I. Principles of quantum mechanics

1° The quantum mechanical formalism

a) States

Axiom 1: The state of a quantum system is described by a ray in a suitable Hilbert space $\mathcal{H}$.

- The state is represented by a normalized state vector $|\psi\rangle \in \mathcal{H}$ with

$$\langle \psi | \psi \rangle = |\psi|^2 = 1$$ scalar product

- Each state can be decomposed into orthonormal basis vectors $|\chi_n\rangle$:

$$|\psi\rangle = \sum_n c_n |\chi_n\rangle, \quad c_n \in \mathbb{C}, \quad \sum_n |c_n|^2 = 1$$

- Each state $|\psi\rangle$ can be associated with a linear form $\langle \psi |$ in the dual space $\mathcal{H}^+$ which acts according to

$$\left.\begin{aligned} \langle \psi | : \mathcal{H} &\to \mathbb{C} \\ |\varphi\rangle &\to \langle \psi | \varphi \rangle \end{aligned}\right\}$$

Examples: - Wave function
- States of a spin-$\frac{1}{2}$-system

Axiom P: The probability that a system prepared in a state $|\psi\rangle$ is found under a measurement to be in state $|\varphi\rangle$ is given by

$$P(\varphi|\psi) = |\langle\psi|\varphi\rangle|^2 \in [0,1]$$

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b) Observables

Axiom O: Physical observables are represented by linear Hermitian operators acting on $\mathcal{H}$.

Reminder: An operator A is Hermitian if

$$A = A^+$$

where the adjoint A^+ of A is defined by

$$\langle\psi|A\varphi\rangle = \langle A^+\psi|\varphi\rangle \quad \forall\, |\psi\rangle, |\varphi\rangle$$

- The possible outcomes of single measurements of A are given by the eigenvalues α:

$$A|\alpha\rangle = \alpha|\alpha\rangle \,, \quad \alpha \in \mathbb{R} \,, \quad |\alpha\rangle \text{ eigenstate}$$

- After a measurement yielding the eigenvalue α, the system is in the corresponding eigenstate $|\alpha\rangle$. Thus it follows from axiom P that the probability to measure α when the system is in state $|\psi\rangle$ is

$$P(\alpha|\psi) = |\langle\alpha|\psi\rangle|^2$$

- As a consequence, the expectation value of A over multiple measurements is

$$\langle A\rangle_\psi = \langle\psi|A\psi\rangle$$

- The uncertainty of an observable A in a state $|\psi\rangle$ is defined by

$$\Delta A_\psi = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$$

For observables A, B the uncertainty relation

$$\Delta A_\psi \cdot \Delta B_\psi \geq \frac{1}{2}|\langle\psi|[A,B]|\psi\rangle|$$

holds, where $[A,B] = AB - BA$.

- If A and B commute, $[A,B]=0$, there are simultaneous eigenstates $|\alpha,\beta\rangle$ such that

$$\left.\begin{aligned} A|\alpha,\beta\rangle &= \alpha|\alpha,\beta\rangle \\ B|\alpha,\beta\rangle &= \beta|\alpha,\beta\rangle \end{aligned}\right\}$$

c) Unitary transformations and time evolution

An operator $U : \mathcal{H} \to \mathcal{H}$ is called unitary if

$$U U^\dagger = U^\dagger U = \mathbb{1}$$

The time evolution of quantum systems is unitary:

Axiom I: The time evolution of a quantum state $|\psi(t)\rangle$ is governed by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle \qquad (SE)$$

where H is the (time-independent) Hamilton operator.

- The formal solution of (SE) is

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

where

$$U(t, t_0) = \exp\left[-\frac{i}{\hbar} (t - t_0) H \right]$$

is the time evolution operator.

U is unitary because H is Hermitian.

- More generally, any one-parameter family of unitary transformations $U(\lambda)$, $\lambda \in \mathbb{R}$ with

(i) $U(\lambda_1 + \lambda_2) = U(\lambda_1) U(\lambda_2)$

(ii) $U(0) = \mathbb{1}$

can be written in the form

$$U(\lambda) = \exp(i\lambda X)$$

where the generator X is a Hermitian operator.

