned along \hat{x}

$$|\psi(t=0)\rangle = \frac{1}{\sqrt{2}} (|e\rangle + |g\rangle)$$

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left(e^{-i\frac{\omega_0 t}{2}} |e\rangle + e^{+i\frac{\omega_0 t}{2}} |g\rangle \right)$$

$$= \frac{1}{\sqrt{2}} e^{-i\frac{\omega_0 t}{2}} \underbrace{\left(|e\rangle + e^{i\omega_0 t} |g\rangle \right)}$$

precession in the xy plane
at frequency ω_0 .

Spin $\frac{1}{2}$ in a rotating magnetic field

$$H_0 = -\vec{\mu} \cdot \vec{B}_0 = -\gamma B_0 \hat{S} \cdot \hat{z}$$

$$= \frac{\hbar \omega_0}{2} \sigma_z = \frac{\hbar \omega_0}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\omega_0 = -\gamma \frac{B_0}{\hbar}$$

Eigenstates $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Eigenenergies $\pm \frac{\hbar \omega_0}{2}$

$$H_1 = -\vec{\mu} \cdot \vec{B}_1 = -\vec{\mu} \cdot \frac{\omega_R}{\gamma} (-\hat{x} \cos(\omega t) - \hat{y} \sin(\omega t))$$

$$= \omega_R (\hat{S}_x \cos(\omega t) + \hat{S}_y \sin(\omega t))$$

$$= \frac{\hbar \omega_R}{2} (\sigma_x \cos(\omega t) + \sigma_y \sin(\omega t))$$

$$= \frac{\hbar \omega_R}{2} \begin{pmatrix} 0 & e^{-i\omega t} \\ e^{i\omega t} & 0 \end{pmatrix}$$

$$\Rightarrow H = H_0 + H_1 = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_R e^{-i\omega t} \\ \omega_R e^{i\omega t} & -\omega_0 \end{pmatrix}$$

• This is exact!

Transform to rotating frame

Rotation about \hat{z} by angle ϑ :

$$e^{-i \hat{S}_z \vartheta} \quad \vartheta = \omega t$$

$$T = e^{-i \hat{S}_z \omega t} = e^{-i \frac{\omega t}{2} \sigma_z}$$

$$= \begin{pmatrix} e^{-i \frac{\omega t}{2}} & 0 \\ 0 & e^{+i \frac{\omega t}{2}} \end{pmatrix}$$

$$|\psi\rangle = T |\tilde{\psi}\rangle$$

$$i\hbar \frac{d}{dt} |\psi\rangle = i\hbar \dot{T} |\tilde{\psi}\rangle + T i\hbar \frac{d}{dt} |\tilde{\psi}\rangle$$

$$= H |\psi\rangle = H T |\tilde{\psi}\rangle$$

$$\Rightarrow i\hbar \frac{d}{dt} |\tilde{\psi}\rangle = (T^\dagger H T - i\hbar T^\dagger \dot{T}) |\tilde{\psi}\rangle$$

$$\Rightarrow \tilde{H} = T^\dagger \left(H - i\hbar \frac{d}{dt} \right) T$$

$$T^\dagger H_0 T = H_0 \quad \text{as } \sigma_z \text{ commutes with } e^{-i \frac{\omega t}{2} \sigma_z}$$

$$T^\dagger H_1 T = \begin{pmatrix} 0 & \omega_K \\ \omega_K & 0 \end{pmatrix} \quad \text{time-independent!}$$

$$T^\dagger \left(-i\hbar \frac{d}{dt} T \right) = \begin{pmatrix} -\omega & 0 \\ 0 & \omega \end{pmatrix}$$

$$\begin{aligned}
 \Rightarrow \tilde{H} &= \frac{\hbar}{2} \begin{pmatrix} -\delta & \omega_R \\ \omega_R & \delta \end{pmatrix} & \delta &= \omega - \omega_0 \\
 &= -\frac{\hbar\delta}{2} \sigma_z + \frac{\hbar\omega_R}{2} \sigma_x \\
 &= \frac{1}{2} \vec{L} \cdot \vec{\sigma} & \text{with } \vec{L} &= \begin{pmatrix} \hbar\omega_R \\ 0 \\ -\hbar\delta \end{pmatrix}
 \end{aligned}$$

\Rightarrow In the frame rotating at frequency ω , the hamiltonian has become time-independent!

