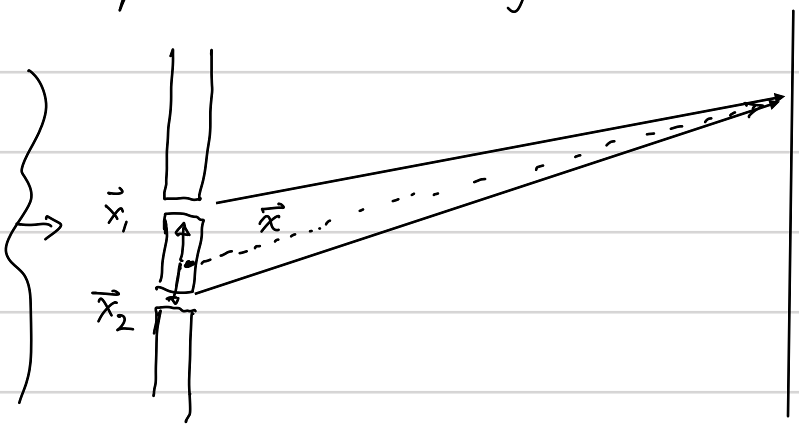
# Physics 566 - Lecture 4

## Quantum Coherence and the Density Matrix

We have defined coherence as the capacity of a system to exhibit interference. For example in the Young's double slit experiment

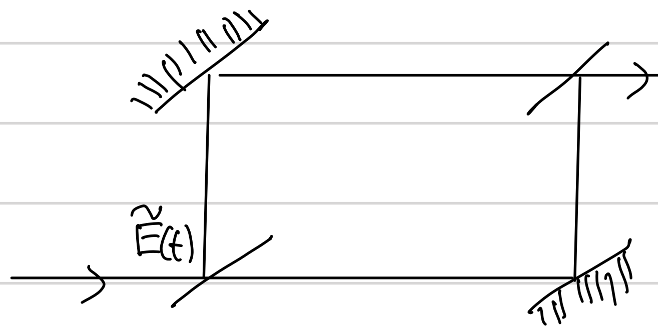



$$\tilde{E}(\vec{x}) = \tilde{E}(\vec{x}_1)\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}_1)} + \tilde{E}(\vec{x}_2)\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}_2)}$$

$$\vec{k} \cong \frac{\omega}{c}\frac{\vec{x}}{|\vec{x}|} \quad \text{(Fraunhoffer)}$$

$$I(\vec{x}) = \langle |\tilde{E}(\vec{x})|^2 \rangle = I_1 + I_2 + 2\,\mathrm{Re}\left(\langle \tilde{E}(\vec{x}_1)\tilde{E}^*(\vec{x}_2)\rangle e^{i\vec{k}\cdot(\vec{x}_1-\vec{x}_2)}\right)$$

In a Mach-Zender (or Michaelson) interferometer




$$\rightarrow \frac{-i}{2}\left(\tilde{E}(t-t_1) + \tilde{E}(t-t_2)\right)$$

$$I_{out} = \frac{1}{2}I + \frac{1}{2}\mathrm{Re}\left(\langle \tilde{E}(0)\tilde{E}^*(t_1-t_2)\rangle\right) \quad \text{stationary}$$

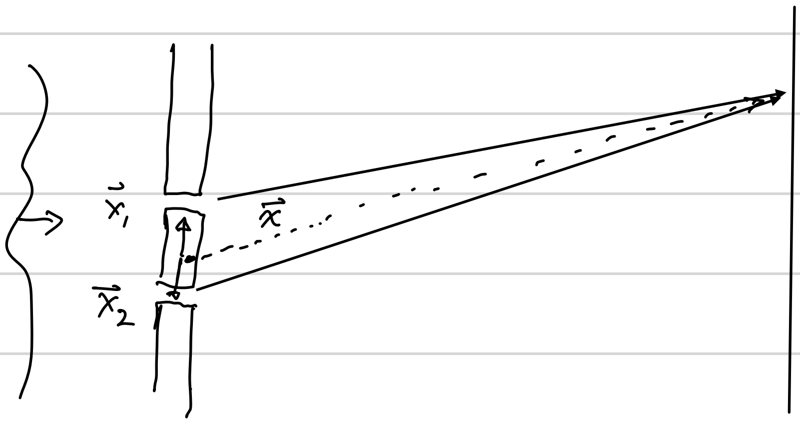
The degree of coherence is quantified by the correlation function

