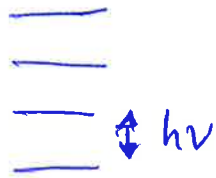
Summary, Advanced Quantum Mechanics

- History of quantum mechanics

  From Planck's radiation law (1900) to quantum computers and quantum technology (2020–)

$$u(\nu,T) = \frac{8\pi}{c^3}\nu^2 \frac{h\nu}{e^{\beta h\nu}-1},$$



- Mathematics of quantum mechanics

  - Hilbert spaces
  - Bra-c-ket (Dirac) notation
  - Superpositions
  - Two level systems

$$|\psi\rangle = \alpha|\uparrow_z\rangle + \beta|\downarrow_z\rangle$$

$$= \alpha\begin{pmatrix}1\\0\end{pmatrix} + \beta\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}\alpha\\\beta\end{pmatrix}$$

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

  - Operators
  - Example: Pauli matrices

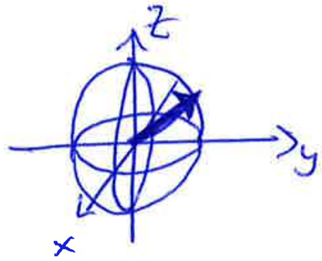
$$\sigma_x = \begin{pmatrix}0&1\\1&0\end{pmatrix};\quad \sigma_y = \begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

- Measurements and expectation values

$$\langle \hat{A} \rangle = \langle \Psi | \hat{A} | \Psi \rangle$$

- Bloch sphere

$$|\psi\rangle = \alpha |\uparrow_z\rangle + \beta |\downarrow_z\rangle$$



- Time-evolution; the Schrödinger equation

$$i\hbar \partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

Hamiltonian

- Solution: (if $\hat{H}$ is time-independent)

$$|\psi(t)\rangle = \hat{U}(t,t_0) |\psi(t_0)\rangle$$

$$\hat{U}(t,t_0) = e^{-i\hat{H}(t-t_0)/\hbar}$$

$$\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = e^{i\hat{H}(t-t_0)/\hbar} e^{-i\hat{H}(t-t_0)/\hbar} = 1$$

- The Schrödinger equation can also be solved for time-dependent problems, although the general procedure is more complicated. We saw one example (ESR), where a rotating magnetic field can be used to flip a spin.

- Harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega_0^2 \hat{x}^2$$

$$= \dots = \hbar\omega_0 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right)$$

with $\hat{a} = \frac{1}{\sqrt{2}}(\hat{q} + i\hat{\rho})$ and $\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{q} - i\hat{\rho})$,

where $\hat{\rho} = \hat{p}\frac{x_0}{\hbar}$ and $\hat{q} = \hat{x}/x_0$.

The oscillator length is $x_0 = \sqrt{\frac{\hbar}{m\omega_0}}$

Eigenenergies: $E_n = \hbar\omega_0 (n + \frac{1}{2})$, $n = 0, 1, 2, 3, \dots$

zero-point energy

Eigenstates: $|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n |0\rangle$

- Coherent states ("most classical states")

$$|z\rangle \equiv \hat{\mathcal{D}}(z) |n=0\rangle; \quad z \in \mathbb{C},$$

where $\hat{\mathcal{D}}(z) \equiv e^{z\hat{a}^\dagger - z^* \hat{a}}$

$$= e^{\frac{i}{\hbar}[p_0 \hat{x} - q_0 \hat{p}]} = \hat{\mathcal{D}}(p_0, q_0)$$

and $p_0 = \sqrt{2\hbar m \omega_0}\, \mathrm{Im}\, z$; $q_0 = \sqrt{\frac{2\hbar}{m\omega_0}}\, \mathrm{Re}\, z$