The hamiltonian is that of a spin $\frac{1}{2}$ in an effective magnetic field $\vec{B}_{\text{eff}} \propto \vec{L} = \begin{pmatrix} \hbar\omega_R \\ 0 \\ -\hbar\delta \end{pmatrix}$, as we had before for classical magnetic moments.

The eigenvalues are

$$E_{\pm} = \pm \frac{1}{2} |\vec{L}| = \pm \frac{\hbar}{2} \sqrt{\omega_R^2 + \delta^2} = \pm \frac{\hbar\Omega_R}{2}$$

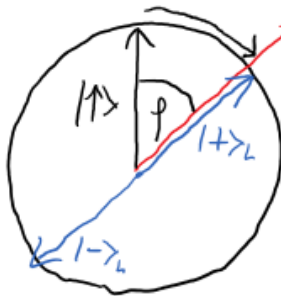
The eigenvectors are the spin eigenstates that are aligned or anti-aligned with \vec{L} :

$$\tilde{H} |+\rangle_L = E_+ |+\rangle_L$$

$$\tilde{H} |-\rangle_L = E_- |-\rangle_L$$

We can obtain them from $|\uparrow\rangle$ and $|\downarrow\rangle$ by rotating about the axis $\hat{z} \times \hat{L} \propto \hat{y}$ by an angle φ with $\cos\varphi = \hat{z} \cdot \hat{L} = \frac{\delta}{\Omega_R}$

Lecture 4 - Magnetic Resonance, the Quantum Way



$$\cos \varphi = \frac{-\sigma}{\Omega_R}; \quad \tan \varphi = \frac{\omega_R}{-\sigma}$$

$$\hat{z} \times \vec{L} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \times \begin{pmatrix} \hbar\omega_R \\ 0 \\ -\hbar\sigma \end{pmatrix} = \begin{pmatrix} 0 \\ \hbar\omega_R \\ 0 \end{pmatrix} = \hbar\omega_R \hat{y}$$

So we need to rotate about \hat{y} by φ :

$$R = e^{-i\varphi S_y} = e^{-i\frac{\varphi}{2}\sigma_y} = \sum_n \frac{1}{n!} (-i\frac{\varphi}{2}\sigma_y)^n$$

Now $\sigma_y^2 = 1$ so $\sigma_y^{2j} = 1$, $\sigma_y^{2j+1} = \sigma_y$.

$$\Rightarrow R = \cos \frac{\varphi}{2} 1 - i \sin \frac{\varphi}{2} \sigma_y$$

$$= \begin{pmatrix} \cos \frac{\varphi}{2} & -\sin \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} & \cos \frac{\varphi}{2} \end{pmatrix}$$

$$|+\rangle_L = R |\uparrow\rangle = \begin{pmatrix} \cos \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} \end{pmatrix} = \cos \frac{\varphi}{2} |\uparrow\rangle + \sin \frac{\varphi}{2} |\downarrow\rangle$$

$$|-\rangle_L = R |\downarrow\rangle = \begin{pmatrix} -\sin \frac{\varphi}{2} \\ \cos \frac{\varphi}{2} \end{pmatrix} = -\sin \frac{\varphi}{2} |\uparrow\rangle + \cos \frac{\varphi}{2} |\downarrow\rangle$$

Note: $\cos \varphi = \cos^2 \frac{\varphi}{2} - \sin^2 \frac{\varphi}{2} = 2 \cos^2 \frac{\varphi}{2} - 1$

$$\Rightarrow \cos \frac{\varphi}{2} = \sqrt{\frac{1 + \cos \varphi}{2}} = \sqrt{\frac{1}{2} + \frac{\sigma}{2\Omega_R}}$$

$$\sin \frac{\varphi}{2} = \sqrt{\frac{1 - \cos \varphi}{2}} = \sqrt{\frac{1}{2} - \frac{\sigma}{2\Omega_R}}$$

Time evolution $|+(t)\rangle = e^{-iE_+t/\hbar} |+\rangle_L = e^{-i\frac{\Omega_R t}{2}} |+\rangle_L$

$$|-(t)\rangle = e^{-iE_-t/\hbar} |-\rangle_L = e^{+i\frac{\Omega_R t}{2}} |-\rangle_L$$