Spatial coherence: $\langle \tilde{E}(\vec{x}_1)\tilde{E}^*(\vec{x}_2)\rangle$

Temporal coherence $\langle \tilde{E}(t_1)\tilde{E}^*(t_2)\rangle$

We compare the complex amplitude at two different space-time points. Here $\langle\ \rangle$ denotes "ensemble average" over the probability distribution of random amplitudes. Coherence depends on the field maintaining a good phase relation at different space-time points.

What about the quantum problem? Lets return to the double slit, now for a single photon. The wavefunction is the prob. amplitude




$$\psi(\vec{x}) = \psi(\vec{x}_1)\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}_1)} + \psi(\vec{x}_2)\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}_2)}$$

$$\vec{k} \cong \frac{\omega}{c}\frac{\vec{x}}{|\vec{x}|} \quad \text{(Fraunhoffer)}$$

$$|\psi(\vec{x})|^2 = |\psi(\vec{x}_1)|^2 + |\psi(\vec{x}_2)|^2 + \underbrace{2\,\mathrm{Re}\left(\psi(\vec{x}_1)\,\psi^*(\vec{x}_2)\, e^{i\vec{k}\cdot(\vec{x}_1-\vec{x}_2)}\right)}_{\text{Quantum interference term}}$$

The quantum coherence is quantified by the autocorrelation of the wave function with itself at different positions. This encodes the the phase information.

The wave function is the representation in the position basis

$$\psi(\vec{x}_1) = \langle \vec{x}_1 | \psi \rangle \Rightarrow |\psi(\vec{x}_1)|^2 = \langle \vec{x}_1 | \psi \rangle \langle \psi | \vec{x}_1 \rangle$$

The quantum interference term $\psi(\vec{x}_1)\,\psi^*(\vec{x}_2) = \langle \vec{x}_1 | \psi \rangle \langle \psi | \vec{x}_2 \rangle$

These are "matrix elements" of the

$$\boxed{\text{density operator } \hat{\rho} \equiv |\psi\rangle\langle\psi|}$$

Probability density $|\psi(\vec{x})|^2 = \langle \vec{x} | \hat{\rho} | \vec{x} \rangle$ (diagonal "matrix element")

Coherence $\psi(\vec{x}_1)\,\psi^*(\vec{x}_2) = \langle \vec{x}_1 | \hat{\rho} | \vec{x}_2 \rangle$ (off-diagonal "matrix element")

Here I have put matrix element in quotes, because $\vec{x}$ is continuous variable, and $|\vec{x}\rangle$ is an improper basis.

If we consider a countable basis for the Hilbert space $\{|\alpha\rangle\}$ in d-dimension (d can be $\infty$)

$$|\psi\rangle = \sum c_\alpha |\alpha\rangle$$

$$\Rightarrow \hat{\rho} = |\psi\rangle\langle\psi| = \sum c_\alpha c_\beta^* \; |\alpha\rangle\langle\beta|$$

$\rho_{\alpha\beta} = c_\alpha c_\beta^*$ : Elements of the "density matrix"

Diagonal matrix element $\quad \rho_{\alpha\alpha} = |c_\alpha|^2 =$ Probability to be in state $|\alpha\rangle$
= "Population"

Off-diagonal matrix element $\quad \rho_{\alpha\beta} = |c_\alpha||c_\beta| e^{i(\phi_\alpha - \phi_\beta)}$ = Coherence between $|\alpha\rangle$ and $|\beta\rangle$

Normalization $\quad \langle\psi|\psi\rangle = \sum_\alpha |c_\alpha|^2 = \sum_\alpha \rho_{\alpha\alpha} = Tr(\hat{\rho}) = 1$