Examples:

U	X
time translation	energy (H)
spatial translation	momentum ($\vec{p}$)
rotation	angular momentum ($\vec{J}$)

- In the Heisenberg picture states are time-independent while operators depend on time according to

$$A_H(t) = U^+(t) A U(t)$$

This leads to the Heisenberg equation of motion

$$\frac{d}{dt} A_H(t) = \frac{i}{\hbar} [H, A_H]$$ exercise

- Noether theorem: If H is invariant under a unitary transformation U, i.e. if

$$U^+ H U = H$$

then the generator X of U is a

conserved quantity, i.e.

$$\frac{d}{dt} X_H(t) = 0.$$

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d) Composite systems

Consider two systems S_1, S_2 described by Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$. Then the composite system S composed of S_1 and S_2 is described by state vectors in the tensor product

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$$

$\mathcal{H}$ is spanned by pure tensors $|\psi\rangle \in \mathcal{H}$ of the form

$$\left.\begin{aligned} |\psi\rangle &= |\psi_1\rangle \otimes |\psi_2\rangle =: |\psi_1\rangle|\psi_2\rangle \\ |\psi_1\rangle &\in \mathcal{H}_1, \quad |\psi_2\rangle \in \mathcal{H}_2 \end{aligned}\right\}$$

For pure tensors the scalar product on $\mathcal{H}$ is defined by

$$\langle\psi|\phi\rangle = (\langle\psi_1|\langle\psi_2|)(|\phi_1\rangle|\phi_2\rangle) =$$

$$=: \langle\psi_1|\phi_1\rangle\langle\psi_2|\phi_2\rangle$$

For linear superpositions of pure tensors, the scalar product follows from linearity.

- Independent subsystems: If S_1 is in state $|\psi_1\rangle$ and S_2 in state $|\psi_2\rangle$ and the two systems do not interact, then the composite system is in the product state

$$|\psi\rangle = |\psi_1\rangle|\psi_2\rangle$$

This state is normalized:

$$\langle\psi|\psi\rangle = \langle\psi_1|\psi_1\rangle\langle\psi_2|\psi_2\rangle = 1$$

Operators A_1, A_2 acting on $\mathcal{H}_1$, $\mathcal{H}_2$ are extended to $\mathcal{H}$ through

$$\left.\begin{aligned} \mathcal{A}_1 &= A_1 \otimes \mathbb{1} \quad , \quad \mathcal{A}_2 = \mathbb{1} \otimes A_2 \\ \mathbb{1} &: \text{identity operator} \end{aligned}\right\}$$

Then the expectation values are

$$\langle\psi|\mathcal{A}_1|\psi\rangle = \langle\psi_1|\langle\psi_2|A_1\otimes\mathbb{1}|\psi_1\rangle|\psi_2\rangle$$

$$= \langle\psi_1|A_1|\psi_1\rangle\langle\psi_2|\psi_2\rangle = \langle A_1\rangle_{\psi_1}$$

and $\langle\psi|\mathcal{A}_2|\psi\rangle = \langle A_2\rangle_{\psi_2}$

$\Rightarrow$ the presence of the second, non-interacting subsystem does not change the expectation values of the first subsystem (independence)

Similarly, the probability to find S in a state $|\phi\rangle = |\phi_1\rangle|\phi_2\rangle$ is

$$P(\phi|\psi) = |\langle\phi|\psi\rangle|^2 = |(\langle\phi_1|\langle\phi_2|)(|\psi_1\rangle|\psi_2\rangle)$$

$$= |\langle\phi_1|\psi_1\rangle|^2 |\langle\phi_2|\psi_2\rangle|^2 = P(\phi_1|\psi_1)\,P(\phi_2|\psi_2)$$

$\Rightarrow$ probabilities of independent events multiply

Examples:

(i) Two-particle wave function for two independent, distinguishable particles:

$$\psi(\vec{r}_1, \vec{r}_2) = \psi_1(\vec{r}_1)\,\psi_2(\vec{r}_2)$$

(ii) Two spin-$\frac{1}{2}$-particles:

$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ spin up

$|\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$ spin down

} in the eigenstates of S_z

$\Rightarrow$ two-particle product states are

$$|\uparrow\uparrow\rangle,\ |\downarrow\downarrow\rangle,\ |\uparrow\downarrow\rangle,\ |\downarrow\uparrow\rangle$$

exercise

2° Mixed states and the density operator

- The state vector $|\psi\rangle$ contains the complete information about the system
- How to describe situations where the available information about the system is incomplete, i.e. where (fundamental) quantum mechanical uncertainty is combined with classical lack of information (ignorance)?

a) The density operator

- We want to describe a situation where the system is in state $|\psi_n\rangle$ with probability p_n. Example: Gibbs state
- The answer is not

$$|\psi\rangle = \sum_n p_n |\psi_n\rangle$$

which is simply a superposition of states.

