Lecture 6

5.3 (Continued)

- Rabi (1936) calculated Probability of a "spin flip":
  spinor originally at north pole $\rightarrow$
  $\rightarrow$ south pole.

- Combination $\vec{B}_0 \parallel \vec{e}_z$ and $\vec{B}_1(t) = B_1 \cos\omega t \, \vec{e}_x +$
  $+ B_1 \sin\omega t \, \vec{e}_y$

- Remind: Arbitrary spinor

$$|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha|0\rangle + \beta|1\rangle$$

qubit: coherent superposition of two bits 0 and 1

$$|\alpha|^2 + |\beta|^2 = 1$$

$|\alpha|^2$ ↑ prob. z-comp in state $|0\rangle$; $|\beta|^2$ ↑ in $|1\rangle$

- Remind: Spinor on the Bloch sphere

$$|\xi_n^+\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}e^{i\phi}|1\rangle$$

- Prob. ~~Spinor~~ spinor to be located at the south pole

$$|\langle 1|\xi_n^+\rangle|^2 = \sin^2\frac{\theta}{2} = \frac{1-\cos\theta(t)}{2} = \frac{1-n_z(t)}{2}$$

At $t=0$ $\quad \vec{n}(0) = (0,0,1) = (n_x(0), n_y(0), n_z(0))$

• Rewind: Larmor precession in const $\vec{B}$

$$\frac{d}{dt}\langle\vec{\sigma}\rangle = \langle\vec{\sigma}\rangle\times\vec{\Omega}, \qquad (*)$$

$$\vec{\Omega} = \frac{g\mu_B}{\hbar}\vec{B},$$ free electron $g=2$

$$\mu_B = \frac{e\hbar}{2m_e}$$

$$\langle\sigma_z\rangle = \langle\xi_n^+|\sigma_z|\xi_n^+\rangle = \cos\theta = n_z$$

• Derivation of $n_z(t)$:

(i) from fixed time-indep. ref. frame →
→ rotating ref. frame with ω;

(ii) in rotating frame use $(*)$;

(iii) go back to the fixed ref. frame

$$\Downarrow$$

$$\sin^2\left(\frac{\theta(t)}{2}\right) = \frac{\sin^2\chi(t)}{2}\left[1-\cos\delta(t)\right] =$$

$$= \frac{\omega_1^2}{2\left[\omega_1^2+(\omega_0-\omega)^2\right]}\left\{1-\cos\left[\sqrt{(\omega-\omega_0)^2+\omega_1^2}\,t\right]\right\}$$

$$\omega_0 = \frac{g\mu_B B_0}{\hbar}, \quad \omega_1 = \frac{g\mu_B B_1}{\hbar}$$

$\max P_{0\to 1}\{|0\rangle \to |1\rangle\}$ at $\omega = \omega_0$

$\parallel$

$\sin^2\left(\frac{\omega_1 t}{2}\right)$

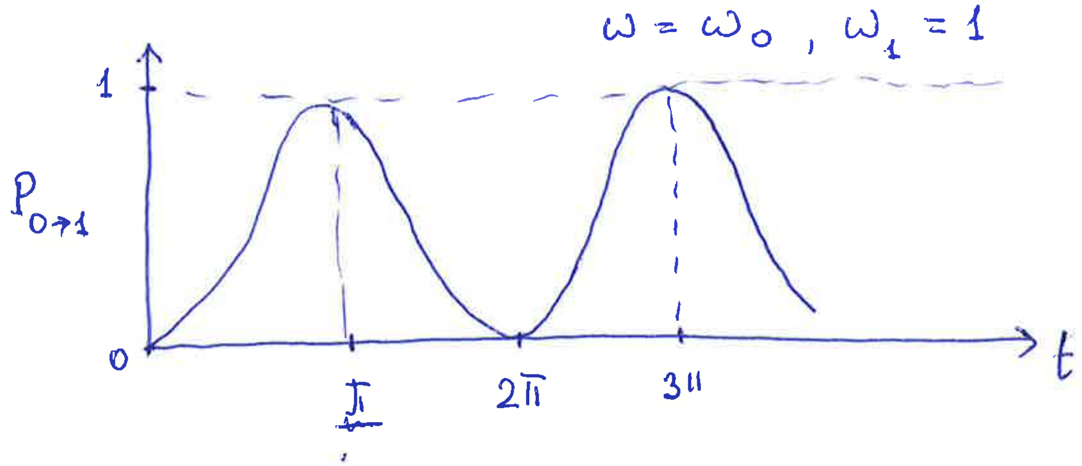
Magnetic field B_1 in $(x-y)$ plane must rotate at frequency equal to Larmor freq. in order for the spinor to reach south pole

- Adjust t such that $\frac{\omega_1 t}{2} = \frac{\pi}{2} \Rightarrow \boxed{t = \frac{\pi}{\omega_1}}$

shortest time to reach south pole

π-pulse

- For $t = \frac{\pi}{2\omega_1}$ $\quad \frac{\pi}{2}$ pulse $\quad |0\rangle \to \frac{|0\rangle + i|1\rangle}{\sqrt{2}}$.