Let us consider the simplest nontrivial Hilbert space with $d=2$, e.g. a spin-½ particle, with standard basis $\{|\uparrow\rangle, |\downarrow\rangle\}$ representing eigenstates of $\hat{\sigma}_z$, spin-up and spin-down.

$$\rho \doteq \begin{bmatrix} c_\uparrow \\ c_\downarrow \end{bmatrix} \otimes \begin{bmatrix} c_\uparrow^* & c_\downarrow^* \end{bmatrix} = \begin{bmatrix} |c_\uparrow|^2 & c_\uparrow c_\downarrow^* \\ c_\downarrow c_\uparrow^* & |c_\downarrow|^2 \end{bmatrix}$$

The off-diagonal elements of $\hat{\rho}$ are the coherences in a given basis. They determine the possibility of quantum interference with respect to the distinguishable alternatives of the basis

Consider $\quad |\uparrow_x\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle + |\downarrow_z\rangle\right) \quad$ (spin-up along x. Standard basis along z.)

$$\hat{\rho} = |\uparrow_x\rangle\langle\uparrow_x| = \underbrace{\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}}_{\text{In the basis } \{|\uparrow_z\rangle, |\downarrow_z\rangle\}} = \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}}_{\text{In the basis } \{|\uparrow_x\rangle, |\downarrow_x\rangle\}}$$

The state has coherence between $|\uparrow_z\rangle, |\downarrow_z\rangle$. This implies that there can be quantum interference between these alternatives.

Consider the probability of finding $|\downarrow_x\rangle$ given the state was prepared $|\uparrow_x\rangle$

$$P(\downarrow_x|\uparrow_x) = \langle \downarrow_x|\hat{\rho}|\downarrow_x\rangle$$

$$= \langle \downarrow_x|\big(|\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\downarrow_z|\big)\,\hat{\rho}\,\big(|\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\downarrow_z|\big)|\downarrow_x\rangle$$

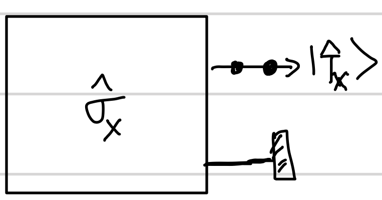
$$= \underbrace{|\langle\downarrow_x|\uparrow_z\rangle|^2}_{P(\downarrow_x|\uparrow_z)}\rho_{\uparrow_z\uparrow_z} + \underbrace{|\langle\downarrow_x|\downarrow_z\rangle|^2}_{P(\downarrow_x|\downarrow_z)}\rho_{\downarrow_z\downarrow_z} + \underbrace{\langle\downarrow_x|\uparrow_z\rangle\langle\downarrow_z|\downarrow_x\rangle\rho_{\uparrow_z\downarrow_z} + \langle\downarrow_x|\downarrow_z\rangle\langle\uparrow_z|\downarrow_x\rangle\rho_{\downarrow_z\uparrow_z}}_{\text{Quantum Interference?}}$$

$$= \left(\tfrac{1}{2}\right)\left(\tfrac{1}{2}\right) + \left(\tfrac{1}{2}\right)\left(\tfrac{1}{2}\right) + \left(+\tfrac{1}{\sqrt{2}}\right)\left(-\tfrac{1}{\sqrt{2}}\right)\left(\tfrac{1}{2}\right) + \left(-\tfrac{1}{\sqrt{2}}\right)\left(\tfrac{1}{\sqrt{2}}\right)\left(\tfrac{1}{2}\right)$$

$$= \tfrac{1}{4} + \tfrac{1}{4} - \tfrac{1}{4} - \tfrac{1}{4} = 0$$ Destructive interference between $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$

