Paramagnetic Resonance and Rabi Oscillations

Last Time: $i\hbar \frac{d}{dt}|\psi(t)\rangle = -\gamma \vec{S}\cdot\vec{B}(t)|\psi(t)\rangle$; $B_a(t) = B(t)\, R_{ab}(t)\, (\vec{n})_b$

Amplitude — t-dept. ord. rotation (3x3 special orthog.) matrix — Fixed reference unit vector

"Boost" into Rotating Frame:

① $\hat{U}^\dagger \hat{S}_a \hat{U} \equiv R_{ab}(t)\, \hat{S}_b$

② $|\psi_R(t)\rangle \equiv \hat{U}^\dagger_{(t)}\, |\psi(t)\rangle$

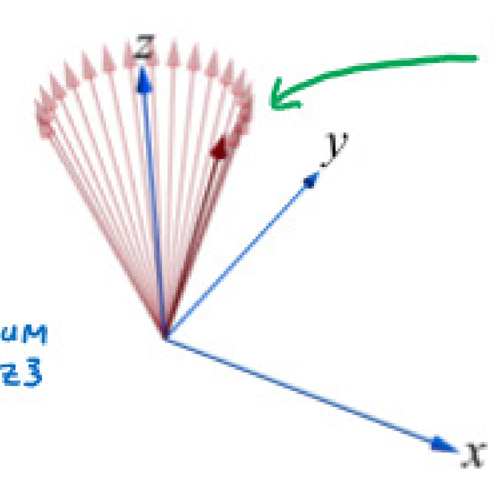
attempts to "undo" rotation of $\vec{B}(t)$ by "boosting" into co-rotating frame

$$\Rightarrow\ i\hbar\frac{d}{dt}|\psi_R(t)\rangle = \hat{H}_R(t)|\psi_R(t)\rangle\ ;\quad H_R(t) = -\gamma\left[B(t)\,\underset{\substack{\Uparrow\\ \text{static orientation } \checkmark}}{\vec{n}}\cdot\hat{\vec{S}} + \underbrace{\frac{i\hbar}{\gamma}\hat{U}^\dagger\frac{d}{dt}\hat{U}}_{\equiv\ \delta\vec{B}(t)\cdot\hat{\vec{S}}}\right]$$

- Extra field induced by the boost
- ~ "Berry Phase" or "Gauge" term

∴ In Rot. Frame, must solve dynamics in $\vec{B}_R(t) = B(t)\,\vec{n} + \delta\vec{B}(t)$

Important Solvable Example: "Paramag. Resonance"



$\vec{B}(t)$ precesses about z-axis at freq. ω

In original frame: $\vec{B}(t) = B_\parallel \vec{n}_z + B_\perp\left[\cos(\omega t)\,\vec{n}_x + \sin(\omega t)\,\vec{n}_y\right]$

$$= R_{ab}(\omega t\,\vec{n}_z)\left[B_\parallel \vec{n}_z + B_\perp \vec{n}_x\right]_b \vec{n}_a$$

Einstein sum $a,b \in \{x,y,z\}$

CCW rot. matrix, $\theta = \omega t$, around z-axis

Corresponding spin-½ rotation:

$$\hat{U}(t) = e^{-i\frac{\hat{S}_z \omega t}{\hbar}} = e^{-i\frac{\hat{\sigma}^3}{2}\omega t} = \hat{\mathbb{I}}\cos\left(\tfrac{\omega t}{2}\right) - i\,\hat{\sigma}^3 \sin\left(\tfrac{\omega t}{2}\right)$$

- $\hat{U}^\dagger_{(t)}\ \hat{S}_a\ \hat{U}(t) = R_{ab}(\omega t\,\vec{n}_z)\ \hat{S}_b$ (HW!!)

$S_{\frac{1}{2}} \equiv \sin\left(\frac{\omega t}{2}\right)$

$C_{\frac{1}{2}} \equiv \cos\left(\frac{\omega t}{2}\right)$

- $\delta\vec{B}(t)\cdot\hat{\vec{S}} = \frac{i\hbar}{\gamma}\hat{U}^\dagger_{(t)}\frac{d}{dt}\hat{U}(t) = \frac{i\hbar}{\gamma}\left(\hat{\mathbb{I}}\,C_{\frac12} + i\,\hat{\sigma}^3 S_{\frac12}\right)\left(\frac{\omega}{2}\right)\left(-\hat{\mathbb{I}}\,S_{\frac12} - i\,\hat{\sigma}^3 C_{\frac12}\right)$