Lecture 4 - Magnetic Resonance, the Quantum Way

To remember: The hamiltonian

$$\tilde{H} = \frac{\hbar}{2} \begin{pmatrix} -\delta & \omega_R \\ \omega_R & \delta \end{pmatrix} = \frac{\hbar}{2} \Omega_R \begin{pmatrix} \cos \varphi & \sin \varphi \\ \sin \varphi & -\cos \varphi \end{pmatrix}$$

with $\cos \varphi = \frac{-\delta}{\Omega_R} = \frac{-\delta}{\sqrt{\omega_R^2 + \delta^2}}$ is diagonalized by

$$R = \begin{pmatrix} \cos \frac{\varphi}{2} & -\sin \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} & \cos \frac{\varphi}{2} \end{pmatrix}$$

$$\tilde{H}' = R^\dagger \tilde{H} R = \frac{\hbar}{2} \begin{pmatrix} \Omega_R & 0 \\ 0 & -\Omega_R \end{pmatrix}$$

$$\begin{aligned} \text{Check } \tilde{H} R |\uparrow\rangle &= \tilde{H} \begin{pmatrix} \cos \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} \end{pmatrix} = \frac{\hbar}{2} \Omega_R \begin{pmatrix} \cos \varphi \cos \frac{\varphi}{2} + \sin \varphi \sin \frac{\varphi}{2} \\ \sin \varphi \cos \frac{\varphi}{2} - \cos \varphi \sin \frac{\varphi}{2} \end{pmatrix} \\ &= \frac{\hbar \Omega_R}{2} \begin{pmatrix} \cos^3 \frac{\varphi}{2} - \sin^2 \frac{\varphi}{2} \cos \frac{\varphi}{2} + 2 \sin^2 \frac{\varphi}{2} \cos \frac{\varphi}{2} \\ 2 \sin \frac{\varphi}{2} \cos^2 \frac{\varphi}{2} - \cos^2 \frac{\varphi}{2} \sin \frac{\varphi}{2} + \sin^3 \frac{\varphi}{2} \end{pmatrix} \\ &= \frac{\hbar \Omega_R}{2} \begin{pmatrix} \cos^3 \frac{\varphi}{2} + \sin^2 \frac{\varphi}{2} \cos \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} \cos^2 \frac{\varphi}{2} + \sin^3 \frac{\varphi}{2} \end{pmatrix} \\ &= \frac{\hbar \Omega_R}{2} \begin{pmatrix} \cos \frac{\varphi}{2} \\ \sin \frac{\varphi}{2} \end{pmatrix} \end{aligned}$$

Say $|\psi(t=0)\rangle = |\uparrow\rangle$ (which is $|\uparrow\rangle_{\text{in lab and rot-frame}}$)

$$\text{Now } |\uparrow\rangle = R^\dagger |+\rangle = \cos \frac{\varphi}{2} |+\rangle - \sin \frac{\varphi}{2} |-\rangle$$

$$\begin{aligned} \Rightarrow |\psi(t)\rangle &= \cos \frac{\varphi}{2} e^{-i \frac{\Omega_R t}{2}} |+\rangle - \sin \frac{\varphi}{2} e^{+i \frac{\Omega_R t}{2}} |-\rangle \\ &= \cos \frac{\varphi}{2} e^{-i \frac{\Omega_R t}{2}} \left(\cos \frac{\varphi}{2} |\uparrow\rangle + \sin \frac{\varphi}{2} |\downarrow\rangle \right) \\ &\quad - \sin \frac{\varphi}{2} e^{+i \frac{\Omega_R t}{2}} \left(-\sin \frac{\varphi}{2} |\uparrow\rangle + \cos \frac{\varphi}{2} |\downarrow\rangle \right) \\ &= \left(\cos^2 \frac{\varphi}{2} e^{-i \frac{\Omega_R t}{2}} + \sin^2 \frac{\varphi}{2} e^{+i \frac{\Omega_R t}{2}} \right) |\uparrow\rangle \\ &\quad + \cos \frac{\varphi}{2} \sin \frac{\varphi}{2} (e^{-i \frac{\Omega_R t}{2}} - e^{+i \frac{\Omega_R t}{2}}) |\downarrow\rangle \end{aligned}$$