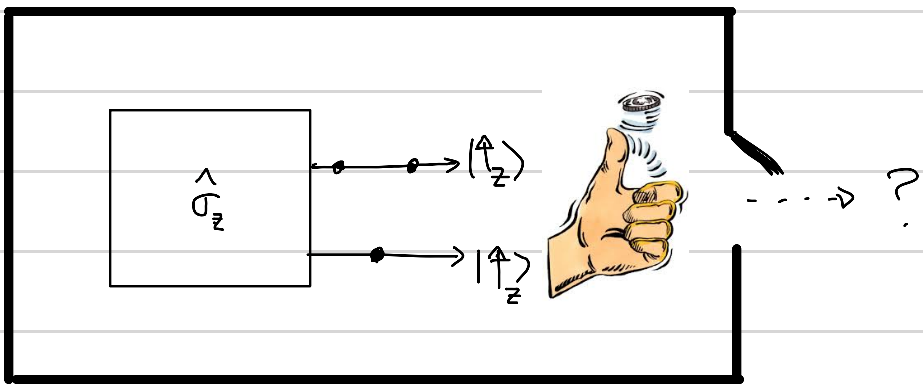
## Pure States vs. Mixed States

So far, all the states of a quantum mechanical system that we have discussed have been pure states, $|\psi\rangle \Rightarrow \hat{\rho} = |\psi\rangle\langle\psi|$. A pure state implies we have maximum possible knowledge of the system, e.g., we prepared the system $|\uparrow_x\rangle$ as the output of a Stern-Gerlach apparatus




The bizarre thing about quantum mechanics is that even with maximal possible knowledge of the system, we have imperfect ability to predict future outcomes, e.g. when we measure $\hat{\sigma}_z$, we has 50-50 to see $|\uparrow_z\rangle$ vs. $|\downarrow_z\rangle$.

Consider another preparation scheme. Suppose the preparer has a Stern–Gerlach device inside a black box that she select either $|\uparrow_z\rangle$ or $|\downarrow_z\rangle$ spins. She then flips a coin and decides which spin to set to me to then measure.




The preparer tells us the weighting of the coin: With probability $p_{\uparrow_z}$ she sends $|\uparrow_z\rangle$ with probability $p_{\downarrow_z}$, she sends $|\downarrow_z\rangle$. The state $\hat{\rho}$ is not a pure state. It is a statistical mixture of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$. We say $\hat{\rho}$ is a mixed state.

If we measure $\hat{\sigma}_z$, then we know that we will find $|\uparrow_z\rangle$ or $|\downarrow_z\rangle$ with probabilities $p_{\uparrow_z}$ and $p_{\downarrow_z}$ respectively. If this is a fair coin, then these are the same outcomes we would see for the pure state $|\uparrow_x\rangle = \frac{1}{\sqrt{2}}|\uparrow_z\rangle + \frac{1}{\sqrt{2}}|\downarrow_z\rangle$.

$|\uparrow_x\rangle$ is a coherent superposition of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$, whereas the state $\hat{\rho}$ out of the black box is a statistical mixture with no quantum coherence between $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$. To calculate the probability of say $|\downarrow_x\rangle$ given the state out of the black box:

$$P(\downarrow_x) = p_{\uparrow_z} P(\downarrow_x|\uparrow_z) + p_{\downarrow_z} P(\downarrow_x|\downarrow_z) = p_{\uparrow_z} |\langle\downarrow_x|\uparrow_z\rangle|^2 + p_{\downarrow_z} |\langle\downarrow_x|\downarrow_z\rangle|^2$$

$$= \frac{1}{2}\left(p_{\uparrow_z} + p_{\downarrow_z}\right) = \frac{1}{2}$$ No interference between $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$

We can assign a density operator to this statistical mixture that represents the state

Note: $P(\downarrow_x) = p_{\uparrow_z} \langle\downarrow_x|\uparrow_z\rangle\langle\uparrow_z|\downarrow_x\rangle + p_{\downarrow_z} \langle\downarrow_x|\downarrow_z\rangle\langle\downarrow_z|\downarrow_x\rangle$

$$= \langle\downarrow_x|\left(p_{\uparrow_z}|\uparrow_z\rangle\langle\uparrow_z| + p_{\downarrow_z}|\downarrow_z\rangle\langle\downarrow_z|\right)|\downarrow_x\rangle$$

