Lecture 7

6. The Density Matrix (continued)

6.6 Generalized Bloch vector

- Reminder: Density matrix for a set of normalized spinors on the Bloch sphere

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| = \sum_j p_j \rho_j \qquad (1)$$

p_j ↑ prob. find spinor in state $|\psi_j\rangle$, $\sum_j p_j = 1$.

- Reminder. Bloch vector: unit vector $\vec{n}$ representing spinor $|\xi_n^+\rangle$ on the Bloch sphere.

- $\vec{V}$: generalized Bloch vector associated with collection of spinors described by d.m. (1)

$$\langle \vec{V} \rangle = \mathrm{Tr}(\rho \vec{V}) = \mathrm{Tr}\Big[\sum_j p_j |\psi_j\rangle\langle\psi_j| \vec{V} \Big] =$$

$$= \sum_j p_j \mathrm{Tr}\Big[|\psi_j\rangle\langle\psi_j| \vec{V} \Big] = \big\{ \mathrm{Tr}(AB) = \mathrm{Tr}(BA) \big\}$$

$$= \sum_j p_j \mathrm{Tr}\Big[\langle\psi_j| \vec{V} |\psi_j\rangle \Big] = \sum_j p_j \langle\psi_j|\vec{V}|\psi_j\rangle$$

$$= \sum_j p_j \vec{v}_j \quad , \quad \vec{v}_j = \langle\psi_j|\vec{V}|\psi_j\rangle \qquad (2)$$

$\Downarrow$

Generalized Bloch vector $\langle \vec{V} \rangle$ corresponding to ensemble of pure states $|\psi_j\rangle$ is the weighted vector sum of Bloch vectors representing members of ensemble.

(6.7) Concept of the Bloch ball

Digression.

A. Trivial decomposition of any 2×2 matrix

$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} =$$

$$= m_{11}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + m_{12}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + m_{21}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + m_{22}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

4 matrices form complete basis for all 2×2 matrices

B. Non-trivial decomposition

$$M = \frac{m_{11}+m_{22}}{2} I + \frac{m_{11}-m_{22}}{2}\sigma_z + \frac{m_{12}+m_{21}}{2}\sigma_x +$$

$$+ i\,\frac{m_{12}-m_{21}}{2}\sigma_y \qquad (B1)$$

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(easy proof)

4 matrices $(I, \sigma_x, \sigma_y, \sigma_z)$ form a complete basis in the space of 2×2 matrices

- In a more condensed form

$$M = a_0 I + \vec{a}\,\vec{\sigma} \qquad (B2)$$

where $a_0 = \frac{1}{2}\mathrm{Tr}(M)$

$$\vec{a} = \frac{1}{2}\mathrm{Tr}(M\vec{\sigma})$$

From (B1) and (B2): M is Hermitian if a_0 and 3 components of $\vec{a}$ are real.

-------- end of digression ----

a) <u>Fact</u>. Density matrices associated with pure or mixed states have general form

$$\rho = \begin{bmatrix} a+b & c-id \\ c+id & a-b \end{bmatrix} \qquad (3)$$

a, b, c, d real.

Take (B1), (B2) and use $Tr(\rho) = 1 \Rightarrow \boxed{a = \frac{1}{2}}$

$$\rho = \frac{1}{2}\underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}_{I} + b\underbrace{\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}}_{\sigma_z} + c\underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{\sigma_x} + d\underbrace{\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}}_{\sigma_y}$$

$$\Downarrow$$

$$\rho = \frac{1}{2}\left[I + 2c\sigma_x + 2d\sigma_y + 2b\sigma_z\right] \qquad (4)$$

find $\Downarrow$ b, c, d via average components of spin operator

$$<\sigma_x> = Tr(\rho\sigma_x) = 2c \qquad (5a)$$

$$<\sigma_y> = Tr(\rho\sigma_y) = 2d \qquad (5b)$$

$$<\sigma_z> = Tr(\rho\sigma_z) = 2b \qquad (5c)$$

b) Proof (5a)

$$\langle \sigma_x \rangle = \mathrm{Tr}(\rho \sigma_x) =$$

$$= \mathrm{Tr}\Big[\frac{1}{2} I \sigma_x + c \underbrace{\sigma_x^2}_{= I} + d \underbrace{\sigma_y \sigma_x}_{-i\sigma_z} + b \underbrace{\sigma_z \sigma_x}_{-i\sigma_y} \Big] = 2c$$

$$I\sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = 0,$$ see lecture 3 properties of Pauli matr

