Lecture 5

Monday, June 10, 2024 9:55 AM

Chapter 5. Evolution of a Spinor on the Bloch Sphere

Rabi formula: probability of a "spin flip", i.e. probability of a spinor originally located at the north pole, to ultimately reach the south pole

Applications: NMR concepts, spin-based quantum computing

5.1 Time evolution of expectation values ($A \equiv \hat{A}$ operator)

$$\langle A(t) \rangle = \int \psi^*(x,t) A \psi(x,t)\, dx \qquad (x \equiv \vec{r})$$

$$\frac{d}{dt}\langle A(t) \rangle = \int \psi^* \frac{\partial A}{\partial t} \psi\, dx + \int \frac{\partial \psi^*}{\partial t} A \psi\, dx + \int \psi^* A \frac{\partial \psi}{\partial t}\, dx \qquad (1)$$

Schrödinger eq $\quad \dfrac{\partial \psi}{\partial t} = \dfrac{1}{i\hbar} H\psi \,, \quad \dfrac{\partial \psi^*}{\partial t} = -\dfrac{1}{i\hbar} H^* \psi^* \qquad (2)$

Plug (2) into (1)

$$\frac{d}{dt}\langle A(t) \rangle = \left\langle \frac{\partial A}{\partial t} \right\rangle - \frac{1}{i\hbar}\int (H^*\psi^*) A \psi\, dx + \frac{1}{i\hbar}\int \psi^* (AH) \psi\, dx \qquad (3)$$

Digression - - - - - - - - - - - - - - - - - - -

Self-adjoint (Hermitian) operators

$$\int u_1^*(x) A u_2(x)\, dx = \int u_2(x) A^* u_1^*(x)\, dx \qquad (4)$$

$\forall u_1, u_2$ integrable, $u_{1,2}(\infty) = \frac{d}{dx} u_{1,2} \Big|_{\pm\infty} = 0$

Only such operators represent physical (real) quantities

<u>Example 1.</u> $p_x = -i\hbar \frac{\partial}{\partial x}$

$$\underbrace{\int_{-\infty}^{\infty} u_1^* p_x u_2\, dx} = -i\hbar \int_{-\infty}^{\infty} u_1^* \frac{\partial u_2}{\partial x}\, dx = \underbrace{-i\hbar u_1^* u_2 \Big|_{-\infty}^{\infty}}_{0} + i\hbar \int_{-\infty}^{\infty} u_2 \frac{\partial u_1^*}{\partial x}\, dx =$$

$$= \underbrace{\int_{-\infty}^{\infty} u_2 p_x^* u_1\, dx}$$

<u>Example 2</u> $\quad \partial/\partial x\,? \quad \displaystyle\int_{-\infty}^{\infty} u_1^* \frac{\partial u_2}{\partial x}\, dx = -\int_{-\infty}^{\infty} u_2 \frac{\partial u_1^*}{\partial x}\, dx \neq + \int_{-\infty}^{\infty} u_2 \frac{\partial u_1^*}{\partial x}\, dx \Rightarrow$

$\Rightarrow$ linear, non-hermitian

- $\hat{C}\psi = \hat{A}(\hat{B}\psi) \Rightarrow \hat{C} = \hat{A}\hat{B}$

  $\hat{C}'\psi = \hat{B}(\hat{A}\psi) \Rightarrow \hat{C}' = \hat{B}\hat{A}$

If $\hat{C} = \hat{C}' \Rightarrow \hat{A}\hat{B} - \hat{B}\hat{A} = 0$ A, B commuting operators

If $\hat{C} \neq \hat{C}' \Rightarrow \hat{F} = \hat{A}\hat{B} - \hat{B}\hat{A} \neq 0$ commutator of A and B

- $AB = \underbrace{\frac{1}{2}(AB + BA)}_{\text{Hermitian (prove with (4))}} + \underbrace{\frac{1}{2}(AB - BA)}_{\text{non-Hermitian (except } =0)}$

$\Rightarrow$ if A Hermitian $\Rightarrow A^n = A \cdot A \cdot \ldots \cdot A$ Hermitian