What we want to achieve is that the expectation value of some operator A is

$$\langle A\rangle = \sum_n p_n \langle \psi_n | A | \psi_n\rangle$$

Using a basis $|\chi_m\rangle$ and the resolution of identity

$$\mathbb{1} = \sum_m |\chi_m\rangle\langle\chi_m|$$

we can write

$$\underline{\langle A\rangle} = \sum_n \sum_m p_n \langle\psi_n|A|\chi_m\rangle\langle\chi_m|\psi_n\rangle$$

$$= \sum_m \sum_n \langle\chi_m|\psi_n\rangle p_n \langle\psi_n|A|\chi_m\rangle$$

$$= \underline{\mathrm{Tr}(\rho A)} \quad \text{where the } \underline{\text{density operator}} \text{ is}$$

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

This generalizes the concept of a quantum state. In the standard case of a (pure) state vector $|\psi\rangle$, ρ is the <u>projection operator</u> onto $|\psi\rangle$:

$$\rho = |\psi\rangle\langle\psi|$$

The <u>density matrix</u> is defined by the matrix elements of ρ w.r.t. some basis:

$$\rho_{mm'} = \langle\chi_m|\rho|\chi_{m'}\rangle = \sum_n p_n \langle\chi_m|\psi_n\rangle \times$$

$$\times \langle\psi_n|\chi_{m'}\rangle$$

Properties of ρ

(i) ρ is Hermitian:

$$\langle \phi | \rho \chi \rangle = \sum_n \langle \phi | \psi_n \rangle p_n \langle \psi_n | \chi \rangle$$

$$= \sum_n \langle \psi_n | \phi \rangle^* p_n \langle \chi | \psi_n \rangle^* =$$

$$= \left(\sum_n \langle \chi | \psi_n \rangle p_n \langle \psi_n | \phi \rangle \right)^* = \langle \chi | \rho \phi \rangle^*$$

$$= \langle \rho \phi | \chi \rangle$$

This is true because ρ is a linear superposition of projection operators with real coefficients.

(ii) ρ is positive semi-definite:

This implies that for any state $|\phi\rangle$

$$\langle \phi | \rho | \phi \rangle = \sum_n \underbrace{p_n}_{\geq 0} \underbrace{|\langle \phi | \psi_n \rangle|^2}_{\geq 0} \geq 0$$

(iii) $\mathrm{Tr}(\rho) = 1$: For any basis $|\chi_m\rangle$

$$\mathrm{Tr}(\rho) = \sum_m \sum_n p_n |\langle \chi_m | \psi_n \rangle|^2 =$$

$$= \sum_n p_n \underbrace{\sum_m |\langle \chi_m | \psi_n \rangle|^2}_{= |\langle \psi_n | \psi_n \rangle|^2 = 1} = \sum_n p_n = 1 .$$

(iv) Von Neumann equation:

The time evolution of ρ can be inferred from that of the $|\psi_n\rangle$:

$$\left.\begin{aligned} i\hbar \frac{\partial}{\partial t} |\psi_n\rangle &= H |\psi_n\rangle \\ -i\hbar \frac{\partial}{\partial t} \langle \psi_n| &= \langle \psi_n | H \end{aligned}\right\}$$

$$\Rightarrow \underline{i\hbar \frac{\partial \rho}{\partial t}} = \sum_n p_n \left\{ (H|\psi_n\rangle)\langle \psi_n| - |\psi_n\rangle\langle \psi_n| H \right\} = \underline{[H, \rho]}$$

which is reminiscent of (but differs from) the Heisenberg equation of motion

$$i\hbar \frac{\partial A_H}{\partial t} = -[H, A_H]$$

b) Pure and mixed states

A state described by a density operator ρ is called pure if there exists a state vector $|\psi\rangle$ such that

$$\rho = |\psi\rangle\langle\psi|$$

Otherwise the state is called mixed.
We now show that

$$\left.\begin{array}{l} \rho \text{ pure} \iff \mathrm{Tr}(\rho^2) = 1 \\ \rho \text{ mixed} \iff \mathrm{Tr}(\rho^2) < 1 \end{array}\right\}$$