• Back to (4):

$$\rho = \frac{1}{2}\left[I + \vec{v}\vec{\sigma} \right], \qquad (6)$$

$$\vec{v} = (v_x, v_y, v_z) = (\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle)$$

c) Density matrix pure state $\mathrm{Tr}(\rho)^2 = 1 \Rightarrow$

$$\Rightarrow (\text{take } (6)) \Rightarrow \mathrm{Tr}(\rho^2) =$$

$$= \frac{1}{4}\mathrm{Tr}\Big[\underbrace{I^2}_{= I} + \underbrace{I(\vec{v}\vec{\sigma})}_{= 0} + \underbrace{(\vec{v}\vec{\sigma})I}_{= 0} + (\vec{v}\vec{\sigma})^2 \Big] =$$

$$= \left\{ \text{Recall } \mathrm{Tr}(\sigma_j) = 0, \ \sigma_x \sigma_y = i\sigma_z, \dots \right\} =$$

$$= \frac{1}{4}\mathrm{Tr}\left[I + v_x^2 \sigma_x^2 + v_y^2 \sigma_y^2 + v_z \sigma_z^2 \right] = \left\{ \mathrm{Tr}[\sigma_j^2] = 1 \right\}$$

$$= \frac{1}{4}\mathrm{Tr}\left[I + I\vec{v}^2 \right] \overset{\mathrm{Tr}\, I = 0}{=} \frac{1}{2}(1 + \vec{v}^2) \overset{\text{pure state}}{=} 1 \Rightarrow \boxed{|\vec{v}| = 1}$$

d) Density matrix mixed state

Back to (3)

- Eigenvalues from $\det(\rho - \lambda I) = 0$

$$\begin{vmatrix} a+b-\lambda & c-id \\ c+id & a-b-\lambda \end{vmatrix} = 0$$

$$(a+b-\lambda)(a-b-\lambda) - (c+id)(c-id) =$$

$$= a^2 - b^2 - \lambda(a-b) - \lambda(a+b) + \lambda^2 - (c^2+d^2) = 0$$

$$\lambda^2 - 2a\lambda + a^2 - b^2 - c^2 - d^2 = 0$$

Recall: $a = 1/2$ since $\mathrm{Tr}\,\rho = 1$

$$\lambda^2 - \lambda + \frac{1}{4} - b^2 - c^2 - d^2 = 0$$

Recall: $x^2 + px + q = 0 \Rightarrow x_{1,2} = -\frac{p}{2} \pm \sqrt{\left(\frac{p}{2}\right)^2 - q}$

$$\lambda_{1,2} = \frac{1}{2} \pm \sqrt{b^2 + c^2 + d^2}$$

Recall: Hermitian matrix $\Rightarrow$ all eigenvalues positive

$$\Downarrow$$

$$\sqrt{b^2+c^2+d^2} \leq 1/2 \overset{(5),(6)}{\Longrightarrow} |\vec{v}| \leq 1$$

Generalized Bloch vector $\vec{v}$ associated with mixed state represent point inside Bloch sphere $\Rightarrow$ Bloch ball

6.8 Time evolution of the density matrix: Case of mixed state

Take ensemble of spinors

$$\frac{d\rho}{dt} = \frac{d}{dt}\left[\sum_j p_j |\psi_j\rangle\langle\psi_j|\right] = \left\{\text{similar to pure state}\right\}$$

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

$$= \sum_j p_j \left[\left(\frac{-i}{\hbar}H|\psi_j\rangle\right)\langle\psi_j| + |\psi_j\rangle\left(\frac{i}{\hbar}\langle\psi_j|H\right)\right] =$$

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

$$\boxed{\frac{d\rho}{dt} = \frac{-i}{\hbar}[H, \rho]} \qquad \text{Liouville eq} \qquad (7)$$

Time evolution of the density matrix for a mixed state is equivalent to that for a pure state (see lecture 6).