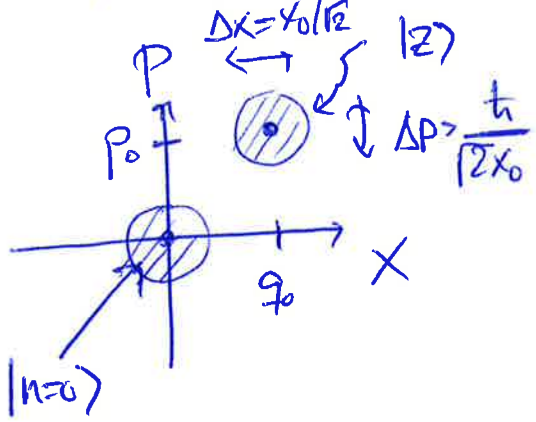
- $\hat{\mathcal{D}}^\dagger(z) \hat{x} \hat{\mathcal{D}}(z) = \hat{x} + q_0$
- $\hat{\mathcal{D}}^\dagger(z) \hat{p} \hat{\mathcal{D}}(z) = \hat{p} + p_0$

$\to$ $\hat{\mathcal{D}}$ is known as the displacement operator

$$|z\rangle \equiv \hat{D}(z)\,|n=0\rangle = \hat{D}(p_0, q_0)\,|n=0\rangle$$

$$\Delta X \Delta P = \sqrt{\langle \hat{X}^2\rangle - \langle X\rangle^2} \cdot \sqrt{\langle \hat{P}^2\rangle - \langle \hat{P}\rangle^2} = \frac{\hbar}{2}$$

minimal uncertainty



- Fock state representation

$$|z\rangle = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}\,|n\rangle$$

- Probability to find the oscillator in the state $|n\rangle$

$$P(n) = |\langle n|z\rangle|^2 = \frac{\bar{n}^n}{n!}\,e^{-\bar{n}} \quad \text{with } \bar{n} = |z|^2$$

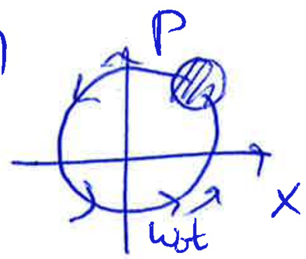
- Time-evolution of coherent states

$$|z(t)\rangle = e^{-i\hat{H}t/\hbar}\,|z\rangle$$

$$= e^{-i\omega_0 t/2}\,|z e^{-i\omega_0 t}\rangle$$

↳ $p_0(t) = \sqrt{2\hbar m\omega_0}\,|z|\,\sin(\varphi_0 - \omega_0 t)$

$q_0(t) = \sqrt{\frac{2\hbar}{m\omega_0}}\,|z|\,\cos(\varphi_0 - \omega_0 t)$



- Orbital & spin angular momentum

  - Orbital angular momentum

$$\hat{\underline{L}} = \hat{\underline{r}} \times \hat{\underline{p}} = \begin{pmatrix} \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{pmatrix} = \frac{\hbar}{i} \begin{pmatrix} y\partial_z - z\partial_y \\ z\partial_x - x\partial_z \\ x\partial_y - y\partial_x \end{pmatrix}$$

  - Commutation relations

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$$

  - $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

$$[\hat{L}^2, \hat{L}_\alpha] = 0 \ , \ \alpha = x, y, z$$

  - Eigenvalues:

$$\hat{L}^2 |l,m\rangle = \hbar^2 l(l+1) |l,m\rangle, \ \overbrace{l = 0, 1, 2, \ldots}^{\text{orbital a.m.}}$$

$$\hat{L}_z |l,m\rangle = \hbar m |l,m\rangle, \ m = \underbrace{-l, -l+1, \ldots, l-1, l}_{2l+1 \text{ values}}$$

- Spin angular momentum

  The Stern-Gerlach experiment showed that the angular momentum can also take half-integer values! $\rightsquigarrow$ spin a.m.

- Operators for the spin angular momentum

$$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$$

$$[\hat{S}_y, \hat{S}_z] = i\hbar \hat{S}_x$$

$$[\hat{S}_z, \hat{S}_x] = i\hbar \hat{S}_y$$

$$\hat{S}^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle; \quad s = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots$$

$$\hat{S}_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle,$$

integer s: bosons
half-integer s: fermions

$$m_s = -s, \ldots, +s$$

Electrons have $s = \frac{1}{2}$, and

$$\hat{S}_x = \frac{\hbar}{2}\hat{\sigma}_x, \quad \hat{S}_y = \frac{\hbar}{2}\hat{\sigma}_y, \quad \hat{S}_z = \frac{\hbar}{2}\hat{\sigma}_z$$

$$= \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Perturbation theory:

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{solved problem}} + \underbrace{\lambda \hat{H}_1}_{\text{perturbation}}, \quad \lambda \ll 1$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots$$

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + \ldots$$

- Non-degenerate perturbation theory

$$E_n^{(1)} = \langle \psi_n^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle$$

$$|\psi_n^{(1)}\rangle = \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} |\psi_m^{(0)}\rangle$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle \psi_m^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

- (WKB method)

- Composite systems, $\mathcal{H}^{12} = \mathcal{H}^1 \otimes \mathcal{H}^2$

For example, for two spin-½'s, we have

$$\hat{\sigma}_x^{(1)} = \hat{\sigma}_x \otimes \mathbb{1} = \left(\begin{array}{cc|cc} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \hline 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{array}\right) = \left(\begin{array}{c|c} \underline{0} & \mathbb{1} \\ \hline \mathbb{1} & \underline{0} \end{array}\right)$$

$$\hat{\sigma}_x^{(2)} = \mathbb{1} \otimes \hat{\sigma}_x = \left(\begin{array}{cc|cc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array}\right) = \left(\begin{array}{c|c} \sigma_x & 0 \\ \hline 0 & \sigma_x \end{array}\right)$$

$$\hat{S}_z = \hat{S}_z^{(1)} + \hat{S}_z^{(2)} = \frac{\hbar}{2}\begin{pmatrix} 2 & & & \\ & 0 & & \\ & & 0 & \\ & & & -2 \end{pmatrix} = \hbar \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & -1 \end{pmatrix}$$

Singlet state:

$$|s=0, m_s=0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Triplet states:

$$|s=1, m_s=1\rangle = |\uparrow\uparrow\rangle$$

$$|s=1, m_s=0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$

$$|s=1, m_s=-1\rangle = |\downarrow\downarrow\rangle$$

- Identical particles:

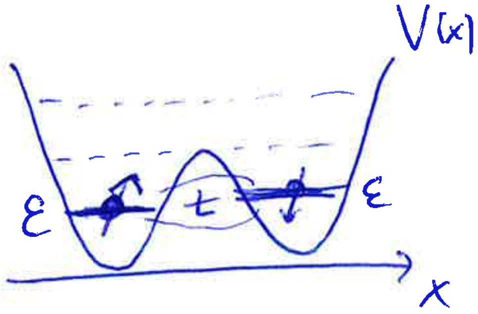
$$\varphi(x_1, x_2) = \pm\, \varphi(x_2, x_1)$$

$+ \rightarrow$ bosons

$- \rightarrow$ fermions

↳ Pauli exclusion principle for fermions

- Exchange coupling



$\psi_{sym}(x_1,x_2) \otimes |\text{singlet}\rangle, E_S$

$\psi_{anti}(x_1,x_2) \otimes |\text{triplet}\rangle; E_T$

$$\hookrightarrow \hat{\mathcal{H}}_{spin} = \frac{J}{\hbar^2}\, \hat{\underline{S}}_1 \cdot \hat{\underline{S}}_2 , \quad J = \underset{\underset{2\varepsilon}{\parallel}}{E_T} - \underset{\underset{2\varepsilon - \frac{4t^2}{U}}{\parallel}}{E_S} \simeq \frac{4t^2}{U}$$

- The exchange coupling can be used to entangle two spins:

$$|\uparrow\rangle_L |\downarrow_R\rangle \xrightarrow[\text{pulse}]{\text{exchange}} \underbrace{\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_L |\downarrow\rangle_R - i |\downarrow\rangle_L |\uparrow\rangle_R \right)}_{\neq |\sigma_L\rangle \otimes |\sigma_R\rangle}$$

$\rightarrow$ entanglement!

- Bell inequality and local realism

Local realism according to Einstein, Podolsky, and Rosen (EPR)

<u>Realism</u>: Observables have definite values before measurements.

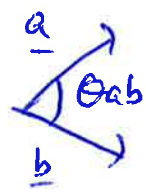
<u>Locality</u>: Distant measurements do not influence each other.