<u>Remark 1</u>. Rabi formula

Time-dependent Pauli (Schrödinger) eq

<u>Remark 2</u>. Can be generalized for a spin transfer between any two points of the Block sphere starting at $t=0$ other than the north pole.

<u>Remark 3</u>. ~~Radi~~ NMR: nuclei in strong const magnetic field perturbed by oscillating magn. field => respond by e/m signal => ~~get information~~ magnetic moment μ

<u>Remark 4</u>. Two level atom in the laser field: full analogy => quantum optics

6. The Density Matrix

- Useful concept to deal with large collection of spinors with ~~p~~ prob. distr. at $t=0$

- Bloch sphere $\xrightarrow{\text{extension}}$ Bloch ball: interior of Block sph.

- interactions between spinors and interaction with environment

- phenomenological Bloch's eqs.

6.1 Density matrix concept: Case of a pure state

- general ket $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

This state is also referred to as <u>pure state</u>, $|\alpha|^2 + |\beta|^2 = 1$

- 2×2 <u>density matrix</u>

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix} =$$

$$= \begin{pmatrix} \alpha\alpha^* & \alpha\beta^* \\ \beta\alpha^* & \beta\beta^* \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \beta\alpha^* & |\beta|^2 \end{pmatrix} \qquad (1)$$

6.12

6.2) Properties of the density matrix

1) definite positive, i.e. for any $|\psi'\rangle$

$$\langle\psi'|\rho|\psi'\rangle \geq 0$$

2) Hermitian => eigenvalues are real and positive

$\rho = \overline{\rho^T}$ transpose & c.c.

3) $\mathrm{Tr}(\rho) = 1$

4) $\rho^2 = \rho$ (exercise)

5) $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$,

Average values of individual spin components,

$$\langle S_x \rangle = \langle \psi | S_x | \psi \rangle = \frac{\hbar}{2}(\alpha\beta^* + \beta\alpha^*) =$$

$$= Tr(\rho S_x), \qquad (2a)$$

$$\langle S_y \rangle = \langle \psi | S_y | \psi \rangle = \frac{\hbar}{2i}(\beta\alpha^* - \alpha\beta^*) =$$

$$= Tr(\rho S_y), \qquad (2b)$$

$$\langle S_z \rangle = \langle \psi | S_z | \psi \rangle = \frac{\hbar}{2}(|\alpha|^2 - |\beta|^2) =$$

$$= Tr(\rho S_z) \qquad (2c)$$

$$\langle S_x \rangle = \left(\frac{\hbar}{2}\alpha^*(1,0) + \frac{\hbar}{2}\beta^*(0,1)\right)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\left(\alpha\begin{pmatrix}1\\0\end{pmatrix} + \beta\begin{pmatrix}0\\1\end{pmatrix}\right) = \qquad (6.8a)$$

$$= \frac{\hbar}{2}\alpha\alpha^*(1,0)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} + \frac{\hbar}{2}\beta^*\alpha(0,1)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} +$$

$$+ \frac{\hbar}{2}\alpha^*\beta(1,0)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} + \frac{\hbar}{2}\beta^*\beta(0,1)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} =$$

$$= \frac{\hbar}{2}|\alpha|^2(0 \;\; 1)\begin{pmatrix}1\\0\end{pmatrix} + \frac{\hbar}{2}\beta^*\alpha(1 \;\; 0)\begin{pmatrix}1\\0\end{pmatrix} + \frac{\hbar}{2}\alpha^*\beta(0 \;\; 1)\begin{pmatrix}0\\1\end{pmatrix} + \frac{\hbar}{2}|\beta|^2(1 \;\; 0)\begin{pmatrix}0\\1\end{pmatrix}$$