6.9 Equations of motion for the generalized Bloch vector

Use (6) $\rho = \frac{1}{2}\left[I + \vec{\nu}\,\vec{\sigma} \right]$, $\vec{\nu} = \langle \vec{\sigma} \rangle$

$$\frac{d\nu_j}{dt} = \frac{d}{dt}\left(\mathrm{Tr}\left[\rho \sigma_j \right] \right) =$$

$$= \mathrm{Tr}\left[\sigma_j \frac{d\rho}{dt} \right] = \frac{-i}{\hbar} \mathrm{Tr}\left[\sigma_j \left[H, \rho \right] \right] \xRightarrow{(6)}$$

$$\frac{d\nu_j}{dt} = -\frac{i}{2\hbar} \mathrm{Tr}\left[\sigma_j \left[H, \left(I + \vec{\nu}\,\vec{\sigma} \right) \right] \right] \qquad (8)$$

<u>Remark</u>. Evolution of 3 components generally is coupled.

6.10 Spin-1/2 particle in magnetic field (spatially independent) 7.9

$$H = -\gamma \vec{S}\cdot\vec{B} = -\gamma \frac{\hbar}{2}(\vec{\sigma}\vec{B}) \qquad (9)$$

γ gyromagnetic factor

$$\frac{d\nu_j}{dt} = -\frac{i}{2\hbar}\mathrm{Tr}\left[\sigma_j\left[-\gamma\frac{\hbar}{2}(\vec{\sigma}\vec{B}),(I+\vec{\nu}\vec{\sigma})\right]\right] =$$

$$= \frac{i\gamma}{4}\mathrm{Tr}\left[\sigma_j(\vec{\sigma}\vec{B})(\cancel{I}+\vec{\nu}\vec{\sigma}) - \sigma_j(\cancel{I}+\vec{\nu}\vec{\sigma})(\vec{\sigma}\vec{B})\right]$$

$$= \frac{i\gamma}{4}\mathrm{Tr}\left[\sigma_j(\sigma_x B_x+\sigma_y B_y+\sigma_z B_z)(I+\nu_x\sigma_x+\nu_y\sigma_y+\nu_z\sigma_z) - \right.$$

$$\left. - \sigma_j(I+\nu_x\sigma_x+\nu_y\sigma_y+\nu_z\sigma_z)(\sigma_x B_x+\sigma_y B_y+\sigma_z B_z)\right]$$

$= \{$ recall $\sigma_x\sigma_y = i\sigma_z, \ldots;$ $\mathrm{Tr}(\sigma_j)=0 \Rightarrow$ quadratic in σ_j terms $\sim \sigma_j\sigma_i$, $i\neq j$ disappear $\}$

Focus on x-component

$$\frac{d\nu_x}{dt} = \frac{i\gamma}{4}\mathrm{Tr}\left[\sigma_x(\sigma_x B_x+\sigma_y B_y+\sigma_z B_z)(I+\nu_x\sigma_x+\nu_y\sigma_y+\nu_z\sigma_z)\right.$$

$$\left. - \sigma_x(I+\nu_x\sigma_x+\nu_y\sigma_y+\nu_z\sigma_z)(\sigma_x B_x+\sigma_y B_y+\sigma_z B_z)\right] =$$