(i) ρ pure $\Rightarrow \rho = |\psi\rangle\langle\psi|$

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

$$\Rightarrow \mathrm{Tr}(\rho^2) = \mathrm{Tr}(\rho) = 1$$

(ii) Consider now a general density operator ρ. Because ρ is Hermitian and positive, there is a basis $|\rho_\mu\rangle$ such that

$$\rho = \sum_\mu \rho_\mu |\rho_\mu\rangle\langle\rho_\mu|, \quad \rho_\mu \geq 0$$

with $\mathrm{Tr}(\rho) = \sum_\mu \rho_\mu = 1$. Thus

$$\rho^2 = \sum_\mu \rho_\mu^2 |\rho_\mu\rangle\langle\rho_\mu|$$

$$\Rightarrow \mathrm{Tr}(\rho^2) = \sum_\mu \rho_\mu^2 \leq \sum_\mu \rho_\mu = 1$$

because $0 \leq \rho_m \leq 1$.

Suppose now that $\mathrm{Tr}(\rho^2) = 1$. Then

$$0 = \sum_m \rho_m - \sum_m \rho_m^2 = \sum_m \rho_m (1 - \rho_m)$$

which is only possible if $\rho_m = 1$ or $\rho_m = 0$ for all m. Because $\sum_m \rho_m = 1$ it follows that

$$\rho_m = \begin{cases} 1 & \text{for some } m_0 \\ 0 & m \neq m_0 \end{cases}$$

$$\Rightarrow \rho = |\rho_{m_0}\rangle\langle\rho_{m_0}| \text{ is pure.}$$

Example: The general density operator of a spin-$\frac{1}{2}$-particle is of the form

$$\rho = \frac{1}{2}(\mathbb{1} + \vec{n} \cdot \vec{\sigma})$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices and $\vec{n}$ is a three-dimensional vector. Then

$$\left.\begin{aligned} &\rho \text{ pure} \Leftrightarrow |\vec{n}| = 1 \\ &\rho \text{ mixed} \Leftrightarrow |\vec{n}| < 1 \end{aligned}\right\} \text{ exercise}$$

