Density Matrix and Decoherence

Quantum Mechanics II

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- **Intrinsic randomness of quantum mechanics:** Unlike classical physics, where probabilities arise solely from lack of knowledge, quantum mechanics involves intrinsic randomness.
- Consider a state $|\psi\rangle \in V$, with V an N-dimensional complex vector space.
- Even with complete knowledge, measurements in quantum mechanics are probabilistic, leading to the concept of an *ensemble*.

- **New Layer of Randomness:**
  - Quantum mechanics adds a new layer of randomness;
  - This arises when describing a *subsystem* that is entangled with the rest of the system.
- **Density Matrix:**
  - To account for this added randomness, we use a *density matrix*—an operator on the state space encoding the quantum state and this extra randomness.
- **Pure vs. Mixed States:**
  - A *pure state* is represented by $|\psi\rangle \in V$, a vector in the Hilbert space.
  - A *mixed state* accounts for additional randomness and cannot be described by a vector in V alone.

Stern-Gerlach Experiment

In the Stern-Gerlach experiment, a beam of silver atoms emerges from a hot oven, unpolarized, with a spin state that is random. If we denote the spin state of an atom as $|\mathbf{n}\rangle$ with $\mathbf{n}$ a unit vector, then atoms have vectors $\mathbf{n}$ pointing in random directions. Can we represent this ensemble of atoms with a quantum state $|\psi\rangle$ that captures this intrinsic randomness?
The answer is **no**. The general state is

$$|\psi\rangle = a_+|+\rangle + a_-|-\rangle, \quad a_+, a_- \in \mathbb{C},$$

where $|\pm\rangle$ are the familiar $\hat{S}_z$ eigenstates. The state $|\psi\rangle$, a pure state, is fixed by a_+ and a_-, thus fixing the direction $\mathbf{n}$ of the spin state. Consequently, $|\psi\rangle$ cannot describe states $|\mathbf{n}\rangle$ with random $\mathbf{n}$.
To simplify, assume an oven with 50% of the atoms polarized as $|+\rangle$ and the other 50% as $|-\rangle$. This can be represented by pairs $(p_i, |\psi_i\rangle)$, where p_i is the probability of a given atom being in the quantum state $|\psi_i\rangle$:

$$E_z = \left\{ \left(\frac{1}{2}, |+\rangle\right), \left(\frac{1}{2}, |-\rangle\right) \right\}.$$

We denote E_z as the **ensemble of z-polarized states**, with each entry specifying a state and its probability. This ensemble represents the mixed state of our system.

General Ensemble for Quantum Systems

For a general ensemble E associated with a quantum system with state space V, we have a list of states and probabilities:

$$E = \{(p_1, |\psi_1\rangle), \ldots, (p_n, |\psi_n\rangle)\}, \quad p_1, \ldots, p_n > 0, \quad p_1 + \cdots + p_n = 1.$$

where $n \geq 1$ is an integer representing the number of entries in the ensemble. This ensemble describes a general mixed state.

- The states $|\psi_a\rangle \in V$ are normalized for all $a = 1, \ldots, n$:

$$\langle\psi_a|\psi_a\rangle = 1.$$

- The states $|\psi_a\rangle$ are **not required** to be orthogonal to each other.
- The integer n does not need to be related to the dimensionality $\dim V$ of the state space.
- If $n = 1$, then $p_1 = 1$, and the ensemble represents a pure state $|\psi_1\rangle$.
- For $n \geq 2$, we have a mixed state.
- We can also have $n > \dim V$ since the states $|\psi_a\rangle$ are not required to be linearly independent.

Expectation Value of a Hermitian Operator in an Ensemble

If $\hat{Q}$ denotes a Hermitian operator we are to measure, its expectation value $\langle \hat{Q} \rangle_E$ in the ensemble E is given by

$$\langle \hat{Q} \rangle_E = \sum_{a=1}^{n} p_a \langle \psi_a | \hat{Q} | \psi_a \rangle = p_1 \langle \psi_1 | \hat{Q} | \psi_1 \rangle + \cdots + p_n \langle \psi_n | \hat{Q} | \psi_n \rangle .$$

This becomes clear if we imagine measuring $\hat{Q}$ on the full ensemble E. The expectation value $\langle \psi_a | \hat{Q} | \psi_a \rangle$ of $\hat{Q}$ in the ath subensemble of states $|\psi_a\rangle$ must be weighted by the probability p_a for states in E.

Now, consider an oven producing 50% of atoms in the state $|x;+\rangle$ and the other 50% in the state $|x;-\rangle$. The ensemble E_x is:

$$E_x = \left\{ \left(\frac{1}{2}, |x;+\rangle \right), \left(\frac{1}{2}, |x;-\rangle \right) \right\} .$$

The expectation value of $\hat{Q}$ in E_x is then

$$\langle \hat{Q} \rangle_{E_x} = \frac{1}{2} \langle x;+ | \hat{Q} | x;+ \rangle + \frac{1}{2} \langle x;- | \hat{Q} | x;- \rangle .$$

Equivalence of Ensembles

An interesting result emerges if we rewrite $\langle \hat{Q} \rangle_{E_x}$ by expressing $|x;+\rangle$ and $|x;-\rangle$ in terms of $|+\rangle$ and $|-\rangle$:

$$\langle \hat{Q} \rangle_{E_x} = \frac{1}{4}\left(\langle + | + \langle - |\right) \hat{Q} \left(|+\rangle + |-\rangle\right) + \frac{1}{4}\left(\langle + | - \langle - |\right) \hat{Q} \left(|-\rangle + |+\rangle\right).$$

The off-diagonal matrix elements cancel, yielding:

$$\langle \hat{Q} \rangle_{E_x} = \frac{1}{2}\langle + | \hat{Q} | + \rangle + \frac{1}{2}\langle - | \hat{Q} | - \rangle = \langle \hat{Q} \rangle_{E_z}.$$

Thus, for any observable, the expectation values in the two ensembles E_z and E_x are identical, making them physically indistinguishable.
Both ensembles represent the same mixed quantum state, despite the different entries. We are led to a deeper understanding of representing a mixed quantum state using density matrices, which we will explore further.

Example: Unpolarized Ensemble

- The oven in the Stern-Gerlach experiment produces **unpolarized silver atoms**. We analyze the expectation value of $\hat{Q}$ for the unpolarized ensemble and compare it with the E_z ensemble.
- In the unpolarized state, the values of $\mathbf{n}$ are uniformly distributed over the solid angle 4π.
- The probability of $\mathbf{n}$ being within a solid angle $d\Omega$ is $\frac{d\Omega}{4\pi}$.