$$= \frac{i\hbar\omega}{2\gamma}\left(-\hat{\mathbb{I}}\,\cancel{C_{\frac12}S_{\frac12}} - i\,\hat{\sigma}^3 C_{\frac12}C_{\frac12} - i\,\hat{\sigma}^3 S_{\frac12}S_{\frac12} + \hat{\mathbb{I}}\,\cancel{C_{\frac12}S_{\frac12}}\right)$$

$$= \frac{\hbar\omega}{2\gamma}\hat{\sigma}^3 = \frac{\omega}{\gamma}\hat{S}^z \Rightarrow \delta\vec{B} = \frac{\omega}{\gamma}\vec{n}_z$$

$$\therefore\quad \vec{B}_R = B_{\parallel}\vec{n}_z + B_\perp \vec{n}_x + \cancel{\delta\vec{B}(t)} = \left(B_{\parallel} + \frac{\omega}{\gamma}\right)\vec{n}_z + B_\perp \vec{n}_\perp$$

CONSTANT FIELD!

$$\Rightarrow\quad i\hbar \frac{d}{dt}|\psi_R(t)\rangle = -\gamma \vec{B}_R \cdot \hat{\vec{S}}\, |\psi_R(t)\rangle$$

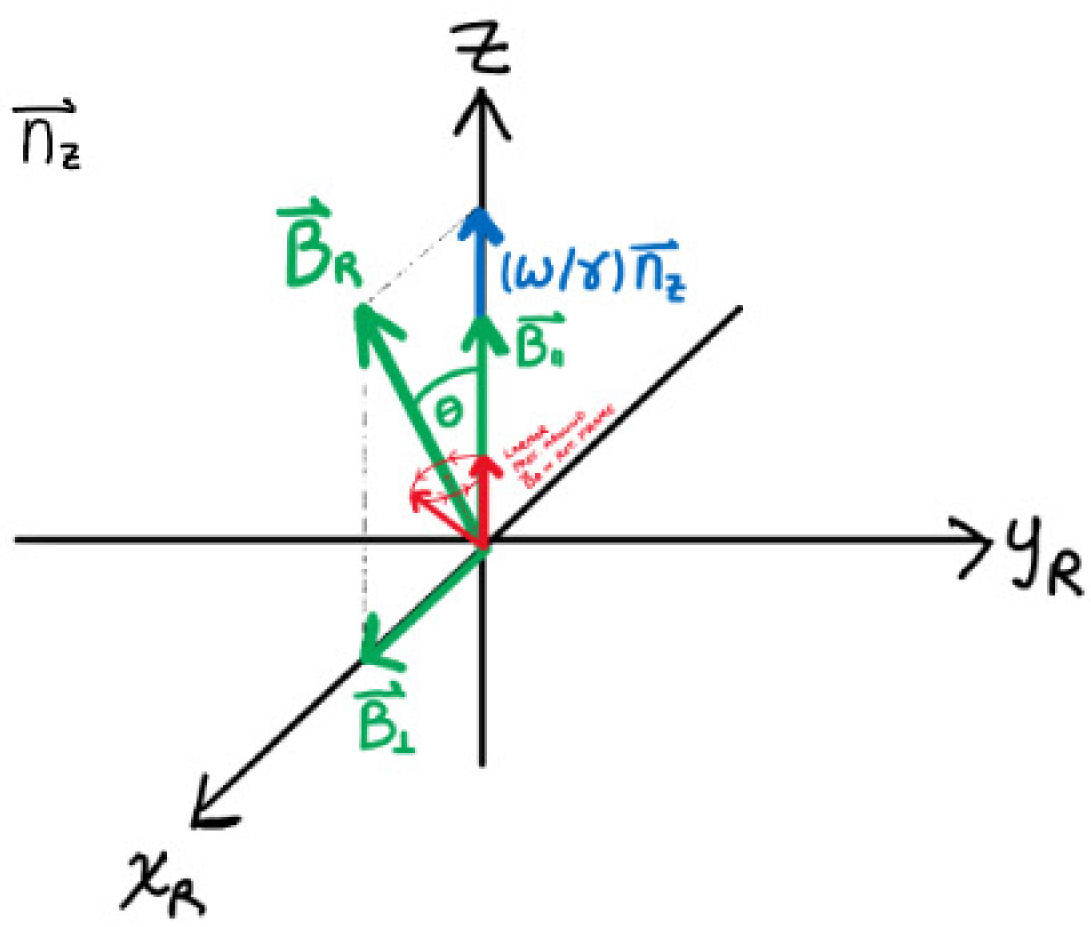
- SOLUTION IN ROTATING FRAME: LARMOR PRECESSION $\quad \gamma\langle\psi_{R(t)}|\hat{\vec{S}}|\psi_{R(t)}\rangle \equiv \vec{\mu}_R$