Terms with I disapper

$$
\begin{aligned}
&= \frac{ig}{4} \mathrm{Tr}\Big[\sigma_x \left(\sigma_x B_x + \sigma_y B_y + \sigma_z B_z\right)\left(\partial_x \sigma_x + \partial_y \sigma_y + \partial_z \sigma_z\right) \\
&\qquad - \sigma_x \left(\partial_x \sigma_x + \partial_y \sigma_y + \partial_z \sigma_z\right)\left(\sigma_x B_x + \sigma_y B_y + \sigma_z B_z\right)\Big] \\
&= \frac{ig}{4} \mathrm{Tr}\Big[\cancel{\sigma_x \sigma_x B_x \partial_x \sigma_x} + \sigma_x \sigma_y B_y \partial_x \sigma_x + \sigma_x \sigma_z B_z \partial_x \sigma_x + \\
&\qquad + \sigma_x \sigma_x B_x \partial_y \sigma_y + \cancel{\sigma_x \sigma_y B_y \partial_y \sigma_y} + \sigma_x \sigma_z B_z \partial_y \sigma_y + \\
&\qquad + \sigma_x \sigma_x B_x \partial_z \sigma_z + \sigma_x \sigma_y B_y \partial_z \sigma_z + \sigma_x \sigma_z B_z \partial_z \sigma_z - \\
&\qquad - \cancel{\sigma_x \partial_x \sigma_x \sigma_x B_x} - \sigma_x \partial_y \sigma_y \sigma_x B_x - \sigma_x \partial_z \sigma_z \sigma_x B_x - \\
&\qquad - \sigma_x \partial_x \sigma_x \sigma_y B_y - \cancel{\sigma_x \partial_y \sigma_y \sigma_y B_y} - \sigma_x \partial_z \sigma_z \sigma_y B_y - \\
&\qquad - \sigma_x \partial_x \sigma_x \sigma_z B_z - \sigma_x \partial_y \sigma_y \sigma_z B_z - \sigma_x \partial_z \sigma_z \sigma_z B_z \Big] \\
&= \frac{ig}{4} \mathrm{Tr}\Big[\sigma_x \sigma_x \sigma_y \left(B_x \partial_y - \partial_x B_y\right) + \sigma_x \sigma_x \sigma_z \left(B_x \partial_z - \partial_x B_z\right) + \\
&\qquad + \sigma_x \sigma_y \sigma_x \left(B_y \partial_x - \partial_y B_x\right)\Big] \\
&+ \frac{ig}{4} \mathrm{Tr}\Big[\sigma_x \sigma_y \sigma_z \left(B_y \partial_z - \partial_y B_z\right) + \sigma_x \sigma_z \sigma_x \left(B_z \partial_x - \partial_z B_x\right) + \\
&\qquad + \sigma_x \sigma_z \sigma_y \left(B_z \partial_y - \partial_z B_y\right)\Big] =
\end{aligned}
$$

have a look at these

$$= \{ \sigma_p \sigma_q + \sigma_q \sigma_p = 0 \,,\ p \neq q \,,\ p,q = x,y,z \} =$$

$$= \frac{i\gamma}{4} \mathrm{Tr} \Big[\sigma_x^2 \sigma_y (B_x \vartheta_y - \vartheta_x B_y) + \sigma_x^2 \sigma_z (B_x \vartheta_z - \vartheta_x B_z)$$

(AB)C = A(BC) $\rightarrow$

$$- \sigma_x^2 \sigma_y (B_y \vartheta_x - \vartheta_y B_x) \Big]$$

$$+ \frac{i\gamma}{4} \mathrm{Tr} \Big[\underline{\sigma_x \sigma_y \sigma_z (B_y \vartheta_z - \vartheta_y B_z)} + \sigma_x^2 \sigma_z (B_z \vartheta_x - \vartheta_z B_x)$$

$$\underline{+ \sigma_x \sigma_z \sigma_y (B_z \vartheta_y - \vartheta_z B_y) \Big]} =$$

$$= \{ \sigma_j^2 = 1 \,,\ \mathrm{Tr}(\sigma_j) = 0 \} = \text{only } 2$$

terms __ remain! $\Rightarrow$

$$\frac{d\vartheta_x}{dt} = \frac{i\gamma}{4} \mathrm{Tr} \Big[\sigma_x \sigma_y \sigma_z (B_y \vartheta_z - \vartheta_y B_z) +$$

$$+ \sigma_x \sigma_z \sigma_y (B_z \vartheta_y - \vartheta_z B_y) \Big] =$$

$$= \frac{i\gamma}{4} (B_y \vartheta_z - \vartheta_y B_z) \mathrm{Tr} \big[\sigma_x \sigma_y \sigma_z - \sigma_x \sigma_z \sigma_y \big] =$$

$$= \{ \sigma_x \sigma_y \sigma_z = iI \,,\ \sigma_x \sigma_z \sigma_y = -iI \,,\ \mathrm{Tr}(I) = 2 \} \Rightarrow$$

$$\Rightarrow \quad \frac{dv_x}{dt} = -\gamma\left(B_y v_z - v_y B_z\right) \qquad (10a)$$