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$$\Rightarrow |\psi(t)\rangle = \cos\left(\frac{\Omega_R t}{2}\right) |\uparrow\rangle - i \sin\left(\frac{\Omega_R t}{2}\right) \cos\varphi |\uparrow\rangle - i \sin\left(\frac{\Omega_R t}{2}\right) \sin\varphi |\downarrow\rangle$$

(*)

In fact, we have

$$\begin{aligned} U(t) &= e^{-i\tilde{H}t/\hbar} = e^{-i\frac{\Omega_R t}{2} \hat{L} \cdot \vec{\sigma}} \\ &= \cos\left(\frac{\Omega_R t}{2}\right) \mathbb{1} - i \sin\left(\frac{\Omega_R t}{2}\right) \hat{L} \cdot \vec{\sigma} \\ &= \cos\left(\frac{\Omega_R t}{2}\right) \mathbb{1} - i \sin\left(\frac{\Omega_R t}{2}\right) \left(\frac{\omega_R}{\Omega_R} \sigma_x - \frac{\omega}{\Omega_R} \sigma_z\right) \end{aligned}$$

From which (*) follows $|\psi(t)\rangle = U(t) |\uparrow\rangle$
with $\cos\varphi = -\frac{\omega}{\Omega_R}$ and $\sin\varphi = \frac{\omega_R}{\Omega_R}$.

Probability for spin-flip:

$$\begin{aligned} P_{\downarrow}(t) &= |\langle \downarrow | \psi(t) \rangle|^2 = |\langle \downarrow | U(t) | \uparrow \rangle|^2 \\ &= \frac{\omega_R^2}{\Omega_R^2} \sin^2\left(\frac{\Omega_R t}{2}\right) \end{aligned}$$

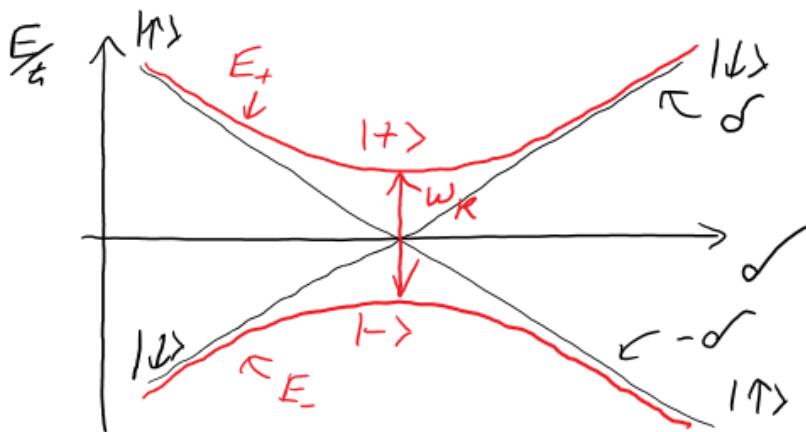
as we found before classically.

Rapid adiabatic passage - the QM version

The Landau - Zener problem -

"Unperturbed" Hamiltonian $H_0 = \frac{\hbar}{2} \begin{pmatrix} -\sigma & 0 \\ 0 & \sigma \end{pmatrix}$

Full Hamiltonian $H = \frac{\hbar}{2} \begin{pmatrix} -\sigma & \omega_R \\ \omega_R & \sigma \end{pmatrix}$



Starting with $|\downarrow\rangle$ at $\sigma \ll -\omega_R$, the adiabatic theorem shows that when I sweep "infinitely" slowly to $\sigma \gg +\omega_R$, I should always stay in the adiabatic eigenstate, i.e. $|-\rangle$, and thus, after the sweep, the spin will have changed to be $|\uparrow\rangle$.

However, if I don't sweep σ infinitely slowly, there is some probability to jump from $|-\rangle$ to $|+\rangle$ and thus end up still in $|\downarrow\rangle$.