$\frac{d}{dt}\vec{\mu}_R = \gamma\vec{\mu}_R \times \vec{B}_R$; CHOOSE COORD. AXES. S.T. $\frac{\vec{B}_R}{|\vec{B}_R|} \equiv \vec{n}_3$; $\vec{\mu}_R = \sum_{i=1}^{3} \mu_{R,i}\vec{n}_i$; $\vec{n}_i \cdot \vec{n}_j = \delta_{ij}$

① $\mu_3(t) = \mu_3(0)$
② $\mu_1(t) = \mu_1(0)\cos(\omega_L t) + \mu_2(0)\sin(\omega_L t)$; $\omega_L = \gamma B_R$
③ $\mu_2(t) = -\mu_1(0)\sin(\omega_L t) + \mu_2(0)\cos(\omega_L t)$

- PRECESSION AROUND $\vec{B}_R$ IN ROTATING FRAME:

- TAKE SOLUTION $\{\mu_{1,2,3}(t)\}$. FOR $\vec{n}_3 = \vec{n}_z$, THIS IS PRECESSION AROUND $\vec{n}_z$
- TO GET $\{\mu_{R,x,y,z}(t)\}$, ROTATE $\vec{n}_z \Rightarrow \vec{B}_R / B_R$



$\vec{B}_R$ IS TILTED FROM $\vec{n}_z$ BY θ IN XZ PLANE

- $\tan\theta = \frac{B_\perp}{B_\parallel + \omega/\gamma}$
- $\cos\theta = \frac{B_\parallel + \omega/\gamma}{B_R}$
- $\sin\theta = \frac{B_\perp}{B_R}$; $B_R^2 = B_\perp^2 + (B_\parallel + \omega/\gamma)^2$

$$\begin{bmatrix} \mu_{R,x}(t) \\ \mu_{R,y}(t) \\ \mu_{R,z}(t) \end{bmatrix} = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix} \begin{bmatrix} \mu_1(0)\cos\omega_L t + \mu_2(0)\sin\omega_L t \\ -\mu_1(0)\sin\omega_L t + \mu_2(0)\cos\omega_L t \\ \mu_3(0) \end{bmatrix}$$

$$= \begin{bmatrix} \cos\theta\left[\mu_1(0)\cos\omega_L t + \mu_2(0)\sin\omega_L t\right] + \sin\theta\,\mu_3(0) \\ -\mu_1(0)\sin\omega_L t + \mu_2(0)\cos\omega_L t \\ -\sin\theta\left[\mu_1(0)\cos\omega_L t + \mu_2(0)\sin\omega_L t\right] + \cos\theta\,\mu_3(0) \end{bmatrix}$$

CHECK: IF $\mu_1(0) = \mu_2(0) = 0$ (SPIN INITIALLY ALIGNED W/ $\vec{B}_R$), THEN
$\vec{\mu}(t) = \vec{\mu}(0) = \mu_3(0)\,\vec{B}_R/B_R$
$= \mu_3(0)\left[\cos\theta\,\vec{n}_{R,z} + \sin\theta\,\vec{n}_{R,x}\right]$

ASSUME THAT INITIALLY $|\psi(0)\rangle = |\uparrow\rangle_z$:

$t=0$: WANT $\mu_{R,x}(0) = \mu_{R,y}(0) = 0$; $\mu_{R,z}(0) = \mu$ (FIXED MAG. MOMENT OF SPIN)

$\therefore\ \mu_2(0) = 0$; $\begin{bmatrix} \mu_1(0) \\ \mu_3(0) \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}\begin{bmatrix} 0 \\ \mu \end{bmatrix} = \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}\mu$ $\Rightarrow$ $\mu_{R,z}(t) = -\sin\theta\left[\mu_1(0)\cos\omega_L t + \mu_2(0)\sin\omega_L t\right] + \cos\theta\,\mu_3(0)$

$\therefore\ \mu_1(0) = -\sin\theta\,\mu$; $\mu_3(0) = \cos\theta\,\mu$

$$\boxed{\mu_{R,z}(t) = \mu\left[\cos^2\theta + \sin^2\theta\cos\omega_L t\right]}$$