$$= \frac{\hbar}{2}|\alpha|^2\cdot 0 + \frac{\hbar}{2}\beta^*\alpha\cdot 1 + \frac{\hbar}{2}\alpha^*\beta\cdot 1 + \frac{\hbar}{2}|\beta|^2\cdot 0 = \frac{\hbar}{2}(\alpha^*\beta + \beta^*\alpha)$$

$$\mathrm{Tr}(\rho S_x) = \frac{\hbar}{2}\mathrm{Tr}(\rho S_x) \underset{(1)}{=} \frac{\hbar}{2}\mathrm{Tr}\left[\begin{pmatrix}\alpha\alpha^* & \alpha\beta^*\\ \beta\alpha^* & \beta\beta^*\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right] =$$

$$= \frac{\hbar}{2}\mathrm{Tr}\begin{bmatrix}\alpha\beta^* & \alpha\alpha^*\\ \beta\beta^* & \beta\alpha^*\end{bmatrix} = \frac{\hbar}{2}(\alpha\beta^* + \beta\alpha^*) \implies \langle S_x \rangle = \mathrm{Tr}(\rho S_x)$$

6. For any pure state

$$\langle S_x \rangle^2 + \langle S_y \rangle^2 + \langle S_z \rangle^2 = \frac{\hbar^2}{4}$$

(consequence of 5.) ~~Exercise 6.9a~~

<u>Exercise</u>. Is there a state of the form

$$|\psi\rangle = \alpha|+\rangle + \beta|-\rangle,$$

which represents a non-polarized spin, i.e. the state

$$\langle S_x \rangle = \langle S_y \rangle = \langle S_z \rangle = 0 \quad ?$$

<u>Solution</u>. 1) For $\langle S_x \rangle = 0 \Rightarrow \alpha^* \beta$ is purely Im

2) For $\langle S_y \rangle = 0 \Rightarrow \alpha^* \beta$ purely Re

$$\Downarrow$$

$$\alpha^* \beta = 0$$

$$\Downarrow$$

- $\alpha = 0, \; |\beta| = 1, \; \langle S_z \rangle = -\frac{\hbar}{2}$ OR
- $\beta = 0, \; |\alpha| = 1, \; \langle S_z \rangle = +\frac{\hbar}{2}$

<u>Conclusion</u>. $\langle S_z \rangle$ cannot be zero simultaneously with $\langle S_x \rangle$ and $\langle S_y \rangle \Rightarrow$ The state $|\psi\rangle = \alpha|+\rangle + \beta|-\rangle$ cannot represent a non-polarized state

~~Proof~~

<u>Exercise.</u> The average value

$\langle M \rangle = \langle \psi | M | \psi \rangle$ of any operator M

can be calculated as (any 2×2 matrix)

$$\langle M \rangle = \mathrm{Tr}(\rho M) = \mathrm{Tr}\left[\begin{pmatrix} \alpha\alpha^* & \alpha\beta^* \\ \beta\alpha^* & \beta\beta^* \end{pmatrix}\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\right]$$

$$\| \qquad\qquad\qquad\qquad \|$$

$$(\alpha^* \;\; \beta^*)\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \ldots \qquad \ldots$$

(6.3) Liouville equation:
Time evolution of the density matrix

$$\frac{d\rho}{dt} = \frac{d}{dt}\left[|\psi\rangle\langle\psi|\right] =$$

$$= \left[\left(\frac{d}{dt}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(\frac{d}{dt}\langle\psi|\right)\right] =$$

$$= \frac{-i}{\hbar}\left[H|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|H\right] \Rightarrow$$

$$= \frac{-i}{\hbar}[H,\rho]$$

commutator

$$\boxed{\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho]}$$

Liouville (3)

[...] commutator

Exercise. With Liouville eq prove Ehrenfest equation (lect. 5)

$$\frac{d}{dt} < M(t) > = -\frac{i}{\hbar} < [M, H] > + < \frac{dM}{dt} >$$

Sol: Start from

$$< M > = \mathrm{Tr}(\rho M)$$

$$\frac{d}{dt} < M > = \frac{d}{dt} \mathrm{Tr}(\rho M) =$$

$$= \mathrm{Tr}\left(\frac{d\rho}{dt} M\right) + \mathrm{Tr}\left(\rho \frac{dM}{dt}\right) \overset{(3)}{=}$$

$$= -\frac{i}{\hbar} \mathrm{Tr}\left([H, \rho] M\right) + < \frac{dM}{dt} > =$$

$$= -\frac{i}{\hbar} \mathrm{Tr}\left(H\rho M - \rho H M\right) + < \frac{dM}{dt} > =$$