The unpolarized ensemble is defined as:

$$E_{\text{unp}} = \left\{ \frac{d\Omega}{4\pi}, |\mathbf{n}(\theta, \phi)\rangle \right\}, \quad |\mathbf{n}(\theta, \phi)\rangle = \cos\frac{\theta}{2}|+\rangle + e^{i\phi}\sin\frac{\theta}{2}|-\rangle.$$

The expectation value of any observable $\hat{Q}$ is given by:

$$\langle \hat{Q} \rangle_{E_{\text{unp}}} = \int \frac{d\Omega}{4\pi} \langle \mathbf{n}(\theta, \phi)|\hat{Q}|\mathbf{n}(\theta, \phi)\rangle.$$

Example: Unpolarized Ensemble (cont.)

Integrating over ϕ eliminates off-diagonal elements of $\hat{Q}$:

$$\langle \hat{Q} \rangle_{E_{\text{unp}}} = \frac{1}{2}\langle + | \hat{Q} | + \rangle + \frac{1}{2}\langle - | \hat{Q} | - \rangle.$$

- This is the same result as for the E_z and E_x ensembles.
- The unpolarized ensemble E_{unp} is equivalent to the ensembles where half the states are polarized in one direction and the other half in the opposite direction.

Entangled States and Ensembles

An even simpler example of quantum states described by ensembles is provided by a pair of entangled states. Let Alice and Bob each have one of two entangled spin one-half states. The entangled state $|\psi_{AB}\rangle$ they share is the singlet state of total spin equal to zero:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\big(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\big).$$

- If Alice measures the spin of her state along the z-direction:
  - If Alice gets $|+\rangle$, then the state of Bob is $|-\rangle$.
  - If Alice gets $|-\rangle$, then the state of Bob is $|+\rangle$.
- If the result of Alice's measurement is unknown, the state of Bob can be described by the ensemble:

$$E_{\text{Bob}} = \left\{\left(\frac{1}{2}, |+\rangle\right), \left(\frac{1}{2}, |-\rangle\right)\right\}.$$

Entangled States and Ensembles (cont.)

- If Alice measures along an arbitrary direction $\mathbf{n}$:
  - Using rotational invariance, the singlet state can be rewritten as:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\big(|\mathbf{n};+\rangle_A|\mathbf{n};-\rangle_B - |\mathbf{n};-\rangle_A|\mathbf{n};+\rangle_B\big).$$

  - The ensemble for Bob's state becomes:

$$E_{\text{Bob}} = \left\{\left(\frac{1}{2}, |\mathbf{n};+\rangle\right), \left(\frac{1}{2}, |\mathbf{n};-\rangle\right)\right\}.$$

There is no pure state representing the quantum state of Alice's particle when entangled (example 22.2).

Density Matrix

Trace identity

- Consider two states $|u\rangle, |w\rangle \in V$. Define the operator $|u\rangle\langle w|$. The trace of this operator is given by:

$$\mathrm{tr}(|u\rangle\langle w|) = \langle w|u\rangle.$$

- Proof:
  - Assume $|i\rangle$ $(i = 1, \ldots, N)$ form an orthonormal basis.
  - Using $\mathrm{tr} M = \sum_i \langle i|M|i\rangle$, for any operator M:

$$\mathrm{tr}(|u\rangle\langle w|) = \sum_i \langle i|(|u\rangle\langle w|)|i\rangle = \sum_i \langle i|u\rangle\langle w|i\rangle.$$

  - Reordering the factors, we find:

$$\mathrm{tr}(|u\rangle\langle w|) = \sum_i \langle w|i\rangle\langle i|u\rangle = \langle w| \left(\sum_i |i\rangle\langle i| \right) |u\rangle.$$

  - Since $\sum_i |i\rangle\langle i| = \mathbb{I}$, this simplifies to:

$$\mathrm{tr}(|u\rangle\langle w|) = \langle w|u\rangle.$$

- Observation: The result follows as a corollary of the generalized cyclicity property of the trace, $\mathrm{tr}(AB) = \mathrm{tr}(BA)$, which holds even when A and B are not square matrices.

The Density Matrix

- The density matrix $\rho \in \mathcal{L}(V)$ is an operator on the Hilbert space V.
- Consider a general ensemble:

$$E = \{(p_1, |\psi_1\rangle), \ldots, (p_n, |\psi_n\rangle)\}, \quad \sum_{a=1}^{n} p_a = 1, \quad p_a > 0.$$

- Expectation value of observable $\hat{Q}$:

$$\langle \hat{Q} \rangle_E = \sum_{a=1}^{n} p_a \langle \psi_a | \hat{Q} | \psi_a \rangle.$$

- Using the trace identity $(\mathrm{tr}(|u\rangle\langle w|) = \langle w \mid u \rangle)$:

$$\langle \hat{Q} \rangle_E = \sum_{a=1}^{n} p_a \mathrm{tr}(\hat{Q} |\psi_a\rangle\langle\psi_a|).$$

The Density Matrix (cont.)

- For a linear operator A and constant p:

$$\mathrm{tr}(pA) = p\,\mathrm{tr}(A).$$

- Rewrite the expectation value:

$$\langle \hat{Q} \rangle_E = \mathrm{tr}\left(\hat{Q} \sum_{a=1}^{n} p_a |\psi_a\rangle\langle\psi_a| \right).$$

- Define the density matrix:

$$\rho_E \equiv \sum_{a=1}^{n} p_a |\psi_a\rangle\langle\psi_a|.$$

- The density matrix contains all relevant information about the ensemble:

$$\langle \hat{Q} \rangle_E = \mathrm{tr}\left(\hat{Q} \rho_E \right)$$

E.g.

$$\rho_{E_z} = \frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-| = \frac{1}{2}\mathbb{I}. \quad \rho_{E_X} = \frac{1}{2}|x;+\rangle\langle x;+| + \frac{1}{2}|x;-\rangle\langle x;-| = \frac{1}{2}\mathbb{I},$$

Remarks on Density Matrix

- The density matrix ρ is a Hermitian operator:

$$\rho^\dagger = \rho.$$

  Hermitian property ensures real eigenvalues and diagonalizability.

- ρ is positive semidefinite:

$$\langle v|\rho|v\rangle \geq 0 \quad \text{for all vectors } v.$$

  Nonnegative eigenvalues derived from:

$$\langle v|\rho|v\rangle = \sum_{a=1}^{n} p_a |\langle v|\psi_a\rangle|^2 \geq 0.$$

Remarks on Density Matrix (cont.)