$$\boxed{\Rightarrow P(\downarrow_x) = \langle \downarrow_x | \hat{\rho} | \downarrow_x \rangle \qquad \hat{\rho} = \underbrace{P_{\uparrow_z} |\uparrow_z\rangle\langle\uparrow_z| + P_{\downarrow_z} |\downarrow_z\rangle\langle\downarrow_z|}_{\text{Statistical mixture of } |\uparrow_z\rangle \text{ and } |\downarrow_z\rangle}}$$

the

Consider $\langle \uparrow_x | \hat{\rho} | \downarrow_x \rangle$ = Coherence between $|\uparrow_x\rangle$ and $|\downarrow_x\rangle$

$$= P_{\uparrow_z} \langle \uparrow_x | \uparrow_z \rangle \langle \uparrow_z | \downarrow_x \rangle + P_{\downarrow_z} \langle \uparrow_x | \downarrow_z \rangle \langle \downarrow_z | \downarrow_x \rangle$$

$$= P_{\uparrow_z} \left(\tfrac{1}{\sqrt{2}}\right)\left(\tfrac{1}{\sqrt{2}}\right) + P_{\downarrow_z} \left(\tfrac{1}{\sqrt{2}}\right)\left(-\tfrac{1}{\sqrt{2}}\right) = \tfrac{1}{2}\left( P_{\uparrow_z} - P_{\downarrow_z} \right)$$

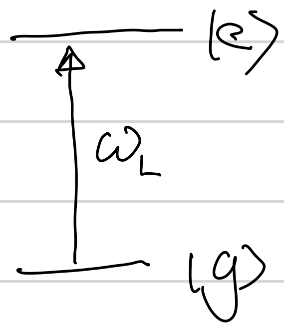
$\Rightarrow$ for a 50-50 statistical mixture of $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$ there is no coherence between $|\uparrow_x\rangle$ and $|\downarrow_x\rangle$. In fact there is no coherence between and two orthogonal states since

$$\hat{\rho} = \tfrac{1}{2}\left( |\uparrow_z\rangle\langle\uparrow_z| + |\downarrow_z\rangle\langle\downarrow_z| \right) = \tfrac{1}{2} \hat{\mathbb{1}} = \tfrac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{in any basis}$$

Since the off-diagonal elements of $\hat{\rho}$ are $0$ in all bases, this state has <u>no coherence</u>. It is said to be the maximally mixed state.

A state is mixed when we don't have complete information about the state. The example we gave is somewhat contrived, involving preparers flipping coins. Mixed states occur natural when we have open quantum system, i.e. a quantum system is interacting with other system (e.g. the environment), whose degrees of freedom we do not or cannot keep track of. For example, consider the collision brodening studied in the classical context. In the quantum problem we consider the coherent oscillation between a ground and excited state, a so-called two level atom, as we will study in the next lectures.

Two-level atom
$|g\rangle$ = ground-state
$|e\rangle$ = excited-state




A coherent field (e.g. laser) with frequency $\omega_L$ tuned near resonance can create a coherent superposition

. A elastic collision will induce a phase shift on one state

$$|\psi\rangle = c_g|g\rangle + c_e|e\rangle \Rightarrow c_g e^{i\phi}|g\rangle + c_e|e\rangle.$$

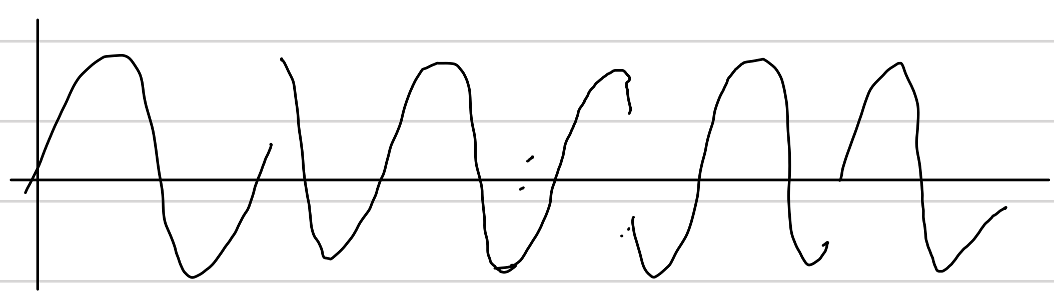
But if we don't know the phase shift we must take the statistical average of the possible phases