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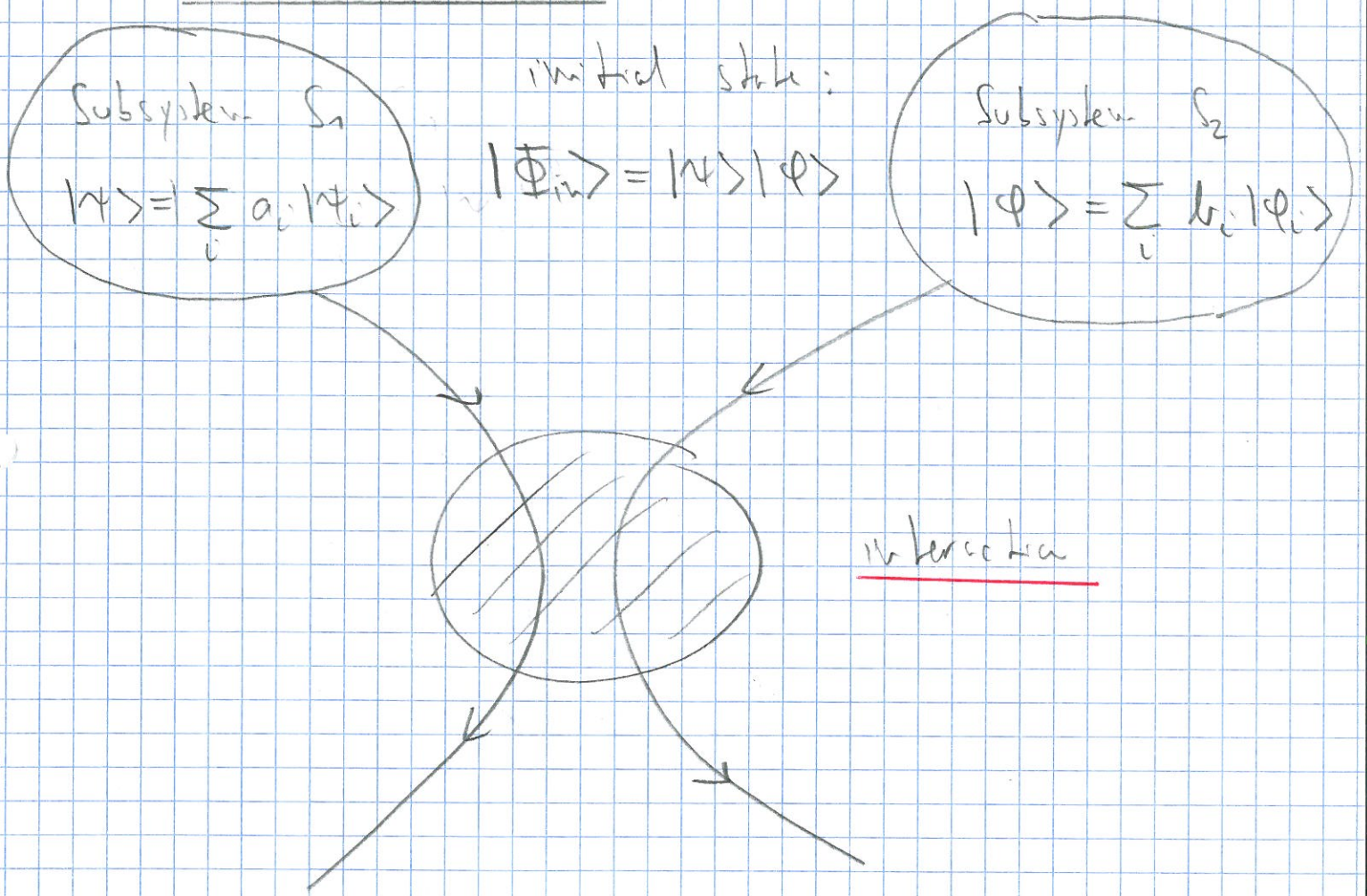
c) The reduced density operator

Question: How can mixed states ever arise, given that the Schrödinger time evolution always takes pure states to pure states?

Answer: Mixed states provide a **reduced description** of the interacting parts of a composite system.

General scenario:



but a product state

Consider the expectation value of an observable acting on S_1:

$$\langle \Phi | A^{(1)} | \Phi \rangle = \sum_{ij} \sum_{kl} c_{ij} c^*_{kl} \langle \psi_k | \langle \varphi_l | A^{(1)} | \psi_i \rangle | \varphi_j \rangle$$

$$= \sum_{ij} \sum_{kl} c_{ij} c^*_{kl} \langle \psi_k | A^{(1)} | \psi_i \rangle \underbrace{\langle \varphi_l | \varphi_j \rangle}_{= \delta_{lj}} =$$

$$= \sum_{ijk} c_{ij} c^*_{kj} \langle \psi_k | A^{(1)} | \psi_i \rangle = \sum_{ik} \rho^{(1)}_{ik} \langle \psi_k | A^{(1)} | \psi_i \rangle$$

with $\rho^{(1)}_{ik} := \sum_j c_{ij} c^*_{kj}$. Defining the reduced density operator of subsystem 1 by

$$\rho^{(1)} = \sum_{ik} \rho^{(1)}_{ik} | \psi_i \rangle \langle \psi_k |$$

it follows that

$$\mathrm{Tr}(\rho^{(1)} A^{(1)}) = \sum_m \langle \psi_m | \rho^{(1)} A^{(1)} | \psi_m \rangle =$$

$$= \sum_m \sum_{ik} \underbrace{\langle \psi_m | \psi_i \rangle}_{\delta_{mi}} \rho^{(1)}_{ik} \langle \psi_k | A^{(1)} | \psi_m \rangle =$$

$$= \sum_{ik} \rho^{(1)}_{ik} \langle \psi_k | A^{(1)} | \psi_i \rangle = \langle A^{(1)} \rangle_\Phi$$