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

Go back to Eq (3), take

$$\int (H^* \psi^*)(A\psi)\, dx = \{\psi = u_1, \; A\psi = u_2\} =$$

$$= \int u_2 H^* u_1^* \, dx = \int u_1^* H u_2 \, dx = \int \psi^* H A \psi \, dx \underset{(3)}{\Rightarrow}$$

$$\Rightarrow \frac{d}{dt} \langle A(t) \rangle = \langle \frac{\partial A}{\partial t} \rangle + \frac{1}{i\hbar} \int \psi^* (AH - HA) \psi \, dx$$

- Poisson bracket $[A, H] = AH - HA$

$$\boxed{\frac{d}{dt} \langle A(t) \rangle = \langle \frac{\partial A}{\partial t} \rangle + \frac{1}{i\hbar} \langle [A, H] \rangle} \quad (5a)$$

Ehrenfest Theorem

Remark 1. In some textbooks $[A, B] = BA - AB$

$$\frac{d}{dt} \langle A \rangle = \langle \frac{\partial A}{\partial t} \rangle + \frac{1}{i\hbar} \langle [H, A] \rangle \quad (5b)$$

Remark 2. In some books

$$[A, H] = \frac{1}{i\hbar}(AH - HA)$$

quantum Poisson brackets

Remark 3. Operator of (full) time derivative of operator A
of operator A

$$(5b) \to \frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{1}{i\hbar}[H, A] \Rightarrow$$

$$\frac{d}{dt}\langle A\rangle = \left\langle \frac{dA}{dt}\right\rangle = \int \psi^* \frac{dA}{dt}\psi\, dx \qquad (5c)$$

Remark 4 (Exercise)

$$\left.\begin{aligned} &\bullet\ C = A + B \Rightarrow \frac{dC}{dt} = \frac{dA}{dt} + \frac{dB}{dt} \\ &\bullet\ C = AB \Rightarrow \frac{dC}{dt} = \frac{dA}{dt}B + A\frac{dB}{dt} \end{aligned}\right\}$$

like "usual" derivative

Digression -

Operators of coordinate and momentum [lecture 1-2]

$$\hat{x} = x, \quad \hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

$$\left.\begin{aligned} &\bullet\ x(p_x\psi) = x\left(-i\hbar\frac{\partial\psi}{\partial x}\right) = -i\hbar x\frac{\partial\psi}{\partial x} \\ &\bullet\ p_x(x\psi) = -i\hbar\frac{\partial}{\partial x}(x\psi) = -i\hbar x\frac{\partial\psi}{\partial x} - i\hbar\psi \end{aligned}\right\} -$$

$$(xp_x - p_x x)\psi = i\hbar\psi$$

$$\boxed{\begin{aligned} xp_x - p_x x &= i\hbar \\ yp_y - p_y y &= i\hbar \\ zp_z - p_z z &= i\hbar \end{aligned}} \qquad (6)$$

Heisenberg permutation rules

Similarly,

$$xp_y - p_y x = 0$$
$$yp_z - p_z y = 0$$
$$zp_y - p_y z = 0 \quad \text{etc}$$

Take $F = F(x, y, z)$

$$Fp_x - p_x F = i\hbar\frac{\partial F}{\partial x}$$
$$Fp_y - p_y F = i\hbar\frac{\partial F}{\partial y}$$
$$Fp_z - p_z F = i\hbar\frac{\partial F}{\partial z}$$

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

end of digression — — — — — — — — — — —

(5.2) Equations of motion in q. mech.

- coordinate operators x, y, z
- momentum operators p_x, p_y, p_z
- Hamiltonian $H = H(p_x, p_y, p_z, x, y, z, t)$

$\hat{x}, \hat{p}_x, \ldots$ do not depend on t explicitly $\Rightarrow \frac{\partial}{\partial t} \ldots = 0$

Via quantum Poisson brackets $[H, A] = \frac{1}{i\hbar}(AH - HA)$

$$\frac{dx}{dt} = [H, x], \ldots$$

$$\frac{dp_x}{dt} = [H, p_x], \ldots$$

quantum Hamilton eqs (7)

Example 1. No magnetic field

- $H = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + U(x, y, z, t)$

- $[H, x] = \frac{1}{i\hbar}(xH - Hx) \underset{[U,x]=0}{\uparrow}{=} \frac{1}{2mi\hbar}(x p_x^2 - p_x^2 x)$ (8)