• Solution in original ("Lab") Frame:

– If $\vec{\mu}_R(t) = \vec{\mu}_R(0)$ (constant — i.e. $\vec{\mu}_R \parallel \vec{B}_R$), then $\vec{\mu}_L(t)$ must Precess with the Rotating Frame

$\therefore$ in general,
$$\begin{bmatrix}\mu_{L,x}(t)\\ \mu_{L,y}(t)\\ \mu_{L,z}(t)\end{bmatrix} = \begin{bmatrix}\cos(\omega t) & -\sin(\omega t) & 0\\ +\sin(\omega t) & \cos(\omega t) & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}\mu_{R,x}(t)\\ \mu_{R,y}(t)\\ \mu_{R,z}(t)\end{bmatrix} \quad \text{or} \quad \mu_{L,a}(t) = R_{ab}(\omega t\, \vec{n}_z)\, \mu_{R,b}(t)$$

Same as rotation of $\vec{B}_\perp$ in lab frame

$$\Rightarrow \mu_{L,z}(t) = \mu_{R,z}(t) = [\cos^2\theta + \sin^2\theta \cos(\omega_L t)]$$

$$\mu_z(t) = \mu \frac{\left[(B_\parallel + \frac{\omega}{\gamma})^2 + B_\perp^2 \cos(\omega_L t)\right]}{B_\perp^2 + (B_\parallel + \omega/\gamma)^2}, \quad \omega_L = \gamma\sqrt{B_\perp^2 + (B_\parallel + \omega/\gamma)^2}$$

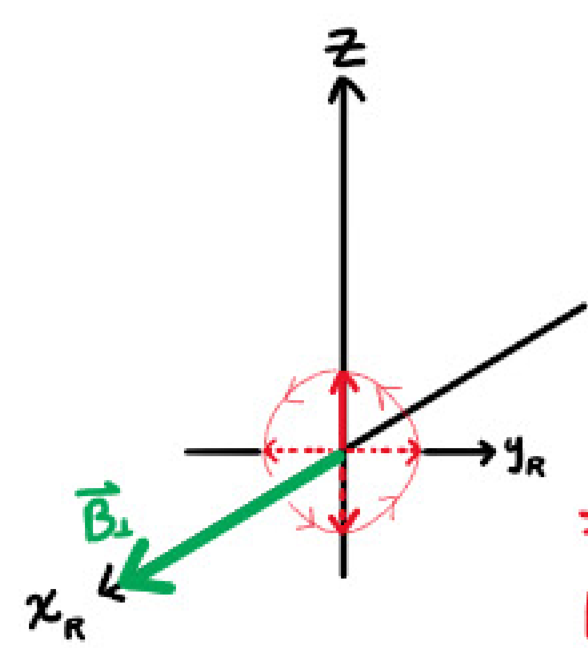
$$= \mu \frac{\left[(\omega_0 + \omega)^2 + (\gamma B_\perp)^2 \cos(\omega_L t)\right]}{(\omega_0 + \omega)^2 + (\gamma B_\perp)^2};$$

where $\omega_0 \equiv \gamma B_\parallel$, Larmor freq. in lab frame for zero rotating comp. of the field: $B_\perp = 0$.

For e^-, $\gamma = -\frac{g_e e}{2 m_e c} < 0 \Rightarrow \omega_0 < 0$

Paramagnetic Resonance: $B_\parallel + \frac{\omega}{\gamma} = 0$ or $\omega = -\omega_0$

$$\mu_z(t) = \mu \cos(\omega_L^{(PR)} t), \quad \omega_L^{(PR)} = \gamma B_\perp$$

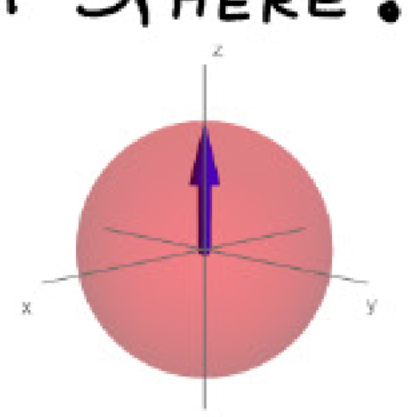
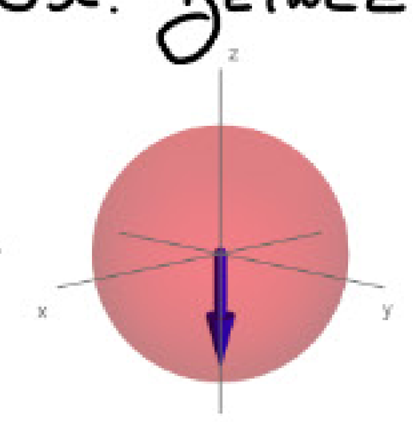


Paramag. Res: $B_\parallel$ canceled by ω/γ in Rot. frame.