- Trace of the density matrix is 1:

$$\mathrm{tr}(\rho) = \sum_{a=1}^{n} p_a \mathrm{tr}(|\psi_a\rangle\langle\psi_a|) = \sum_{a=1}^{n} p_a = 1.$$

- Removes redundancies:

$$\rho = \sum_{i,j=1}^{N} \rho_{ij} |i\rangle\langle j|,$$

where ρ_{ij} are elements of a Hermitian $N \times N$ matrix. ρ is specified by $N^2 - 1$ real numbers (trace $= 1$).

Remarks on Density Matrix (cont.)

- Phases of ensemble states $|\psi_a\rangle$ are irrelevant:

$$\rho_E = \rho_{E'} \quad \text{if } |\psi_a\rangle \to e^{i\alpha_a}|\psi_a\rangle.$$

- Physicists often refer to ρ as the "state" or "state operator" of the system.

Density Matrix for a Pure State

- For a pure state $|\psi\rangle$, the ensemble collapses to a single entry:

$$E = \{(1, |\psi\rangle)\},$$

  and the associated density matrix is:

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

- Properties of the density matrix ρ for a pure state:
  - It is a **rank-one orthogonal projector** onto the subspace generated by $|\psi\rangle$.
  - ρ is Hermitian and satisfies:

$$\rho^2 = |\psi\rangle\langle\psi||\psi\rangle\langle\psi| = \rho.$$

  - Trace property:

$$\operatorname{tr}\rho^2 = \operatorname{tr}\rho = 1.$$

- **Theorem:** For any state,

$$\operatorname{tr}\rho^2 \leq 1,$$

  with the inequality saturated only for pure states.

Purity of the Density Matrix

- Key relations for traces of the density matrix:

$$\operatorname{tr}\rho^2 \leq \operatorname{tr}\rho = 1.$$

- **Purity** $\zeta(\rho)$ of a density matrix:

$$\zeta(\rho) \equiv \operatorname{tr}\rho^2.$$

  - $\zeta = 1$: The state is pure.
  - $\zeta < 1$: The state is mixed.
- **Maximally mixed state:** The density matrix is proportional to the identity matrix $\mathbb{I}$:

$$\bar{\rho} = \frac{1}{N}\mathbb{I},$$

where N is the dimension of the state space.

Derivation of the Maximally Mixed State

- Assume $\rho = \mathrm{diag}(p_1, p_2, \ldots, p_N)$, where $p_i \geq 0$ and $\sum_{i=1}^{N} p_i = 1$.
- Minimize $\sum_{i=1}^{N} p_i^2$ under these constraints using the Lagrange multiplier λ:

$$L(p_1, \ldots, p_N; \lambda) = \sum_{i=1}^{N} p_i^2 - \lambda \left(-1 + \sum_{i=1}^{N} p_i \right).$$

- Stationary conditions:

$$\frac{\partial L}{\partial p_i} = 2p_i - \lambda = 0, \quad i = 1, \ldots, N; \quad \frac{\partial L}{\partial \lambda} = 1 - \sum_{i=1}^{N} p_i = 0.$$

- Solve for p_i:

$$p_i = \frac{\lambda}{2}, \quad N\frac{\lambda}{2} = 1 \implies p_i = \frac{1}{N}.$$

- Resulting density matrix:

$$\bar{\rho} = \frac{1}{N}\mathbb{I}.$$

Example: Density Matrix for Spin One-Half Pure States

- The density matrix for a pure spin state $|\mathbf{n}\rangle$, pointing along the unit vector $\mathbf{n}$, is expressed as:

$$|\mathbf{n}\rangle\langle\mathbf{n}| \equiv \frac{1}{2}a_0\mathbb{I} + \frac{1}{2}\sum_{i=1}^{3} a_i\sigma_i,$$

  where:
  - $\mathbb{I}$ is the identity matrix.
  - σ_i $(i = 1, 2, 3)$ are the Pauli matrices.
  - a_0 and a_i are real constants.
- Using the projector $P_n = |\mathbf{n}\rangle\langle\mathbf{n}|$, the expression simplifies to:

$$|\mathbf{n}\rangle\langle\mathbf{n}| \equiv \frac{1}{2}\big(\mathbb{I} + \mathbf{n}\cdot\boldsymbol{\sigma}\big).$$

Theorem: Density Matrix and Ensembles

Theorem: For any unit trace, positive semidefinite matrix $M \in \mathcal{L}(V)$, we can associate an ensemble for which M is the density matrix.

Proof:

- The matrix M, being Hermitian and positive semidefinite, can be diagonalized. It has nonnegative eigenvalues $\lambda_i \geq 0$ with $i = 1, \ldots, N$, where $N = \dim V$.
- Denote $|e_i\rangle$ as the eigenvectors associated with λ_i. The matrix M is expressed as:

$$M = \sum_{i=1}^{N} \lambda_i |e_i\rangle\langle e_i|, \quad \sum_{i=1}^{N} \lambda_i = 1.$$

- Consider the ensemble E_M defined by:

$$E_M \equiv \{(\lambda_1, |e_1\rangle), \ldots, (\lambda_N, |e_N\rangle)\}.$$

  This definition is consistent as the λ_i are nonnegative and sum to one.
- The density matrix ρ_{E_M} associated with E_M is constructed as:

$$\rho_{E_M} \equiv \sum_{i=1}^{N} \lambda_i |e_i\rangle\langle e_i| = M.$$

Thus, the claim of the theorem is confirmed.

Example: Density Matrix for General Spin One-Half States

- The density matrix ρ for a general 2×2 Hermitian matrix is written as:

$$\rho = \frac{1}{2}(a_0\, \mathbb{I} + \mathbf{a} \cdot \boldsymbol{\sigma}), \quad a_0, a_1, a_2, a_3 \in \mathbb{R}.$$

- The trace condition $\operatorname{tr} \rho = 1$ fixes $a_0 = 1$. The eigenvalues of $\mathbf{a} \cdot \boldsymbol{\sigma}$ are $\pm|\mathbf{a}|$. The positivity of ρ requires the eigenvalues of $\mathbf{a} \cdot \boldsymbol{\sigma}$ to satisfy:

$$\frac{1}{2}(1 \pm |\mathbf{a}|) \geq 0, \quad \text{or equivalently} \quad |\mathbf{a}| \leq 1.$$

- The general density matrix for mixed or pure states becomes:

$$\text{Spin one-half density matrix:} \;\; \rho = \frac{1}{2}(\mathbb{I} + \mathbf{a} \cdot \boldsymbol{\sigma}), \quad |\mathbf{a}| \leq 1.$$

The Bloch Ball:

- The set of allowed pure and mixed states forms the *Bloch ball*, a unit ball in the Euclidean three-dimensional space $\{a_1, a_2, a_3\}$.
- Boundary ($|\mathbf{a}| = 1$): Represents pure states.
- Interior ($|\mathbf{a}| < 1$): Represents mixed states.
- Center ($\mathbf{a} = 0$): Represents the unpolarized (maximally mixed) state.