$$\Rightarrow \hat{\rho} = \int d\phi\, P(\phi)\left(c_g e^{i\phi}|g\rangle + c_e|e\rangle\right)\left(c_g^* e^{-i\phi}\langle g| + c_e^*\langle e|\right)$$

$$= \int d\phi\, P(\phi)\left(|c_g|^2|g\rangle\langle g| + |c_e|^2|e\rangle\langle e| + c_g c_e^* e^{i\phi}|g\rangle\langle e| + c_e c_g^* e^{-i\phi}|e\rangle\langle g|\right)$$

$$= |c_g|\;|g\rangle\langle g| + |c_e|^2|e\rangle\langle e| + \overline{c_g c_e^* e^{i\phi}}\,|g\rangle\langle e| + \overline{c_e c_g^* e^{-i\phi}}\,|e\rangle\langle g|$$

The statistical mixture of random phases $\Rightarrow$ loss of coherence between $|g\rangle$ & $|e\rangle$
This dephasing process is the quantum analog of collision dephasing of the Lorentz oscillator that we studied classically.
If we knew the phase at each collision time, the probability amplitude we be determined. In that case we have a pure state, conditioned on the phase jumps



When we don't have the phase information, we have a mixed state.
Generally, if we expect the state is one of an ensemble of possible states $|\psi_i\rangle$ with probability $p_i$ we assign the mixed state

$$\hat{\rho} \equiv \sum p_i |\psi_i\rangle\langle\psi_i| \qquad \text{Statistical mixture of } \{|\psi_i\rangle\}$$

$$\rho_{\alpha\beta} = \sum_i p_i\, c_\alpha^{(i)} c_\beta^{(i)*} = \overline{c_\alpha c_\beta^*} \quad \text{Ensemble average}$$

- A statistical mixture should be distinguished from a coherent superposition
- The states in the ensemble need not be orthogonal, e.g. statistical mixture of $|\uparrow_x\rangle$ and $|\uparrow_z\rangle$.
- The ensemble decomposition is not unique; different mixtures lead to the same $\hat{\rho}$.

More generally, for an "Open quantum system" information about one quantum subsystem that is part of the whole system is not generally a pure state. This can be true even if the state of the whole is pure. E.g. bipartite A+B : $|\Psi\rangle_{AB}$ pure, but $\hat{\rho}_A, \hat{\rho}_B$ mixed. This is a uniquely quantum phenomenon: entanglement. We can have maximum possible information about the whole but an incomplete description of the parts. We will revisit this in much greater detail in the next semester.

## Formal Properties of the Density Operator

- Hermitian $\hat{\rho}^\dagger = \hat{\rho}$

- Positive: $\hat{\rho} \geq 0 \Rightarrow \langle\phi|\hat{\rho}|\phi\rangle \geq 0 \Rightarrow$ The eigenvalues of $\hat{\rho}$

- Normalization: $\mathrm{Tr}(\hat{\rho}) = 1$

- Diagonalization: $\hat{\rho} = \sum_{i=1}^{d} \lambda_i |e_i\rangle\langle e_i|$ = Unique ensemble decomposition into orthogonal vectors $\{|e_i\rangle\}$ with probabilities $\{\lambda_i\}$, $\sum \lambda_i = 1$

- Pure vs. mixed state:

A pure state $\Rightarrow \exists |\psi\rangle$ s.t. $\hat{\rho} = |\psi\rangle\langle\psi| \Rightarrow$ One eigenvector $|e_1\rangle = |\psi\rangle$, eigenvalue 1

All other eigenvalues are 0

$$\hat{\rho}_{pure} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 \cdots & 0 \\ & & \ddots & \\ & & & 0 \end{bmatrix}$$