- $\underbrace{p_x^2 x} = p_x(p_x x) \underset{(6)}{\uparrow}{=} p_x(x p_x - i\hbar) = p_x x p_x - i\hbar p_x =$

$= (p_x x) p_x - i\hbar p_x \underset{(6)}{\uparrow}{=} (x p_x - i\hbar) p_x - i\hbar p_x = \underbrace{x p_x^2 - 2 i\hbar p_x}$ plug into (8)

$\Rightarrow [H, x] = \frac{p_x}{m} \Rightarrow \{$plug into (7)$\} \Rightarrow$

$$\Rightarrow \boxed{\frac{dx}{dt} = \frac{p_x}{m}, \quad \frac{dy}{dt} = \frac{p_y}{m}, \quad \frac{dz}{dt} = \frac{p_z}{m}}$$

analogous to class mech (but now for operators!) (9)

- $[H, p_x] = \frac{1}{i\hbar}(p_x U - U p_x) = \frac{1}{i\hbar}\left(-i\hbar \frac{\partial}{\partial x}(Ux) + i\hbar U \frac{\partial}{\partial x}\right) = -\frac{\partial U}{\partial x}$

go to (7)

$$\boxed{\frac{dp_x}{dt} = -\frac{\partial U}{\partial x}, \quad \frac{dp_y}{dt} = -\frac{\partial U}{\partial x}, \quad \frac{dp_z}{dt} = -\frac{\partial U}{\partial z}}$$

(10) Newton eqs in operator form

• mean values of time derivatives of operators (see (5c))

$$\begin{cases} \left\langle \frac{dx}{dt} \right\rangle = \frac{d}{dt}\langle x\rangle = \frac{\langle p_x\rangle}{m} & (11) \\ \left\langle \frac{dp_x}{dt} \right\rangle = \frac{d}{dt}\langle p_x\rangle = -\left\langle \frac{\partial U}{\partial x}\right\rangle = \langle F_x\rangle \end{cases}$$

$$m\frac{d^2}{dt^2}\langle x\rangle = -\left\langle \frac{\partial U}{\partial x}\right\rangle = \langle F_x\rangle \quad \text{quantum Newton eq} \qquad (12)$$

<u>Example 2.</u> Quantum eqs of motion of spin-1/2 particle in magnetic field

Remind lecture 3 $\quad H = H_0 + H_B = H_0 - \frac{g_e}{2}\underset{\substack{\uparrow \\ \text{Bohr magneton}}}{\mu_B}\vec{B}\vec{\sigma}$

Ehrenfes Theorem $\quad \vec{S} = \frac{\hbar}{2}\vec{\sigma}$

$$\frac{d}{dt}\langle\sigma_x\rangle = \frac{1}{i\hbar}\langle[\sigma_x, H]\rangle = \frac{1}{i\hbar}\langle\sigma_x H - H\sigma_x\rangle =$$

$$= \frac{1}{i\hbar}\langle\sigma_x H_B - H_B\sigma_x\rangle = -\frac{g\mu_B}{2i\hbar}\langle\sigma_x\left(\cancel{B_x\sigma_x} + \underline{B_y\sigma_y} + B_z\sigma_z\right) -$$

$$-\left(\cancel{B_x\sigma_x} + \underline{B_y\sigma_y} + B_z\sigma_z\right)\sigma_x\rangle =$$

$$= -\frac{g\mu_B}{2i\hbar}\langle B_y\underbrace{(\sigma_x\sigma_y - \sigma_y\sigma_x)}_{2i\sigma_z} + B_z\underbrace{(\sigma_x\sigma_z - \sigma_z\sigma_x)}_{-2i\sigma_y}\rangle =$$

$$= -\frac{g\mu_B}{\hbar}\left[B_y\langle\sigma_z\rangle - \langle\sigma_y\rangle B_z\right] \qquad (13a)$$

$$\frac{d}{dt}\langle\sigma_y\rangle = \frac{g\mu_B}{\hbar}\left(B_z\langle\sigma_x\rangle - B_x\langle\sigma_z\rangle\right) \qquad (13b)$$

$$\frac{d}{dt}\langle\sigma_z\rangle = \frac{g\mu_B}{\hbar}\left(B_x\langle\sigma_y\rangle - B_y\langle\sigma_x\rangle\right) \qquad (13c)$$