This probability of a non-adiabatic transition from one level to the other is given by

$$P_{na} = e^{-\frac{\pi}{2} \frac{\omega_R^2}{\dot{\sigma}}}$$

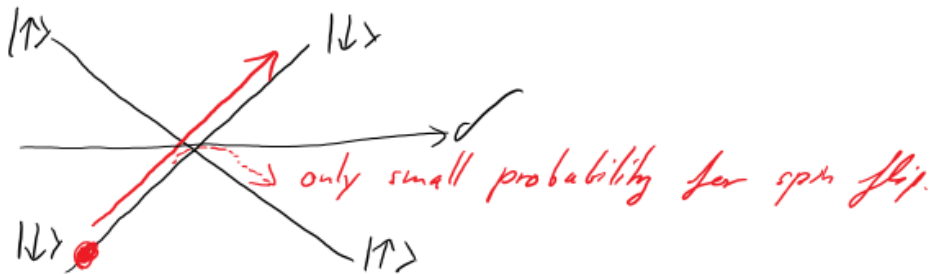
Lecture 4 - Magnetic Resonance, the Quantum Way

Note that this implies a criterion identical to the one we had found classically to have a successful rapid adiabatic passage:

$$\dot{\omega} \ll \omega_R^2 \Rightarrow P_{na} \ll 1$$

\Rightarrow evolution is to good approximation adiabatic.

For faster sweeps, we have $\dot{\omega} \gg \omega_R^2$:



$P_{flip} = 1 - P_{na}$ will then be small.

\Rightarrow Calculate P_{flip} perturbatively, assuming $\omega_R^2 \ll \dot{\omega}$.

Hamiltonian:
$$H = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_R e^{-i\varphi(t)} \\ \omega_R e^{i\varphi(t)} & -\omega_0 \end{pmatrix} \text{ in lab frame}$$

$\varphi(t)$ - phase of my driving field
 $\hat{=}$ rotation angle of field \vec{B}_1

In frame rotating at $\dot{\varphi}$:
$$\tilde{H} = \frac{\hbar}{2} \begin{pmatrix} -\delta(t) & \omega_R \\ \omega_R & \delta(t) \end{pmatrix}$$

with $\delta(t) = \dot{\varphi}(t) - \omega_0$

In frame rotating at $-\omega_0$:
$$\bar{H} = \frac{\hbar}{2} \begin{pmatrix} 0 & \omega_R e^{-i(\varphi(t) - \omega_0 t)} \\ \omega_R e^{i(\varphi(t) - \omega_0 t)} & 0 \end{pmatrix}$$

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Easiest is to use \bar{H} , the hamiltonian in the frame rotating at ω_0 .

Take $|\psi(t)\rangle = a(t) |\uparrow\rangle + b(t) |\downarrow\rangle$

$$\dot{a} = -i \frac{\omega_R}{2} e^{-i(\varphi(t) - \omega_0 t)} b$$

$$\dot{b} = -i \frac{\omega_R}{2} e^{+i(\varphi(t) - \omega_0 t)} a$$

Let's assume a linear sweep $\dot{\varphi}(t) = \dot{\varphi} - \omega_0 = \alpha t$
 $\Rightarrow \varphi(t) = \omega_0 t + \frac{1}{2} \alpha t^2$ ($\alpha = \dot{\omega} = \text{const.}$)

$$\boxed{\begin{aligned} \dot{a} &= -i \frac{\omega_R}{2} e^{-i \frac{1}{2} \alpha t^2} b \\ \dot{b} &= -i \frac{\omega_R}{2} e^{+i \frac{1}{2} \alpha t^2} a \end{aligned}}$$

Perturbative calculation: Let's assume we start in $|\downarrow\rangle$, and we have weak coupling so $b \approx 1$ throughout. Then

$$\dot{a} \approx -i \frac{\omega_R}{2} e^{-i \frac{1}{2} \alpha t^2}$$

We see that a will only grow significantly for times such that $\alpha t^2 \lesssim 1$, so in a range $\Delta t \sim \frac{1}{\sqrt{\alpha}} = \frac{1}{\sqrt{\dot{\omega}}}$ around $t=0$ where we are on resonance. Outside this time interval a oscillates rapidly and a no longer accumulates amplitude.

Lecture 4 - Magnetic Resonance, the Quantum Way

We can thus estimate $a \approx \omega_R \cdot \Delta t \approx \frac{\omega_R}{\sqrt{\omega}}$.