The reduced density operator $\rho^{(1)}$ is obtained from the density operator of the full system

$$\rho = | \Phi \rangle \langle \Phi |$$

by taking a partial trace w.r.t. the subsystem 2:

$$\rho^{(1)} = \mathrm{Tr}_2(\rho) := \sum_j \langle \phi_j | \Phi \rangle \langle \Phi | \phi_j \rangle =$$

$$= \sum_j \sum_{ik} \sum_{\ell m} \underbrace{\langle \phi_j | \psi_i \rangle | \phi_k \rangle}_{\sigma_{jk}} c_{ik} c^*_{\ell m} \langle \psi_\ell | \underbrace{\langle \phi_m | \phi_j \rangle}_{\delta_{mj}}$$

$$= \sum_{i\ell} |\psi_i\rangle \underbrace{\left(\sum_j c_{ij} c^*_{\ell j} \right)}_{\rho^{(1)}_{i\ell}} \langle \psi_\ell | .$$

The information available about a subsystem is incomplete because the two subsystems have become entangled by the interaction.

Examples:

(i) Singlet state of two spin-$\frac{1}{2}$-particles

The initial state is

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

Reduced density operator for particle 1:

$$\rho^{(1)} = \mathrm{Tr}_1 \left(|\psi_{0,0}\rangle\langle\psi_{0,0}| \right) =$$

$$= \mathrm{Tr}_1 \left(\frac{1}{2} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \left(\langle\uparrow\downarrow| - \langle\downarrow\uparrow| \right) \right) =$$

$$= \frac{1}{2}\,\mathrm{Tr}_1\Big[\,|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow| - |\uparrow\downarrow\rangle\langle\downarrow\uparrow| - |\downarrow\uparrow\rangle\langle\uparrow\downarrow|\Big] = \frac{1}{2}\left(|\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\uparrow|\right)$$

$$= \frac{1}{2}\,\mathbb{1}$$

which is of the general form $\rho = \frac{1}{2}(\mathbb{1} + \vec{n}\cdot\vec{\sigma})$ with $\vec{n} = 0$. Measurement w.r.t. any coordinate system yields $\sigma_z = \pm\frac{1}{2}$ with equal probability

$\Rightarrow$ state is maximally mixed / uncertain.

(ii) Measurement process

A measurement can be schematically described as an interaction between a system S with a apparatus A. Basis states of S and A are $|s_i\rangle$ and $|a_i\rangle$, and a measurement $\hat{H}$ induces a correlation between S and A that does not perturb S (ideal measurement)

If A is initially in state $|a\rangle$ and S in an eigenstate $|s_i\rangle$, then

$$|s_i\rangle|a\rangle \xrightarrow[\hat{H}]{} |s_i\rangle|a_i\rangle$$

Suppose now that S is initially in a superposition of eigenstates

$$|s\rangle = \sum_i c_i |s_i\rangle$$

then the effect of the measurement is

$$|s\rangle|a\rangle = \underbrace{\sum_i c_i |s_i\rangle|a\rangle}_{\text{product state}} \xrightarrow{\hat{M}} \underbrace{\sum_i c_i |s_i\rangle|a_i\rangle}_{\text{non-product state}}$$

and the reduced density operator of the system after the measurement is

$$\rho^{(s)} = Tr_A(\rho) = Tr_A\left(\sum_{ij} c_i c_j^* |s_i\rangle|a_i\rangle\langle s_j|\langle a_j|\right)$$

$$= \sum_i |c_i|^2 |s_i\rangle\langle s_i|$$

$\Rightarrow$ S is in state $|s_i\rangle$ with probability $|c_i|^2$.

The measurement transforms the (quantum) superposition $|s\rangle$ into a (classical) mixture $\rho^{(s)}$

Similarly the reduced density operator of the apparatus is

$$\rho^{(A)} = \sum_i |c_i|^2 |a_i\rangle\langle a_i|$$

$\Rightarrow$ A is found in state $|a_i\rangle$ with probability $|c_i|^2$.