Measurement Along an Orthonormal Basis

- Recall: Measuring a pure state $|\psi\rangle$ along an orthonormal basis $\{|i\rangle\}_{i=1}^{N}$ gives the probability of the system collapsing to state $|i\rangle$ as:

$$p(i) = |\langle i|\psi\rangle|^2.$$

- For a mixed state described by the density matrix ρ, this probability is generalized to:

$$p(i) = \sum_{a=1}^{n} p_a \left|\langle i \mid \psi_a\rangle\right|^2 = \sum_{a=1}^{n} p_a \langle i \mid \psi_a\rangle \langle \psi_a \mid i\rangle = \langle i| \sum_{a=1}^{n} p_a |\psi_a\rangle \langle \psi_a \mid i\rangle = \langle i|\rho|i\rangle.$$

  this probability depends only on ρ and not on the ensemble that defines ρ.
- After the measurement, the state will be in one of the basis states $|i\rangle$. The corresponding orthogonal projector for this state is:

$$M_i \equiv |i\rangle\langle i|, \quad \text{with} \quad M_i^\dagger = M_i, \quad M_i M_i = M_i, \quad \sum_i M_i = \mathbb{I}.$$

- If the measurement outcome is not available, the post-measurement state is a mixed state described by the ensemble:

$$\tilde{E} = \{(p(1), |1\rangle), \ldots, (p(N), |N\rangle)\}.$$

Measurement Along an Orthonormal Basis (cont.)

- The new density matrix $\tilde{\rho}$ after measurement is constructed as:

$$\tilde{\rho} = \sum_i p(i)|i\rangle\langle i| = \sum_i |i\rangle\langle i|\rho|i\rangle\langle i| = \sum_i M_i \rho M_i,$$

  This passage from ρ to $\tilde{\rho}$ gives us the effect of measurement along a basis on a quantum system when the result is not available.

- Properties:
  1. The trace of the new density matrix remains one:

$$\operatorname{tr}\tilde{\rho} = \sum_i \operatorname{tr}(M_i \rho M_i) = \sum_i \operatorname{tr}(\rho M_i M_i) = \sum_i \operatorname{tr}(\rho M_i) = \operatorname{tr}\left(\rho \sum_i M_i\right) = \operatorname{tr}\rho = 1.$$

- In summary, measurement modifies the density matrix as:

$$\tilde{\rho} = \sum_i M_i \rho M_i,$$

  capturing the effect of quantum measurements when the outcome is unavailable.

Dynamics of Density Matrices

Dynamics of Density Matrices

- The time evolution of a quantum state is governed by the Schrödinger equation:

$$\frac{\partial}{\partial t}|\psi\rangle = -\frac{i}{\hbar}\hat{H}|\psi\rangle, \quad \frac{\partial}{\partial t}\langle\psi| = \frac{i}{\hbar}\langle\psi|\hat{H}.$$

- Using these equations, the time derivative of the projector $|\psi\rangle\langle\psi|$ becomes:

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

- For a density matrix ρ associated with an ensemble:

$$\rho = \sum_{a=1}^{n} p_a|\psi_a\rangle\langle\psi_a|,$$

the time derivative generalizes to:

$$\frac{\partial\rho}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \rho].$$

Properties of Density Matrix Evolution

- The equation $\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \rho]$ preserves:
  - **Hermiticity**: Since $\frac{\partial \rho}{\partial t}$ is proportional to the commutator of ρ with $\hat{H}$, which is anti-Hermitian, ρ remains Hermitian.
  - **Trace Conservation**: The trace remains constant:

$$\frac{d}{dt}\operatorname{tr}\rho = \operatorname{tr}\left(\frac{\partial \rho}{\partial t}\right) = -\frac{i}{\hbar}\operatorname{tr}[\hat{H}, \rho] = 0.$$

- The density matrix evolves using the unitary operator $\hat{U}(t)$:

$$\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t}, \quad \rho(t) = \hat{U}(t)\rho(0)\hat{U}^\dagger(t).$$

Purity of the Density Matrix

- The purity of a density matrix is defined as:

$$\zeta(\rho) \equiv \mathrm{tr}(\rho^2).$$

- For a pure state, $\zeta = 1$. If $\zeta < 1$, the state is mixed.
- Under unitary evolution, the purity remains constant:

$$\frac{d\zeta}{dt} = \frac{d}{dt}\mathrm{tr}(\rho\rho) = \mathrm{tr}\left(\frac{d\rho}{dt}\rho + \rho\frac{d\rho}{dt}\right) = 2\,\mathrm{tr}\left(\rho\frac{d\rho}{dt}\right).$$

- Substituting $\frac{\partial\rho}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \rho]$, we find:

$$\frac{d}{dt}\zeta = \frac{2}{i\hbar}\mathrm{tr}(\rho[\hat{H}, \rho]) = \frac{2}{i\hbar}\mathrm{tr}(\rho\hat{H}\rho - \rho\rho\hat{H}) = 0.$$

- Conclusion: Pure states remain pure under unitary evolution.