Then $P_{\text{flip}} = |a|^2 \sim \frac{\omega_R^2}{\omega}$, which is correct.

Let's do it with prefactors:

$$\dot{a} = -i \frac{\omega_R}{2} e^{-i \frac{1}{2} \omega t^2}$$

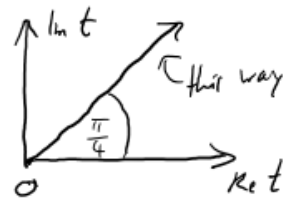
$$\Rightarrow a(t) = -i \frac{\omega_R}{2} \int_{-\infty}^{\infty} dt e^{-i \frac{1}{2} \omega t^2} = -i \omega_R \int_0^{\infty} dt e^{-i \frac{1}{2} \omega t^2}$$

change of variables $\tau^2 = i t^2 \Rightarrow \tau = e^{i \frac{\pi}{4}} t$

$$d\tau = e^{i \frac{\pi}{4}} dt$$

$$a(t) = -i e^{-i \frac{\pi}{4}} \omega_R \int_0^{e^{i \frac{\pi}{4}} \infty} d\tau e^{-\frac{1}{2} \omega \tau^2}$$

$$= -i e^{-i \frac{\pi}{4}} \omega_R \sqrt{\frac{\pi}{2\omega}}$$



$$\Rightarrow \boxed{P_{\text{flip}} = |a|^2 = \frac{\pi}{2} \frac{\omega_R^2}{\omega}}$$

perturbative result!

exact limit of
 $1 - e^{-\frac{\pi}{2} \frac{\omega_R^2}{\omega}}$ (the non-perturbative result)

Non-perturbative calculation

First, let's point out that since we are after the probability of being in $|1\rangle$ or $|0\rangle$, we know that our problem is classical at heart. We can map the question on the spin-flip probability to the problem of a classical spin precessing in a time-varying magnetic field where B_x is static but B_z is varied from large and negative to large and positive. We saw the solutions in the last lecture. Mathematically, we could thus attempt solving the equation

$$\dot{\vec{L}} = \vec{L} \times \gamma \vec{B}(t)$$

and read off the answer from $P_e = \frac{1}{2} \left(\frac{L_z}{L} + 1 \right)$.

The equations are however even less transparent than what we derived for the spin $\frac{1}{2}$ case, so let's proceed with those:

Start again with the two coupled equations

$$\begin{aligned} \dot{a} &= -i \frac{\omega_R}{2} e^{-i\frac{1}{2}\alpha t^2} b \\ \dot{b} &= -i \frac{\omega_R}{2} e^{+i\frac{1}{2}\alpha t^2} a \end{aligned} \quad \text{with boundary condition} \quad \begin{aligned} a(-\infty) &= 0; \quad b(-\infty) = 1 \end{aligned}$$

$$t = \sqrt{\frac{2}{\alpha}} \frac{\Omega}{\omega_R}$$

$$\Rightarrow \ddot{a} = -i \frac{\omega_R}{2} e^{-i\frac{1}{2}\alpha t^2} \dot{b} - i\alpha t \dot{a}$$

$$\boxed{\ddot{a} = -\frac{\omega_R^2}{4} a - i\alpha t \dot{a}}$$

$$\begin{aligned} \frac{\alpha t^2}{4} &= 2\pi h \\ \frac{1}{2}\alpha t &= \frac{1}{\sqrt{2}} \frac{\Omega}{\omega_R} = \frac{1}{\sqrt{2}} \frac{\Omega}{\omega_R} \end{aligned}$$

$$\begin{aligned} \text{Substituting } a &= e^{-i\frac{1}{4}\alpha t^2} c \Rightarrow \dot{a} = e^{-i\frac{1}{4}\alpha t^2} \dot{c} - \frac{1}{2}\alpha t e^{-i\frac{1}{4}\alpha t^2} c \\ \ddot{a} &= e^{-i\frac{1}{4}\alpha t^2} \ddot{c} - i\alpha t e^{-i\frac{1}{4}\alpha t^2} \dot{c} - \left(\frac{1}{4}\alpha^2 t^2 + i\frac{\alpha}{2}\right) e^{-i\frac{1}{4}\alpha t^2} c \end{aligned}$$

$$\Rightarrow \ddot{c} - i\alpha t \dot{c} - \frac{1}{4}\alpha^2 t^2 c - i\frac{\alpha}{2} c = -\frac{\omega_R^2}{4} c - i\alpha t \dot{c} - \frac{1}{4}\alpha^2 t^2 c$$

$$\Rightarrow \ddot{c} + \left(\frac{\omega_R^2}{4} - i\frac{\alpha}{2} + \frac{\alpha^2}{4} t^2 \right) c = 0 \quad \text{Weber equation}$$