$\Longrightarrow$ Spin initially polarized along z precesses in circle in z-y_R plane

• For spin-$\frac{1}{2}$, state $|\psi(t)\rangle$ completely characterized by motion on Bloch sphere

Bloch Sphere: sinusoidal osc. between

$|\uparrow\rangle_z$:  $\Longleftrightarrow$ $|\downarrow\rangle_z$: 

"Rabi Oscillations"

P.R. as a Periodically-Driven Two-Level Quantum System (Periodic Driving: "Floquet" Quantum Dynamics)

$$\hat{H}(t) = -\gamma \hat{\vec{S}}\cdot[B_\parallel \vec{n}_z + B_\perp(\cos(\omega t)\vec{n}_x + \sin(\omega t)\vec{n}_y)]; \quad \hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}}, \quad \hat{\sigma}^1 \Rightarrow \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad \hat{\sigma}^2 \Rightarrow \begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}, \quad \hat{\sigma}^3 \Rightarrow \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$

$$\therefore \hat{H}(t) \Rightarrow -\frac{\gamma\hbar}{2}\begin{bmatrix}B_\parallel & B_\perp e^{-i\omega t}\\ B_\perp e^{i\omega t} & -B_\parallel\end{bmatrix} \equiv \begin{bmatrix}-E_0/2 & V e^{-i\omega t}\\ V e^{i\omega t} & +E_0/2\end{bmatrix} = \underbrace{-\frac{E_0}{2}|1\rangle\langle 1| + \frac{E_0}{2}|2\rangle\langle 2|}_{\text{Describes "unperturbed" two-lvl system, energies } \pm \frac{E_0}{2}} + \underbrace{V e^{-i\omega t}|1\rangle\langle 2| + V e^{i\omega t}|2\rangle\langle 1|}_{\text{Periodic driving due (e.g.) to ext. E+M field} \Rightarrow \text{induces transitions}}$$

$\{|\uparrow\rangle_z, |\downarrow\rangle_z\}$ basis

Here: (1) $E_0 \equiv \hbar\gamma B_\parallel = \hbar\omega_0$, $V \equiv -\frac{\hbar}{2}\gamma B_\perp$

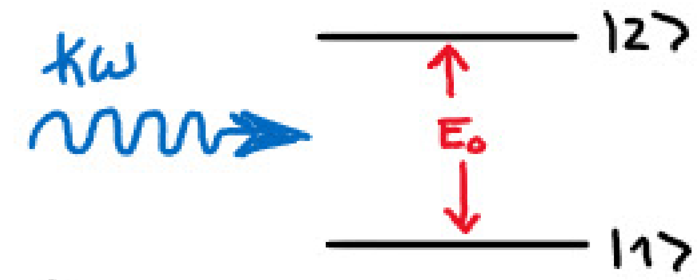
(2) $|1\rangle = |\uparrow\rangle_z$, $|2\rangle = |\downarrow\rangle_z$

Rabi Osc.: $\langle\psi(t)|\hat{\sigma}^3|\psi(t)\rangle = \cos(\Omega t) \Rightarrow |\langle 1|\psi(t)\rangle|^2 = \frac{1 + \cos(\Omega t)}{2}$,

• $\hbar\omega = -E_0$

• $\Omega = -\frac{2V}{\hbar}$

$$\hat{H} = -\frac{E_0}{2}|1\rangle\langle 1| + \frac{E_0}{2}|2\rangle\langle 2| + V e^{-i\omega t}|1\rangle\langle 2| + V e^{i\omega t}|2\rangle\langle 1|$$



Rabi Osc. Summary

(1) Maximal Transition (coh. osc. between $|\psi(0)\rangle = |1\rangle$ and $|\psi(t)\rangle = |2\rangle$) occurs only "on Resonance":

$-\hbar\omega = E_0$
- (Mod. of) drive freq. must match energy gap / $\hbar$.
- Stimulated emission, absorption of quanta ("photons") $\hbar\omega$ of the drive.