Subsystems and Schmidt Decomposition

Subsystems

- In quantum mechanics, a composite system AB can be described as the tensor product of its subsystems:

  $$\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B,$$

  where $\mathcal{H}_A$ and $\mathcal{H}_B$ represent the state spaces of the subsystems A and B.

  $$\dim \mathcal{H}_A = d_A, \quad \left(e_1^A, \ldots, e_{d_A}^A\right) \text{ orthonormal basis,}$$
  $$\dim \mathcal{H}_B = d_B, \quad \left(e_1^B, \ldots, e_{d_B}^B\right) \text{ orthonormal basis.}$$

- For a density matrix ρ_{AB} representing the full composite system, the **reduced density matrix** of subsystem A is defined by tracing out the degrees of freedom of subsystem B:

  $$\rho_A = \mathrm{tr}_B\, \rho_{AB} = \sum_k \left\langle e_k^B \middle| \rho_{AB} \middle| e_k^B \right\rangle \in \mathcal{L}\left(\mathcal{H}_A\right),$$

Reduced Density Matrix Properties

- The reduced density matrix ρ_A satisfies the following key properties:
  1. **Trace:**
  $$\mathrm{tr}_A\, \rho_A = \mathrm{tr}_A\, \mathrm{tr}_B\, \rho_{AB} = \mathrm{tr}\, \rho_{AB} = 1,$$
  2. **Positive semidefinite:**
  $$\langle v_A | \rho_A | v_A \rangle = \langle v_A | \sum_k \left\langle e_k^B \right| \rho_{AB} \left| e_k^B \right\rangle | v_A \rangle = \sum_k \langle v_A | \left\langle e_k^B \right| \rho_{AB} | v_A \rangle \left| e_k^B \right\rangle \geq 0, \quad \forall\, | v_A \rangle \in \mathcal{H}_A,$$
- The reduced density matrix allows us to compute expectation values of observables acting only on subsystem A:
$$\mathrm{tr}_A(\rho_A\, \mathcal{O}_A) = \mathrm{tr}_{AB}(\rho_{AB}\, \mathcal{O}_A \otimes \mathbb{I}_B), \quad \text{with} \quad \mathcal{O}_A \in \mathcal{L}\left(\mathcal{H}_A\right) \tag{1}$$
- This property ensures that measurements on subsystem A can be accurately described without reference to the full system AB.

Proof

- The general density matrix ρ_{AB} for the composite system $\mathcal{H}_A \otimes \mathcal{H}_B$ is expressed as:

$$\rho_{AB} = \sum_{i,j,k,l} \rho_{ij,kl} |e_i^A\rangle\langle e_j^A| \otimes |e_k^B\rangle\langle e_l^B|,$$

  where $|e_i^A\rangle$ and $|e_k^B\rangle$ are orthonormal bases of $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively.
- Taking the partial trace over subsystem B yields the reduced density matrix for subsystem A:

$$\rho_A = \mathrm{tr}_B \rho_{AB} = \sum_{i,j,k} \rho_{ij,kk} |e_i^A\rangle\langle e_j^A|.$$

Proof (cont.)

- Computing the left-hand side of the identity in equation (1):

$$\mathrm{tr}_A(\rho_A \mathcal{O}_A) = \sum_{i,j,k} \rho_{ij,kk} \langle e_j^A | \mathcal{O}_A | e_i^A \rangle.$$

- Computing the right-hand side of the same identity:

$$\mathrm{tr}(\rho_{AB} \mathcal{O}_A \otimes \mathbb{I}_B) = \mathrm{tr}_B \mathrm{tr}_A \sum_{i,j,k,l} \rho_{ij,kl} |e_i^A\rangle\langle e_j^A| \mathcal{O}_A \otimes |e_k^B\rangle\langle e_l^B|.$$

- After simplifications:

$$\mathrm{tr}(\rho_{AB} \mathcal{O}_A \otimes \mathbb{I}_B) = \sum_{i,j,k} \rho_{ij,kk} \langle e_j^A | \mathcal{O}_A | e_i^A \rangle.$$

- This verifies that:

$$\mathrm{tr}_A(\rho_A \mathcal{O}_A) = \mathrm{tr}(\rho_{AB} \mathcal{O}_A \otimes \mathbb{I}_B).$$

Theorem: Subsystem Expectation Values

- **Theorem:** For any operator $S_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$, let $S_A = \mathrm{tr}_B(S_{AB})$. Then for any observable $\hat{O}_A \in \mathcal{L}(\mathcal{H}_A)$:

$$\mathrm{tr}_A(S_A \hat{O}_A) = \mathrm{tr}_{AB}(S_{AB}\, \hat{O}_A \otimes \mathbb{I}_B).$$

- **Implications:**
  1. The reduced density matrix ρ_A provides a consistent framework for computing observables localized on subsystem A.
  2. This consistency applies regardless of the entanglement or mixed-state nature of the full system ρ_{AB}.

Example: Two Entangled Spins

- Consider the pure state $|\psi_{AB}\rangle$ of two entangled spins:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\big(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\big).$$

- The density matrix for the composite system AB is $\rho_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}|$. Explicitly, this is written as:

$$\begin{aligned}\rho_{AB} =& \frac{1}{\sqrt{2}}\left(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\right)\frac{1}{\sqrt{2}}\Big(\langle+|_A\langle-|_B - \langle-|_A\langle+|_B\Big)\\ =& \frac{1}{2}(|+\rangle\langle+|)_A \otimes (|-\rangle\langle-|)_B - \frac{1}{2}(|+\rangle\langle-|)_A \otimes (|-\rangle\langle+|)_B\\ &- \frac{1}{2}(|-\rangle\langle+|)_A \otimes (|+\rangle\langle-|)_B + \frac{1}{2}(|-\rangle\langle-|)_A \otimes (|+\rangle\langle+|)_B.\end{aligned}$$

- **Reduced Density Matrix for Subsystem B:** By tracing out subsystem A, we obtain:

$$\rho_B = \operatorname{tr}_A \rho_{AB} = \frac{1}{2}|-\rangle\langle-| + \frac{1}{2}|+\rangle\langle+|$$

- This shows that subsystem B is in a maximally mixed state, irrespective of the entangled nature of the full state $|\psi_{AB}\rangle$.

Schmidt decomposition

The **pure** states $|\Psi_{AB}\rangle$ of a bipartite system AB can be expressed in an insightful and simplified manner, using the following guiding principles:

- The associated density matrices ρ_A and ρ_B of the subsystems A and B are utilized to guide the decomposition.
- The decomposition is referred to as the **Schmidt decomposition** of the pure state $|\Psi_{AB}\rangle$, named after Erhard Schmidt (1876–1959), who is also credited with the Gram-Schmidt procedure for constructing orthonormal basis vectors.
- The Schmidt decomposition provides a structure that is simpler than the general tensor product of the two subsystems.
  1. The state $|\Psi_{AB}\rangle$ is written in terms of an orthonormal basis $\{|k_A\rangle\}$ of $\mathcal{H}_A$ and an orthonormal basis $\{|k_B\rangle\}$ of $\mathcal{H}_B$ that, respectively, make the reduced density matrices ρ_A and ρ_B diagonal.
  2. The decomposition defines an integer r, called the Schmidt index, that characterizes the degree of entanglement of the subsystems A and B.