Similarly, $$\frac{dv_y}{dt} = -\gamma\left(B_z v_x - v_y B_z\right) \qquad (10b)$$

$$\frac{dv_z}{dt} = -\gamma\left(B_x v_y - v_x B_y\right) \qquad (10c)$$

$$\Downarrow$$

$$\frac{d\vec{v}}{dt} = \gamma\left(\vec{v} \times \vec{B}\right) \qquad (11)$$

6.11 Collection of spinors in constant magnetic field $\vec{B}_0 \parallel \vec{e}_z$

$$\frac{d\nu_x}{dt} = -\gamma B_0 \nu_y$$

$$\frac{d\nu_y}{dt} = -\gamma B_0 \nu_x$$

$$\frac{d\nu_z}{dt} = -\cancel{\gamma} 0$$

$$\frac{d}{dt}\left(\nu_x^2 + \nu_y^2\right) = 0$$

generalized Bloch vector rotates on a cone centered around z-axis with Larmor frequency

Expected result

Digression ----------

- self-rotation of charged entity $\Rightarrow$
  $\Rightarrow$ magnetic moment $\vec{\mu}_e$
- magnetic moment interact with external magnetic field $\vec{B}$ $\Rightarrow$

$$E_{int} = -\vec{\mu}_e \vec{B}$$

- Landé $\quad \dfrac{\vec{\mu}_e}{\mu_B} = g_e \dfrac{\vec{S}}{\hbar}$ $\quad \vec{S}$ = angular momentum of self-rotation

g_e ↑ gyromagnetic factor, number

$$\mu_B = \frac{e\hbar}{2mc} \;\; \text{CGS} \;\; = \frac{e\hbar}{2m} \;\; \text{SI}$$

Bohr magneton (see lect. 3)

$$H_B = -\frac{g_e \mu_B}{\hbar} \vec{S}\vec{B} = -\frac{g_e}{2}\mu_B (\vec{\sigma}\vec{B})$$

~~For a single spin g=2~~

$$\vec{\mu}_e = g_e \frac{\mu_B}{\hbar} \vec{S}, \quad \vec{\mu}_e \text{ magnetic moment}$$

g_e ↑ electron spin g-factor, $g_s = |g_e| = -g_e = 2$

$+\frac{2\mu_B}{\hbar} B S_z$ High Energy state north pole

South pole ; low energy state

6.12 Bloch equations and relaxation times

In equilibrium:

$$(\nu_x, \nu_y, \nu_z) = (0, 0, \nu_{z0})$$

$$\frac{d\nu_z}{dt} = \gamma(\vec{\nu} \times \vec{B})_z + \frac{\nu_{z0} - \nu_z}{T_1}$$

longitudinal relaxation time T_1

$$\frac{d\nu_x}{dt} = \gamma(\vec{\nu} \times \vec{B})_x - \frac{\nu_x}{T_2}$$

transverse relaxation time

$$\frac{d\nu_y}{dt} = \gamma(\vec{\nu} \times \vec{B})_y - \frac{\nu_y}{T_2}$$

Stochastic Bloch eqs

$$\frac{d\nu_z}{dt} = \gamma(\vec{\nu} \times \vec{B})_z + \frac{\nu_z - \nu_{z0}}{T_1} + \xi_1(t)$$

FDT?

$$\frac{d\vec{\nu}_\perp}{dt} = \gamma(\vec{\nu} \times \vec{B})_\perp - \frac{\vec{\nu}_\perp}{T_2} + \vec{\xi}_\perp(t)$$

Interesting analogy.

$\vec{B}_0 \parallel \vec{e}_z$

$$\frac{d\vartheta_x}{dt} = \cancel{\gamma(\vec{\vartheta}_0 \times} \; \gamma B_0 \vartheta_y - \frac{\vartheta_x}{T_2}$$

$$\frac{d\vartheta_y}{dt} = -\gamma B_0 \vartheta_x - \frac{\vartheta_y}{T_2}$$

$$\vartheta_x = \vartheta_0 e^{-t/T_2} \cos\omega t, \quad \vartheta_y = -\vartheta_0 e^{-t/T_2} \sin\omega t$$