(2) Osc. frequency of state $|\psi(t)\rangle$ between $\{|1\rangle, |2\rangle\}$ determined by V, amplitude of drive

$$-\hbar\omega = E_0, \quad |\langle 1|\psi(t)\rangle|^2 = \frac{1+\cos(\Omega t)}{2}, \quad \Omega = -\frac{2V}{\hbar}$$

$\Rightarrow$ Freq. of drive determines Amp. of Rabi osc. away from initial state

$\Rightarrow$ Amp. of drive determines Freq. of real-time probability osc.

Quantum Mech. and Projective Measurements

Postulates of Q.M. so far (Lec. 9, p. 4-5; Lec. 12)

① State is a vector $|\psi\rangle$ in a L.V. or Hilbert Space

② Physical obs. are Hermitian Operators $\hat{\Omega} = \hat{\Omega}^\dagger$; $\hat{\Omega}|\omega_i\rangle = \omega_i|\omega_i\rangle$

③ The probability that eigenvalue ω_i of obs. $\hat{\Omega}$ is measured in an Ideal Projective Measurement is given by $|\langle\omega_i|\psi\rangle|^2$

④ Time evolution of an isolated quantum system [between measurements] is unitary, det. by the Schrödinger Equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle,$$ where $\hat{H}(t)$ is the "Hamiltonian", an obs. that measures energy

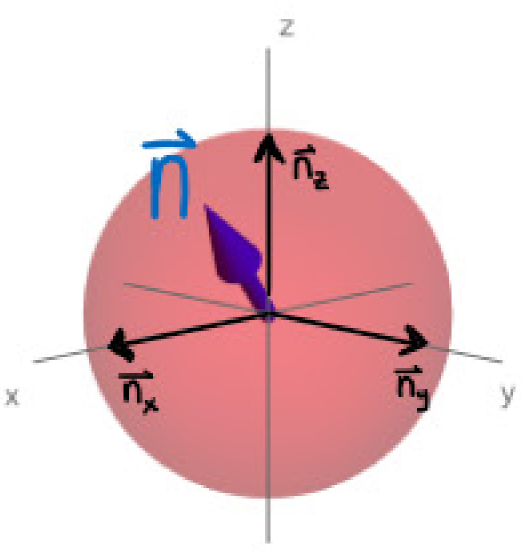
(Energy eigenval.'s are only well-defined if $\hat{H}(t) = \hat{H}$, indep. of time; $\Delta E \Delta t \geq \frac{\hbar}{2}$) (Lec. 9, p. 3)

- So far we have mainly focused on ①, ②, and ④; now we have to confront ③.

Dogma: The "Copenhagen" Interpretation

- System $|\psi(t)\rangle$ evolves unitarily according to the S.E. until we measure observable $\hat{\Omega}$
- The measurement of $\hat{\Omega}$ produces a random result, but the result must be an eigenvalue ω_i. The assoc. probability is $|\langle\omega_i|\psi\rangle|^2$.
- Assume the spectrum $\{\omega_i\}$ of $\hat{\Omega}$ is non-degenerate. Then, if ω_i is the measured value, "Immediately" after the measurement the state of the system is $|\psi\rangle = e^{i\phi}|\omega_i\rangle$, where $e^{i\phi}$ is a pure phase. $\Rightarrow$ "Collapse of the State Vector"

ex:) Single spin-$\frac{1}{2}$ in Time-Indept. Field:



$$\hat{H} = -\gamma \hat{S}^z B^z = -\frac{E_0}{2}\left(|\uparrow\rangle_z {}_z\langle\uparrow| - |\downarrow\rangle_z {}_z\langle\downarrow| \right)$$

$$= -\frac{E_0}{2}\left(\hat{\mathbb{P}}_{\vec{n}_z} - \hat{\mathbb{P}}_{-\vec{n}_z} \right) ; \quad \hat{\mathbb{P}}_{\vec{n}} \equiv |\vec{n}\rangle\langle\vec{n}| \text{ projects onto the Bloch sphere state } \vec{n}$$

- Generic Time-Evolving State: $|\psi(t)\rangle = \alpha |\uparrow\rangle_z e^{+i\frac{E_0 t}{2\hbar}} + \beta |\downarrow\rangle_z e^{-i\frac{E_0 t}{2\hbar}}$

(1) a) Measure $\hat{\sigma}^z$ at time t_0:

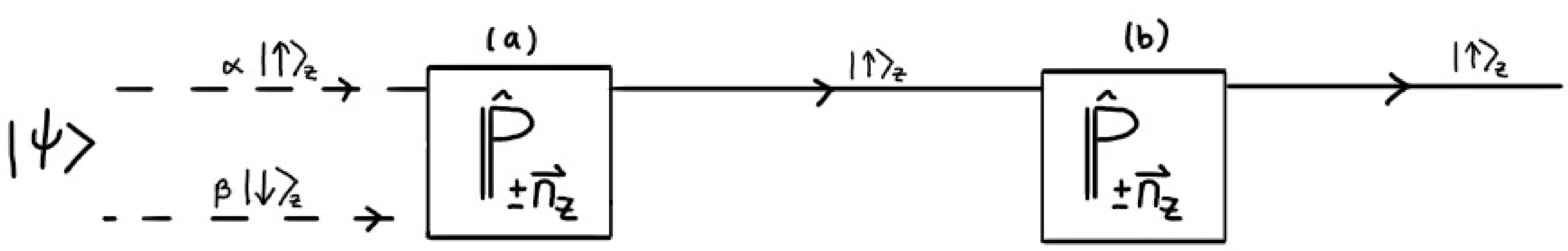
- Prob $|\alpha|^2$, $\sigma^z = +1$; Prob. $|\beta|^2$, $\sigma^z = -1$
- Suppose $\sigma^z = +1$ is measured. State after measurement:

$$|\psi_{a,1}(t)\rangle = e^{+\frac{iE_0(t-t_0)}{2\hbar}} |\uparrow\rangle_z$$

b) Measure $\hat{\sigma}^z$ at time t_1:

- Prob. 1, $\sigma^z = +1$; Prob. 0, $\sigma^z = -1$

$\Longrightarrow$ Will never measure $-1 \Longleftrightarrow |\psi\rangle = |\downarrow\rangle_z$ after initial projective meas. gives $+1$



$\Longrightarrow$ Information is Destroyed by the Measurement, i.e. (α/β)

$\therefore$ Projective Meas. is Not Unitary! Act of measuring changes state, destroys info.

(2) a) Same as above. $\sigma^z = +1$

b) Measure $\hat{\sigma}^x$. $|\uparrow\rangle_x = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z + |\downarrow\rangle_z)$; $|\downarrow\rangle_x = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z - |\downarrow\rangle_z)$

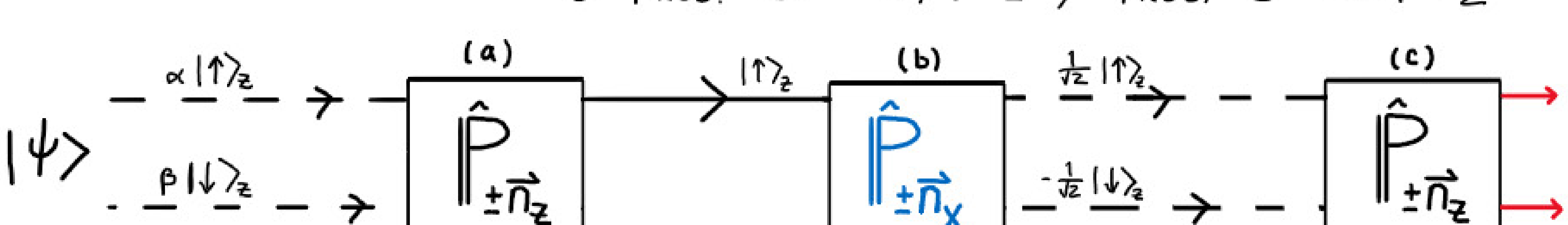
$\Rightarrow$ Before Measurement: $|\psi\rangle \propto |\uparrow\rangle_z = \frac{1}{\sqrt{2}}(|\uparrow\rangle_x + |\downarrow\rangle_x)$

- Prob. $\sigma^x = +1$: $\frac{1}{2}$; Prob. $\sigma^x = -1$: $\frac{1}{2}$
- Suppose $\sigma^x = -1$ is measured. State After Measurement:

$$|\psi_{b,-1}(t)\rangle \propto \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_z e^{+i\frac{E_0 t}{2\hbar}} - |\downarrow\rangle_z e^{-i\frac{E_0 t}{2\hbar}} \right)$$

c) Measure $\hat{\sigma}^z$

- Prob. $\sigma^z = +1$: $\frac{1}{2}$; Prob. $\sigma^z = -1$: $\frac{1}{2}$



Both outcomes $\{|\uparrow\rangle_z, |\downarrow\rangle_z\}$ equally probable.