For a mixed states $\hat{\rho} = \sum \lambda_i |e_i\rangle\langle e_i|$, where $\lambda_i < 1 \quad \forall i$

$$\Rightarrow \hat{\rho}^2 = \sum_i \lambda_i^2 |e_i\rangle\langle e_i| \Rightarrow \mathrm{Tr}(\hat{\rho}^2) = \sum_i \lambda_i^2 < 1 \text{ for mixed states}$$

"purity"

Maximally mixed $\Rightarrow$ Equal mixture of all basis states, $\lambda_i = \frac{1}{d} \ \forall i \Rightarrow \mathrm{Tr}(\hat{\rho}^2)_{min} = \frac{1}{d}$

## Using $\hat{\rho}$ to make predictions

Aside: The trace operation: $\mathrm{Tr}(\hat{A}) = \sum_i \langle e_i|\hat{A}|e_i\rangle$ (independent of basis $\{|e_i\rangle\}$)

$$\mathrm{Tr}(|\psi\rangle\langle\phi|\hat{A}) = \langle\phi|\hat{A}|\psi\rangle$$

$$\mathrm{Tr}(\hat{A}\hat{B}\hat{C}) = \mathrm{Tr}(\hat{C}\hat{A}\hat{B}) = \mathrm{Tr}(\hat{B}\hat{C}\hat{A})$$

See homework

From these properties it follows

- Probability to find outcome $|a\rangle$: $P_a = \langle a|\hat{\rho}|a\rangle = \mathrm{Tr}(\hat{\rho}\,|a\rangle\langle a|)$

- Expectation value of an observable:

$$\langle\hat{A}\rangle = \sum a P_a = \sum_a a\,\mathrm{Tr}(|a\rangle\langle a|\hat{\rho}) = \mathrm{Tr}\left(\sum_a a|a\rangle\langle a|\,\hat{\rho}\right) \Rightarrow \langle\hat{A}\rangle = \mathrm{Tr}(\hat{\rho}\hat{A})$$

## Schrödinger Eqn for $\hat{\rho}$

The Heisenberg equation of motion for an operator (Heisenberg picture)

$$\frac{\partial}{\partial t}\hat{A} = -\frac{i}{\hbar}[\hat{A},\hat{H}] \Rightarrow \frac{\partial}{\partial t}\langle\hat{A}\rangle = -\frac{i}{\hbar}\left(\langle\hat{A}\hat{H}\rangle - \langle\hat{H}\hat{A}\rangle\right)$$

$$\Rightarrow \frac{\partial}{\partial t}\mathrm{Tr}(\hat{\rho}\hat{A}) = -\frac{i}{\hbar}\left[\mathrm{Tr}(\hat{A}\hat{H}\hat{\rho}) - \mathrm{Tr}(\hat{H}\hat{A}\hat{\rho})\right] = -\frac{i}{\hbar}\left[\mathrm{Tr}(\hat{H}\hat{\rho}\hat{A}) - \mathrm{Tr}(\hat{\rho}\hat{H}\hat{A})\right] = \frac{-i}{\hbar}\mathrm{Tr}\left([\hat{\rho},\hat{H}]\hat{A}\right)$$

$\Rightarrow$ In the Schrödinger picture $\hat{A}$ is constant and

$$\boxed{\frac{\partial}{\partial t}\hat{\rho} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}]} \qquad \boxed{\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t)}$$

## Why is $\hat{\rho}$ called the density operator?

Classical Mechanics: State of the system: $P(\vec{q},\vec{p},t)$: Probability density on phase space.

Liouville Eqn of motion: $\frac{\partial}{\partial t}P(\vec{q},\vec{p},t) = \{H(\vec{q},\vec{p}), P(\vec{q},\vec{p},t)\}$ ← Poisson Bracket

$\hat{\rho}$ is the quantum mechanical analog of $P(\vec{q},\vec{p})$. $\frac{\partial\hat{\rho}}{\partial t} = -i[\hat{H},\hat{\rho}]$ is sometimes called the Liouville eqn. We will study representations of $\hat{\rho}$ in phase space in great detail when we study the contrasts of classical vs. nonclassical light.