- Based on local realism, Bell derived the inequality

$$P(\uparrow_{\underline{a}}, \uparrow_{\underline{b}}) \leq P(\uparrow_{\underline{a}}, \uparrow_{\underline{c}}) + P(\uparrow_{\underline{c}}, \uparrow_{\underline{b}})$$

for the probability $P(\uparrow_{\underline{a}}, \uparrow_{\underline{b}})$ to measure two spins along the directions $\underline{a}$ and $\underline{b}$.

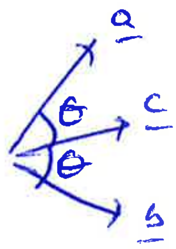
- For a singlet state, one finds



$$P(\uparrow_{\underline{a}}, \uparrow_{\underline{b}}) = \frac{1}{2} \sin^2(\theta_{ab}/2)$$

based on a quantum mechanical calculation.

- Using $\theta_{ac} = \theta_{bc} = \theta$ and $\theta_{ab} = 2\theta$,



one finds

$$P(\uparrow_{\underline{a}}, \uparrow_{\underline{b}}) = \frac{1}{2} \sin^2\theta \simeq \frac{\theta^2}{2} \quad \text{for } \theta \ll 1$$

and

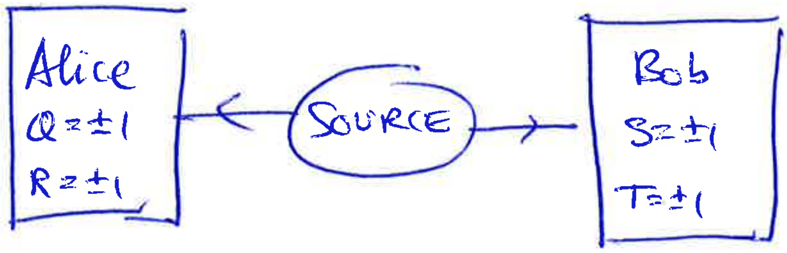
$$P(\uparrow_{\underline{a}}, \uparrow_{\underline{c}}) + P(\uparrow_{\underline{c}}, \uparrow_{\underline{b}}) = 2\,\frac{1}{2} \sin^2\left(\frac{\theta}{2}\right) \simeq \left(\frac{\theta}{2}\right)^2 = \frac{\theta^2}{4}$$

which clearly violates Bell's inequality

$\longrightarrow$ local realism cannot be true.

- CHSH inequality

  Another test of local realism was developed by Clauser, Horne, Shimony, and Holt. (CHSH)



$$\langle QS\rangle + \langle RS\rangle + \langle RT\rangle - \langle QT\rangle \leq 2$$

- For a singlet state, using

$$Q = \hat{\sigma}_z,\ R = \hat{\sigma}_x;\ S = \frac{-(\hat{\sigma}_x + \hat{\sigma}_z)}{\sqrt{2}},\ T = \frac{\hat{\sigma}_z - \hat{\sigma}_x}{\sqrt{2}},$$

one finds $2\sqrt{2} > 2$ and thus a violation of the CHSH inequality.

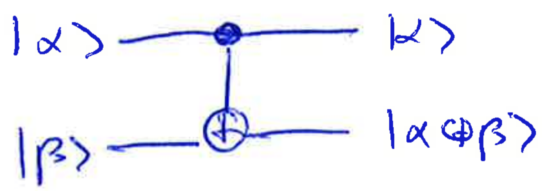
- Quantum computers

  Qu-bits; $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

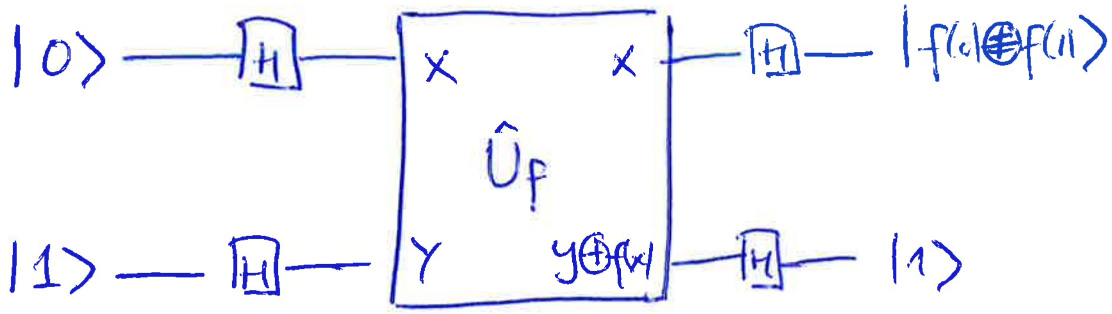
Hadamard-gate $\quad \alpha|0\rangle + \beta|1\rangle — \boxed{H} — \alpha\frac{|0\rangle + |1\rangle}{\sqrt{2}} + \beta\frac{|0\rangle - |1\rangle}{\sqrt{2}}$