Expansion of Bipartite Pure States

- Consider a bipartite system AB with a pure state $|\Psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, where $\mathcal{H}_A$ and $\mathcal{H}_B$ are the Hilbert spaces of subsystems A and B, respectively.
- Assume $d_A \leq d_B$, where $d_A = \dim(\mathcal{H}_A)$ and $d_B = \dim(\mathcal{H}_B)$.
- The state $|\Psi_{AB}\rangle$ can be expressed in terms of the basis states of $\mathcal{H}_A \otimes \mathcal{H}_B$:

$$|\Psi_{AB}\rangle = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} \psi_{ij} |e_i^A\rangle \otimes |e_j^B\rangle,$$

  where ψ_{ij} are the expansion coefficients.
- In the Schmidt decomposition, the state can be rewritten as:

$$|\Psi_{AB}\rangle = \sum_{i=1}^{d_A} |\psi_i^B\rangle \otimes |e_i^A\rangle, \quad \text{with} \quad |\psi_i^B\rangle = \sum_{j=1}^{d_B} \psi_{ij} |e_j^B\rangle.$$

- Observations:
  - The vectors $|\psi_i^B\rangle \in \mathcal{H}_B$ are not necessarily orthonormal.
  - The Schmidt decomposition provides a more structured representation, reducing the sum to an integer $r \leq d_A$, the **Schmidt rank**.

Schmidt Decomposition Derivation

To derive the Schmidt decomposition, we consider the pure state $|\Psi_{AB}\rangle$ and its associated density matrices:

$$\rho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}|, \quad \rho_A = \mathrm{tr}_B \rho_{AB}, \quad \rho_A = \mathrm{tr}_B(|\Psi_{AB}\rangle\langle\Psi_{AB}|).$$

- By construction, ρ_A is a Hermitian positive semidefinite $d_A \times d_A$ matrix and can therefore be diagonalized.
- Let $(p_k, |k_A\rangle)$, with $k = 1, \ldots, d_A$, be the eigenvalues and eigenvectors of ρ_A, where $|k_A\rangle$ forms an orthonormal basis for $\mathcal{H}_A$, and $p_k \geq 0$.
- The density matrix ρ_A is expressed as:

$$\rho_A = \sum_{k=1}^{d_A} p_k |k_A\rangle\langle k_A|, \quad \sum_{k=1}^{d_A} p_k = 1.$$

- If ρ_A is a pure state, only one eigenvalue p_k is nonzero. In general, we assume $r \leq d_A$ eigenvalues are nonzero:

$$\rho_A = \sum_{k=1}^{r} p_k |k_A\rangle\langle k_A|, \quad r \leq d_A, \quad p_{k>r} = 0. \tag{2}$$

Schmidt Decomposition Derivation (cont.)

- Since $|k_A\rangle$ span $\mathcal{H}_A$, we can express the pure state $|\Psi_{AB}\rangle$ as:

$$|\Psi_{AB}\rangle = \sum_{k=1}^{d_A} |k_A\rangle \otimes |\psi_k^B\rangle,$$

  where $|\psi_k^B\rangle$ are states in $\mathcal{H}_B$.
- Note: The number of terms is at most d_A, not $d_A \cdot d_B$, as $|\psi_k^B\rangle$ does not necessarily span $\mathcal{H}_B$.
- The density matrix for $|\Psi_{AB}\rangle$ can then be written as:

$$\rho_{AB} = \sum_{k,\tilde{k}=1}^{d_A} |k_A\rangle \otimes |\psi_k^B\rangle\langle \tilde{k}_A| \otimes \langle \psi_{\tilde{k}}^B|.$$

  Taking the trace over B, we now get

$$\rho_A = \mathrm{tr}_B\, \rho_{AB} = \sum_{k,\tilde{k}=1}^{d_A} |k_A\rangle\langle \tilde{k}_A|\langle \psi_{\tilde{k}}^B \mid \psi_k^B\rangle$$

Schmidt Decomposition Derivation (cont.)

- Compare the previous expression for ρ_A in equation (2), where no state $|k_A\rangle$ with $k > r$ appears.
- This implies that the ansatz for $|\Psi_{AB}\rangle$ must exclude such states; otherwise, nonvanishing terms in ρ_A not included in equation (2) would appear.
- Therefore, $|\Psi_{AB}\rangle$ is rewritten as:

$$|\Psi_{AB}\rangle = \sum_{k=1}^{r} |k_A\rangle \otimes |\psi_k^B\rangle.$$

Schmidt Decomposition Derivation (cont.)

- Substituting the new form of $|\Psi_{AB}\rangle$ into ρ_{AB}, we obtain:

$$\rho_{AB} = \sum_{k,\tilde{k}=1}^{r} |k_A\rangle \otimes |\psi_k^B\rangle\langle\tilde{k}_A| \otimes \langle\psi_{\tilde{k}}^B| \Rightarrow \rho_A = \sum_{k,\tilde{k}=1}^{r} |k_A\rangle \langle\tilde{k}_A|\langle\psi_{\tilde{k}}^B \mid \psi_k^B\rangle$$

- To ensure consistency with ρ_A, states $|\psi_k^B\rangle$ must satisfy:

$$\langle\psi_{\tilde{k}}^B \mid \psi_k^B\rangle = p_k\delta_{k\tilde{k}}, \quad k, \tilde{k} = 1, \ldots, r.$$

- Define normalized versions of $|\psi_k^B\rangle$ as:

$$|k_B\rangle \equiv \frac{|\psi_k^B\rangle}{\sqrt{p_k}}, \quad k = 1, \ldots, r.$$

- These states satisfy:

$$\langle k_B|k'_B\rangle = \delta_{kk'}, \quad k, k' = 1, \ldots, r.$$

- If $r < d_B$, additional orthonormal vectors can complete the basis for $\mathcal{H}_B$, but these extra vectors are not involved here.

Schmidt Decomposition Derivation (cont.)