Lecture 4 - Magnetic Resonance, the Quantum Way

We can introduce a scaled time

$$z = \sqrt{2} e^{-i\frac{\pi}{4}} t$$

We did a similar change of variables for the perturbative calculation: $\Delta t = \frac{1}{\sqrt{2}}$ was the characteristic time spent near resonance ($\delta \approx 0$) where the phase $\varphi(t)$ did not change much and the amplitude a was able to grow appreciably. The $e^{-i\frac{\pi}{4}}$ factor was used to turn $e^{-i\frac{1}{2}\Delta t^2}$ into a real gaussian $e^{-\frac{1}{2}\Delta \tau^2}$.

$$\Rightarrow dz = \sqrt{2} e^{-i\frac{\pi}{4}} dt$$

$$\begin{aligned} \frac{d^2 c}{dt^2} &= \frac{d^2 c}{dz^2} \underbrace{2 e^{-i\frac{\pi}{2}}}_{-i} = -\left(\frac{\omega_R^2}{4} - \frac{i2}{2} + \frac{z^2}{4} z^2 \cdot \frac{1}{2} e^{i\frac{\pi}{2}}\right) c \\ &= -2i\left(i\frac{\omega_R^2}{42} - \frac{1}{2} + \frac{z^2}{4}\right) c \end{aligned}$$

$$\Rightarrow \boxed{\frac{d^2 c}{dz^2} + \left(i\frac{\omega_R^2}{42} + \frac{1}{2} - \frac{z^2}{4}\right) c = 0}$$

Compare to harmonic oscillator: $-\frac{\hbar^2}{2m} \psi'' + \frac{1}{2} m \omega^2 x^2 \psi = E \psi$

$$\text{or } \frac{d^2 \psi}{d\tilde{x}^2} + \left(n + \frac{1}{2} - \frac{\tilde{x}^2}{4}\right) \psi = 0 \quad \text{with } E = \hbar \omega \left(n + \frac{1}{2}\right)$$

$$\tilde{x} = \sqrt{\frac{2\hbar}{m\omega}}$$

\Rightarrow here $n = i\frac{\omega_R^2}{42}$ imaginary.

Boundary conditions $a = e^{-i\frac{1}{2}\Delta t^2} c = 0$ at $t = -\infty$

$$\Rightarrow c(-\infty \cdot e^{-i\frac{\pi}{4}}) = 0$$

Also: $b(-\infty) = 1 \Rightarrow \dot{a} = -i\frac{\omega_R}{2} e^{-\frac{1}{2}i\Delta t^2} = -i\frac{\omega_R}{2} e^{\frac{z^2}{4}}$ at $t = -\infty$

$$\begin{aligned} &= e^{-\frac{1}{2}i\Delta t^2} \dot{c} = e^{\frac{z^2}{4}} \frac{dc}{dz} \sqrt{2} e^{-i\frac{\pi}{4}} \\ &\Rightarrow \frac{dc}{dz}(-\infty e^{-i\frac{\pi}{4}}) = \frac{\omega_R}{2\sqrt{2}} e^{\frac{z^2}{4}} e^{-i\frac{\pi}{4}} \end{aligned}$$

Solution: Parabolic cylinder functions $c(z) = \frac{\omega_R}{2\sqrt{2}} e^{-\frac{\pi}{4}\frac{\omega_R^2}{42}} D_{-1-i\frac{\omega_R^2}{42}}(iz)$
(assume $2 > 0$).

With these one finds $\boxed{|a(\infty)|^2 = 1 - e^{-\frac{\pi}{2}\frac{\omega_R^2}{42}}}$