$$= \cancel{-\frac{i}{\hbar} \mathrm{Tr}} \left\{ \mathrm{Tr}(AB) = \mathrm{Tr}(BA) \right\} =$$

$$= -\frac{i}{\hbar} \mathrm{Tr}\left(\rho M H - \rho H M\right) + < \frac{dM}{dt} > =$$

$$= -\frac{i}{\hbar} \mathrm{Tr}\left(\rho [M, H]\right) + < \frac{dM}{dt} > =$$

$$= -\frac{i}{\hbar} < [M, H] > + < \frac{dM}{dt} >$$ Ehrenfest

6.4 Density matrix associated with the spinor on the Bloch sphere

(general form of)

(Intospin 5.24)

- Recall that $|\psi\rangle = |\xi_n^{\dagger}\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}e^{i\phi}|1\rangle$

dagger

- By definition

$$\rho(\theta,\phi) = |\psi\rangle\langle\psi| = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix} \left(\cos\frac{\theta}{2},\ \sin\frac{\theta}{2}e^{-i\phi}\right)$$

$$= \begin{pmatrix} \cos^2\frac{\theta}{2} & \cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{-i\phi} \\ \cos\frac{\theta}{2}\sin\frac{\theta}{2}e^{i\phi} & \sin^2\frac{\theta}{2} \end{pmatrix} \qquad (4)$$

Exercise. Show explicitly that $\rho(\theta,\phi)$ satisfy the properties 1-4 of the density matrix.

6.5 Pure versus mixed state

a) Example 1

- Start from (Y),
  - Assumption: uniform distributions of spinors on Bloch sphere
- Introduce

$$\rho = \frac{1}{4\pi}\int d\Omega\, \rho(\theta,\varphi) = \frac{1}{4\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta\, \rho(\theta,\varphi)$$

- $\rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$

- Check properties 1–4 of the density matrix
  1) for any ψ $\langle\psi|\rho|\psi\rangle \geq 0$ OK
  2) Hermitian, $\rho = \overline{\rho^T}$ (transpose and c.c)
     => eigenvalues are real and positive OK
  3) $Tr(\rho) = 1$ OK
  4) $\rho^2 = \rho$ NO: $\rho^2 = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}$,

$$Tr(\rho^2) = 0.5$$

  5) Averaged values of spin components

$$\langle S_i \rangle = Tr(\rho S_i) = 0, \quad i = x, y, z$$

Conclusions:

1. The density matrix obtained by averaging over the angles seems to represent a collection of spinors uniformly distributed on the Bloch sphere.

2. For that distribution, we do not expect an average magnetic moment for the collection of spinors

b) Example 2.

- start from (normalized) kets

$$|a_1\rangle = \sqrt{\frac{3}{5}}\,|0\rangle + \sqrt{\frac{2}{5}}\,|1\rangle$$

non-orthogonal

$$|a_2\rangle = \sqrt{\frac{3}{5}}\,|0\rangle - \sqrt{\frac{2}{5}}\,|1\rangle$$

- Consider

$$\rho = \frac{1}{2}|a_1\rangle\langle a_1| + \frac{1}{2}|a_2\rangle\langle a_2|$$

- Exercise

1) $\rho = \frac{3}{5}|0\rangle\langle 0| + \frac{2}{5}|1\rangle\langle 1|$ (5)

2) $\mathrm{Tr}(\rho) = 1$

3) $\mathrm{Tr}(\rho^2) < 1$

4) $\langle S_x\rangle = \langle S_y\rangle = 0,\ \langle S_z\rangle = \frac{\hbar}{4} \Rightarrow$

$$\Rightarrow \langle S_x^{\cancel{2}}\rangle^2 + \langle S_y^{\cancel{2}}\rangle^2 + \langle S_z\rangle^2 = \frac{\hbar^2}{16} < \frac{\hbar^2}{4}$$

for the case of pure state

- Eq. (5): superposition of the density matrices associated with the spinors $|0\rangle$ and $|1\rangle$ with additional property that the sum of coef. for individual matrices is 1.

c) Generalization of (5):
set of normalized spinors on Bloch sphere,

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| = \sum_j p_j \rho_j, \qquad (6)$$

p_j: prob. find spinor in state $|\psi_j\rangle$

$$\sum_j p_j = 1.$$

<u>Exercises.</u>

1. Properties 1-3 for density matrix are still satisfied
2. Using Eq (6) show that $\mathrm{Tr}(\rho^2) < 1$.