- The pure state $|\Psi_{AB}\rangle$ of the bipartite system AB can always be written as:

$$|\Psi_{AB}\rangle = \sum_{k=1}^{r} \sqrt{p_k}|k_A\rangle \otimes |k_B\rangle, \quad r \le d_A \le d_B.$$

- Here:

$$\sum_{k=1}^{r} p_k = 1, \quad p_k > 0, \quad k = 1, \dots, r,$$

and the states $|k_A\rangle \in \mathcal{H}_A$ and $|k_B\rangle \in \mathcal{H}_B$ form orthonormal sets:

$$\langle k_A|k'_A\rangle = \delta_{kk'}, \quad \langle k_B|k'_B\rangle = \delta_{kk'}.$$

Properties of the Schmidt Decomposition

- The Schmidt decomposition:
  - Involves $r \leq d_A$ terms, each a basis state of $\mathcal{H}_A$ multiplied by some state in $\mathcal{H}_B$.
  - Ensures $|k_B\rangle$ states form an orthonormal set, like $|k_A\rangle$.
- The density matrices ρ_A and ρ_B are given by:

$$\rho_A = \sum_{k=1}^{r} p_k |k_A\rangle\langle k_A|, \quad \rho_B = \sum_{k=1}^{r} p_k |k_B\rangle\langle k_B|.$$

- Both ρ_A and ρ_B have the same nonzero eigenvalues $\{p_k\}$, determined by the Schmidt number r.
- Interpretation:
  - $r = 1$: A and B subsystems are not entangled, and the state is a tensor product.
  - $r > 1$: A and B are entangled; ρ_A and ρ_B are mixed.

Example: Schmidt Decomposition

We revisit the pure state $|\Psi_{AB}\rangle$ of a bipartite system AB:

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}|+\rangle_A|+\rangle_B + \frac{1}{2}|-\rangle_A|+\rangle_B - \frac{1}{2}|-\rangle_A|-\rangle_B. \tag{3}$$

- The diagonalized reduced density matrix ρ_A is found to be (Exercise 22.5, 22.6):

$$\rho_A = \frac{1}{2}\left(1 + \frac{1}{\sqrt{2}}\right)|x;+\rangle\langle x;+| + \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)|x;-\rangle\langle x;-|.$$

- Using this, we construct an ansatz for $|\Psi_{AB}\rangle$:

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}}\sqrt{1 + \frac{1}{\sqrt{2}}}|x;+\rangle_A|1_B\rangle + \frac{1}{\sqrt{2}}\sqrt{1 - \frac{1}{\sqrt{2}}}|x;-\rangle_A|2_B\rangle,$$

where $|1_B\rangle$ and $|2_B\rangle$ are orthonormal states to be determined.

Example: Schmidt Decomposition

- Writing the $|\pm\rangle_A$ states in (3) in terms of $|x;\pm\rangle_A$

$$
\begin{aligned}
|\Psi_{AB}\rangle = &\frac{1}{2}|x;+\rangle_A \otimes \left(\left(1+\frac{1}{\sqrt{2}}\right)|+\rangle_B - \frac{1}{\sqrt{2}}|-\rangle_B\right) \\
&+ \frac{1}{2}|x;-\rangle_A \otimes \left(\left(1-\frac{1}{\sqrt{2}}\right)|+\rangle_B + \frac{1}{\sqrt{2}}|-\rangle_B\right).
\end{aligned}
$$

- After rewriting to make orthonormality manifest:

$$
\begin{aligned}
|\Psi_{AB}\rangle = &\frac{1}{\sqrt{2}}\sqrt{1+\frac{1}{\sqrt{2}}}|x;+\rangle_A \otimes \sqrt{1-\frac{1}{\sqrt{2}}}\left(\left(1+\frac{1}{\sqrt{2}}\right)|+\rangle_B - \frac{1}{\sqrt{2}}|-\rangle_B\right) \\
&+ \frac{1}{\sqrt{2}}\sqrt{1-\frac{1}{\sqrt{2}}}|x;-\rangle_A \otimes \sqrt{1+\frac{1}{\sqrt{2}}}\left(\left(1-\frac{1}{\sqrt{2}}\right)|+\rangle_B + \frac{1}{\sqrt{2}}|-\rangle_B\right).
\end{aligned}
$$

Conclusion: The Schmidt number is 2, and subsystems A and B are entangled.

Open Systems and Decoherence

Open Systems and Decoherence

- Open systems interact with an **environment** E. The total system AE consists of:
  - Subsystem A: The focus of interest.
  - Subsystem E: The environment interacting with A.
- Reduced density matrix of subsystem A is obtained by tracing over E:

$$\rho_A = \mathrm{tr}_E(\rho_{AE}),$$

where ρ_{AE} is the density matrix of the full system AE.

Time Evolution of the Reduced Density Matrix

The time evolution of the reduced density matrix $\rho_A(t)$ is governed by:

$$\rho_A(t) = \mathrm{tr}_E\big(U\rho_{AE}(0)U^\dagger\big),$$

where:

- $U = \mathcal{U}(t)$ is the unitary operator describing the evolution of the full system.
- $\rho_{AE}(0)$ is the initial density matrix of the system AE.

Consistency Checks:

- **Trace Preservation:** $\mathrm{tr}\,\rho_A(t) = 1$.
- **Positivity:** $\rho_A(t)$ remains a positive semidefinite operator.

Example: Decoherence of a Qubit

Consider a spin-$\frac{1}{2}$ particle (qubit) in the state:

$$|\psi_A\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle, \quad |\alpha|^2 + |\beta|^2 = 1.$$

The qubit interacts with an environment initially in the pure state $|0_E\rangle$. The total initial state of the system is:

$$|\psi_{AE}\rangle = |\psi_A\rangle \otimes |0_E\rangle = \alpha|\uparrow\rangle \otimes |0_E\rangle + \beta|\downarrow\rangle \otimes |0_E\rangle.$$

The density matrix is:

$$\begin{aligned} \rho_A &= \mathrm{tr}_E\, \rho_{AE} = \mathrm{tr}_E\, |\psi_{AE}\rangle\langle\psi_{AE}| = \mathrm{tr}_E\, |\psi_A\rangle \otimes |0_E\rangle\langle\psi_A| \otimes \langle 0_E| \\ &= |\psi_A\rangle\langle\psi_A| = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \beta\alpha^* & |\beta|^2 \end{pmatrix}, \end{aligned}$$

Example: Decoherence of a Qubit (cont.)

Assume the interaction changes the environment state for $|\downarrow\rangle$. The total state becomes:

$$|\psi'_{AE}\rangle = \alpha|\uparrow\rangle \otimes |0_E\rangle + \beta|\downarrow\rangle \otimes |1_E\rangle.$$

The reduced density matrix of the qubit is obtained by tracing out the environment:

$$\rho'_A = \mathrm{tr}_E\left(|\psi'_{AE}\rangle\langle\psi'_{AE}|\right).$$

Expanding $|\psi'_{AE}\rangle\langle\psi'_{AE}|$, we have:

$$|\psi'_{AE}\rangle\langle\psi'_{AE}| = |\alpha|^2|\uparrow\rangle\langle\uparrow| \otimes |0_E\rangle\langle 0_E| + |\beta|^2|\downarrow\rangle\langle\downarrow| \otimes |1_E\rangle\langle 1_E|$$

$$+\alpha\beta^*|\uparrow\rangle\langle\downarrow| \otimes |0_E\rangle\langle 1_E| + \alpha^*\beta|\downarrow\rangle\langle\uparrow| \otimes |1_E\rangle\langle 0_E|.$$

Example: Decoherence of a Qubit (cont.)