CNOT gate $\quad \text{CNOT}|\alpha\rangle|\beta\rangle \to |\alpha\rangle|\alpha \oplus \beta\rangle$ addition modulo 2

↑ creates entanglement



- Deutsch's algorithm



If $f(0) = f(1)$ ($= 0$ or 1) $\rightarrow$ $|f(0)\oplus f(1)\rangle = |0\rangle$

If $f(0) \neq f(1)$ $\rightarrow$ $|f(0)\oplus f(1)\rangle = |1\rangle$

- Grover's search algorithm.

  More complicated, but see lecture notes for details

  $\rightarrow$ Finds an item in an unsorted database in $\mathcal{O}(\sqrt{N})$ attempts vs $\mathcal{O}(N)$ classically.

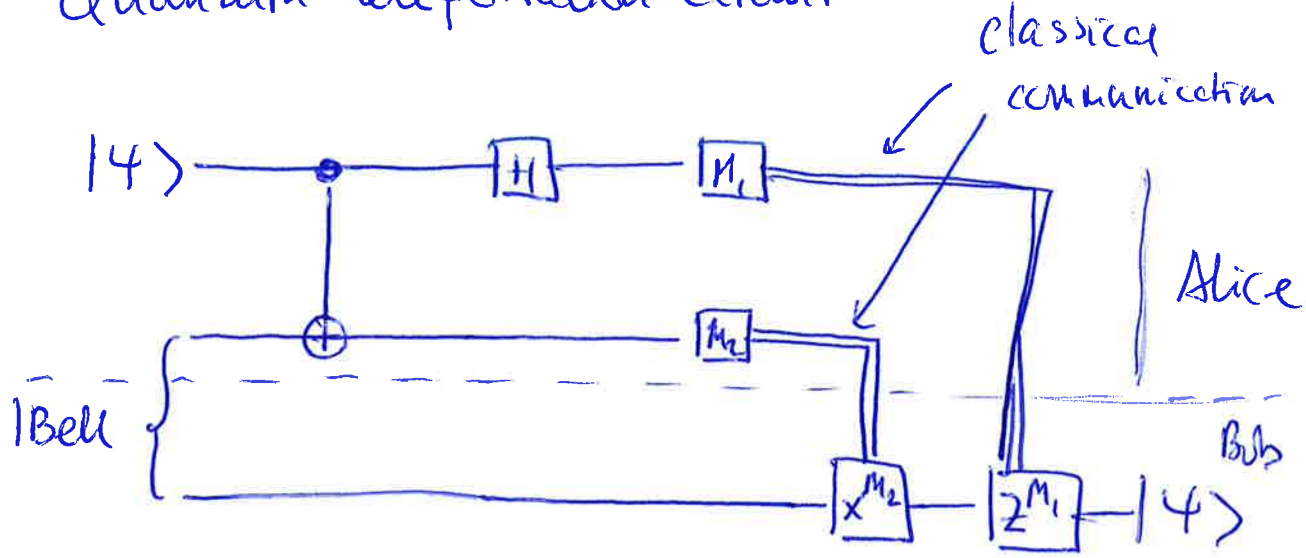
- No-cloning theorem

  $\rightarrow$ Cloning of a state is not possible in quantum mechanics.

- Quantum teleportation.

  Alice can teleport a qubit state to Bob, if they share an entangled state.