$\langle \ldots \rangle \Rightarrow \langle \sigma_n \rangle = \langle \xi_n^+ | \sigma_n | \xi_n^+ \rangle$

average of the operator over the ket $|\xi_n^+\rangle$ representing spinor on the Bloch sphere

$$\frac{d}{dt}\langle \vec{\sigma} \rangle = \frac{g\mu_B}{\hbar}\left(\langle \vec{\sigma} \rangle \times \vec{B}\right) = \langle \vec{\sigma} \rangle \times \vec{\Omega} \qquad (14)$$

$$\vec{\Omega} = \frac{g\mu_B}{\hbar}\vec{B} = \frac{e\vec{B}}{m_e} \quad \text{for free electron } g = 2$$

Since $S_n = \frac{\hbar}{2}\sigma_n$

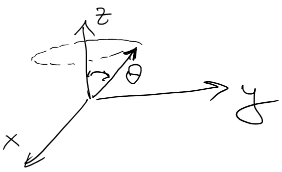
$$\frac{d}{dt}\langle \vec{S} \rangle = \frac{g\mu_B}{\hbar}\left(\langle \vec{S} \rangle \times \vec{B}\right) = \langle \vec{S} \rangle \times \vec{\Omega} \qquad (15)$$

expected value of the spin angular momentum

<u>Exercise</u> $\vec{B} \parallel \vec{e}_z$, $|\vec{B}| = \text{const}$

From (15) $\vec{B}\frac{d}{dt}\langle \vec{S} \rangle = 0 \Rightarrow \frac{d}{dt}\left(\langle \vec{S} \rangle \cdot \vec{B}\right) = 0$

$\angle\theta = \hat{S}\,\hat{B} = \text{const}$



$\Downarrow$ use spherical coordinates

$$\frac{d\phi}{dt} = \frac{g\mu_B}{\hbar}B_z$$

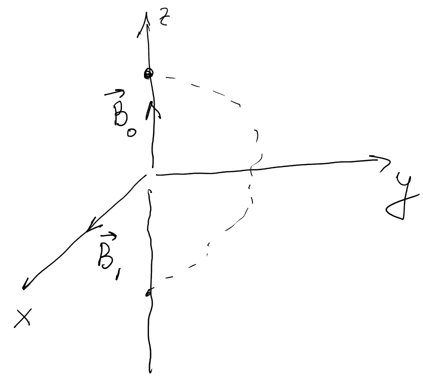
$\vec{S}$ rotates with Larmor processing frequency on a cone making a fixed angle θ with magnetic field $\vec{B}$.

5.3 Rotation on Bloch. Rabi cycle

- Spinor initially at the north pole
- How to flip it to the south pole using some combination of magnetic fields ?

- $\vec{B}_0 \parallel \vec{e}_z$: remains at the north pole ($\theta = 0$)
- Suggestion : apply $\vec{B}_1$ in equatorial plane of Bloch sphere ($x-y$)

Example: $\vec{B}_1 \parallel \vec{e}_x$, $|\vec{B}_1| = \text{const} \Rightarrow$ spinor rotates on circle through north and south in $(y-z)$ plane $\Rightarrow$ periodic spin flips (if no $\vec{B}_0$!)



- Take now both $\vec{B}_1$ and $\vec{B}_0$

  $\vec{B}_1$: spinor starts to rotate in $(y-z)$

  $\vec{B}_0$: spinor move on a cone around z-axis

  $\Downarrow$

  it comes out of $(y-z)$

Rabi $\Downarrow$

$\vec{B}_1$ needs to rotate in $(x-y)$ to keep up with the spinor that tries to rotate on a cone around z

$\Rightarrow \vec{B}_1$: should be magnetic field, $|\vec{B}_1| = \text{const}$, rotating in $(x-y)$ plane at $\omega = \frac{g\mu_B}{\hbar} B_0$

Rabi cycle: spinor $\vec{n}$ rotates in a circle with frequency $\propto B_1$, periodically visit north and south poles with period $\propto 1/B_1$ $\Rightarrow$ basics of NMR $\Rightarrow$

$\Rightarrow$ numerous applications, also in quantum computers

$\boxed{\text{Next lecture on Monday, July 1st at } 10^{15}}$!