Taking the partial trace over the environment, we obtain:

$$\rho'_A = |\alpha|^2 |\uparrow\rangle\langle\uparrow| + |\beta|^2 |\downarrow\rangle\langle\downarrow|.$$

As a matrix, ρ'_A takes the form:

$$\rho'_A = \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}.$$

This is a **mixed state** if $\alpha \neq 0$ and $\beta \neq 0$.

$$\mathrm{tr}\,(\rho'_A)^2 = |\alpha|^4 + |\beta|^4 = \left(|\alpha|^2 + |\beta|^2\right)^2 - 2|\alpha|^2|\beta|^2 = 1 - 2|\alpha|^2|\beta|^2 < 1.$$

The qubit experienced decoherence. It is worth comparing the density matrices ρ_A and ρ'_A. The former has off-diagonal matrix elements, storing the information about the relative phases of the different components of the wave function. The latter does not.

Example: Two Coupled Spin-One-Half Particles

Consider two spin-$\frac{1}{2}$ particles interacting through an Ising Hamiltonian:

$$\hat{H} = -\hbar\omega\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}, \quad \omega > 0.$$

At $t = 0$, the state of the two particles is a pure state:

$$|\psi_{12}(0)\rangle = \frac{1}{2}\Big(a_+|\uparrow\uparrow\rangle + a_-|\uparrow\downarrow\rangle + b_+|\downarrow\uparrow\rangle + b_-|\downarrow\downarrow\rangle\Big),$$

where the first arrow represents particle one, and the second represents particle two. The coefficients a_+, a_-, b_+, b_- are complex numbers satisfying the normalization condition:

$$|a_+|^2 + |a_-|^2 + |b_+|^2 + |b_-|^2 = 4.$$

At $t = 0$, the density matrix ρ_{12} of the system is:

$$\rho_{12}(0) = \frac{1}{4}\Big(a_+|\uparrow\uparrow\rangle + a_-|\uparrow\downarrow\rangle + b_+|\downarrow\uparrow\rangle + b_-|\downarrow\downarrow\rangle\Big)\Big(a_+^*\langle\uparrow\uparrow| + a_-^*\langle\uparrow\downarrow| + b_+^*\langle\downarrow\uparrow| + b_-^*\langle\downarrow\downarrow|\Big).$$

Example: Two Coupled Spin-One-Half Particles (cont.)

The evolution operator $\mathcal{U}(t)$ is given by:

$$\mathcal{U}(t) = \exp(-i\hat{H}t/\hbar) = e^{i\omega t\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}}, \quad \mathcal{U}^\dagger = e^{-i\omega t\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}}.$$

The density matrix $\rho_{12}(t)$ evolves as:

$$\rho_{12}(t) = \mathcal{U}\rho_{12}(0)\mathcal{U}^\dagger,$$

resulting in:

$$\begin{aligned}\rho_{12}(t) =& \frac{1}{4}\Big(a_+e^{i\omega t}|\uparrow\uparrow\rangle + a_-e^{-i\omega t}|\uparrow\downarrow\rangle + b_+e^{-i\omega t}|\downarrow\uparrow\rangle + b_-e^{i\omega t}|\downarrow\downarrow\rangle\Big)\\ &\times\Big(a_+^*e^{-i\omega t}\langle\uparrow\uparrow| + a_-^*e^{i\omega t}\langle\uparrow\downarrow| + b_+^*e^{i\omega t}\langle\downarrow\uparrow| + b_-^*e^{-i\omega t}\langle\downarrow\downarrow|\Big).\end{aligned}$$

Taking the trace over the second state space, the time-dependent density matrix $\rho_1(t)$ for the first particle is:

$$\begin{aligned}\rho_1(t) =& \mathrm{Tr}_2\rho_{12}(t) = \frac{1}{4}\Big((|a_+|^2 + |a_-|^2)|\uparrow\rangle\langle\uparrow| + (a_+b_+^*e^{2i\omega t} + a_-b_-^*e^{-2i\omega t})|\uparrow\rangle\langle\downarrow|\\ &+ (a_+^*b_+e^{-2i\omega t} + a_-^*b_-e^{2i\omega t})|\downarrow\rangle\langle\uparrow| + (|b_+|^2 + |b_-|^2)|\downarrow\rangle\langle\downarrow|\Big).\end{aligned}$$

Example: Two Coupled Spin-One-Half Particles (cont.)

Let us consider the case when $a_+ = a_- = b_+ = b_- = 1$, consistent with normalization. Then the initial state is:

$$|\psi_{12}(0)\rangle = \frac{1}{2}\Big(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle\Big) = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle + |\downarrow\rangle\Big) \otimes \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle + |\downarrow\rangle\Big) = |x;+\rangle \otimes |x;+\rangle.$$

The two particles are not entangled at $t = 0$. The density matrix for the first particle can be obtained

$$\rho_1(t) = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}\cos 2\omega t\Big(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\Big) + \frac{1}{2}|\downarrow\rangle\langle\downarrow|.$$

The diagonal terms lead to the required trace, and the off-diagonal terms oscillate. At $t = 0$, the density matrix is $\rho_1(0) = |x;+\rangle\langle x;+|$, as expected, since the two particles are not entangled, and this is the density matrix for the pure state $|x;+\rangle$ of the first particle.

For arbitrary times it is useful to compute $\mathrm{tr}\rho_1^2$

$$\mathrm{tr}\rho_1^2 = 1 - \frac{1}{2}\sin^2 2\omega t \leq 1.$$

Since the density matrix represents a pure state if and only if the above inequality is saturated, we see that the state is pure when $\sin 2\omega t = 0$.

The Lindblad Equation

The Lindblad equation describes the dynamics of the density matrix $\rho(t)$ for an open quantum system, generalizing unitary evolution:

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar}[H, \rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\} \right).$$

- L_k: Lindblad operators describing interaction with the environment (not necessarily Hermitian).
- The anticommutator is defined as $\{A, B\} = AB + BA$.
- If $L_k = 0$, the evolution is purely unitary.

Properties:

- **Hermiticity:** $\rho(t)$ remains Hermitian since the right-hand side of the equation is Hermitian.
- **Trace Preservation:** The trace of $\rho(t)$ is conserved