- Quantum teleportation circuit



- Open quantum systems

  - Density matrix

$$\hat{\rho} = \sum_n p_n |\psi_n\rangle\langle\psi_n|$$

probabilities, $\sum_n p_n = 1$

$\Rightarrow \mathrm{Tr}\{\hat{\rho}\} = 1$

  - Observables:

$$\langle\hat{O}\rangle = \mathrm{Tr}\{\hat{O}\hat{\rho}\} = \sum_n p_n \langle\psi_n|\hat{O}|\psi_n\rangle$$

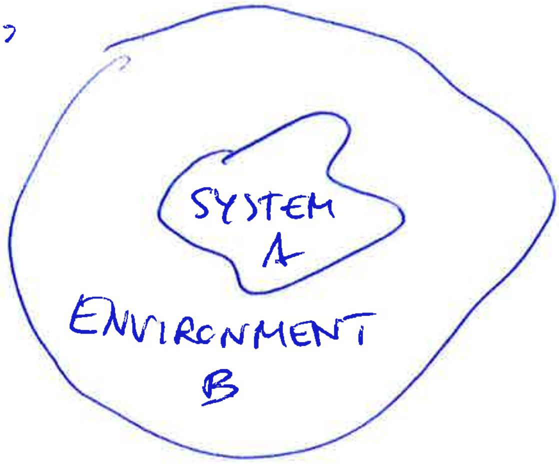
  - Pure state: $\hat{\rho} = |\psi\rangle\langle\psi|$

$$\Rightarrow \hat{\rho}^2 = |\psi\rangle\underbrace{\langle\psi|\psi\rangle}_{1}\langle\psi| = |\psi\rangle\langle\psi| = \hat{\rho}$$

$+ \mathrm{Tr}\{\hat{\rho}^2\} = 1$

  - Mixed state: $\hat{\rho}^2 \neq \hat{\rho}$ $+ \mathrm{Tr}\{\hat{\rho}^2\} < 1$

- Reduced density matrix:



$$\langle \hat{O}_A \rangle = \mathrm{Tr}\{\hat{O}_A \hat{\rho}\}$$

$$= \mathrm{Tr}_A\{\hat{O}_A \hat{\rho}_A\}$$

where $\hat{\rho}_A = \mathrm{Tr}_B\{\hat{\rho}\}$ is the reduced density matrix of A, defined by

$$\langle m_A|\hat{\rho}_A|n_A\rangle \equiv \sum_{n_B} \langle n_B|\langle m_A|\hat{\rho}|n_A\rangle|n_B\rangle$$

- Lindblad equation for reduced density matrix

$$\frac{d}{dt}\hat{\rho} = \frac{1}{i\hbar}[\hat{H},\hat{\rho}] + \mathcal{D}\hat{\rho}$$

system Hamiltonian

Dissipator due to interactions with environment

$$\mathcal{D}\hat{\rho} = \gamma\left(\hat{L}\hat{\rho}\hat{L}^{\dagger} - \frac{1}{2}\{\hat{L}^{\dagger}\hat{L},\hat{\rho}\}\right)$$ for some operator $\hat{L}$.

- Example: Pure dephasing

$$\frac{d}{dt}\hat{\rho} = -\frac{i\omega_0}{2}[\hat{\sigma}_z,\hat{\rho}] + \frac{\gamma}{2}\left(\hat{\sigma}_z\hat{\rho}\hat{\sigma}_z - \hat{\rho}\right)$$

- With $\hat{\rho}(t) = \frac{1}{2}(\mathbb{I} + \underline{a} \cdot \underline{\hat{\sigma}})$, we find

$$\frac{d}{dt}\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \begin{pmatrix} -\gamma & -\omega_0 & 0 \\ \omega_0 & -\gamma & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix}$$

$\hookrightarrow$ $a_z(t) = \text{const}$ & $\begin{pmatrix} a_x(t) \\ a_y(t) \end{pmatrix} = \underbrace{e^{-\gamma t}}_{\to 0 \text{ for } t \to \infty\,!} \begin{pmatrix} \cos(\omega_0 t) & -\sin(\omega_0 t) \\ \sin(\omega_0 t) & \cos(\omega_0 t) \end{pmatrix}\begin{pmatrix} a_x(0) \\ a_y(0) \end{pmatrix}$