$\Rightarrow$ MEASURING NON-COMMUTING OBSERVABLES IN SUCCESSION SCRAMBLES SUBSEQUENT OUTCOMES.

(3) a) SAME AS ABOVE. $\sigma^z = +1$

b) MEASURE $\hat{\sigma}^x$. $|\uparrow\rangle_x = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z + |\downarrow\rangle_z)$; $|\downarrow\rangle_x = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z - |\downarrow\rangle_z)$

$\Rightarrow$ BEFORE MEASUREMENT: $|\psi\rangle \propto |\uparrow\rangle_z = \frac{1}{\sqrt{2}}(|\uparrow\rangle_x + |\downarrow\rangle_x)$

- PROB. $\sigma^x = +1 : \frac{1}{2}$; PROB. $\sigma^x = -1 : \frac{1}{2}$
- SUPPOSE $\sigma^x = -1$ IS MEASURED. STATE AFTER MEASUREMENT:

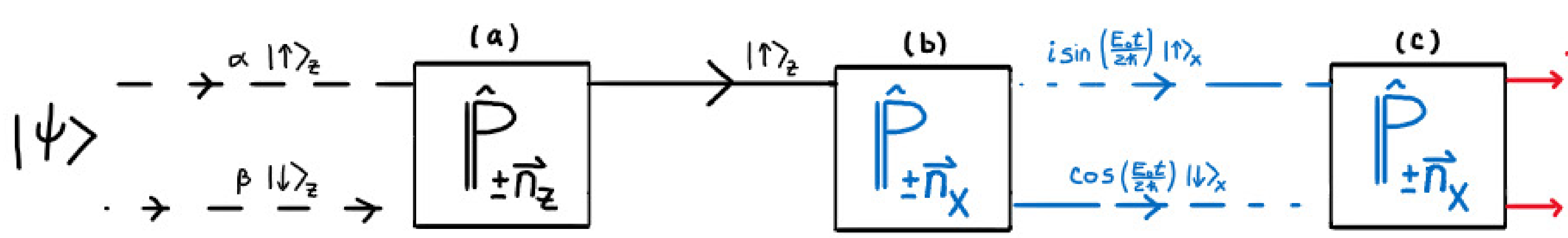
$$|\psi_{b,-1}(t)\rangle \propto \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_z e^{+i\frac{E_0 t}{2\hbar}} - |\downarrow\rangle_z e^{-i\frac{E_0 t}{2\hbar}}\right)$$

c) MEASURE $\hat{\sigma}^x$ AGAIN, TIME t LATER.

$$|\psi_{b,-1}(t)\rangle = \frac{1}{2}(|\uparrow\rangle_x + |\downarrow\rangle_x)e^{i\frac{E_0 t}{2\hbar}} - \frac{1}{2}(|\uparrow\rangle_x - |\downarrow\rangle_x)e^{-i\frac{E_0 t}{2\hbar}}$$

$$= i\sin\left[\frac{E_0 t}{2\hbar}\right]|\uparrow\rangle_x + \cos\left[\frac{E_0 t}{2\hbar}\right]|\downarrow\rangle_x$$

- PROB. $\sigma^x = +1 :\ \sin^2\left(\frac{E_0 t}{2\hbar}\right)$; PROB. $\sigma^x = -1 :\ \cos^2\left(\frac{E_0 t}{2\hbar}\right)$



BOTH OUTCOMES $\{|\uparrow\rangle_x, |\downarrow\rangle_x\}$ POSSIBLE; PROBABILITIES DEPEND ON TIME t, BECAUSE OF PREV. $\hat{\sigma}^x$ MEASUREMENT, AND: $[\hat{H}, \hat{\sigma}^x] \neq 0$.

TAKEAWAYS:

(1) PROJECTIVE MEASUREMENT DETERMINES THE STATE IMMEDIATELY AFTER THE MEASUREMENT IS PERFORMED. THE MEASUREMENT IS NOT UNITARY, AND DESTROYS INFORMATION (i.e., PROB. AMP. TO HAVE FOUND $|\psi\rangle$ IN ANY OTHER STATE)

(2) SUCCESSIVE MEASUREMENTS OF NON-COMMUTING OBSERVABLES SCRAMBLE PROBABILITIES.

(3) MEASUREMENT PROBABILITIES FOR OBSERVABLES THAT DO NOT COMMUTE WITH THE HAMILTONIAN $\hat{H}$ CHANGE WITH TIME