This addition section covers

all the mathematical details concerning

the Density Matrix and Decoherence

Density Matrix and Decoherence

Incomplete knowledge about a quantum system adds a new layer of randomness to the state of the system, which can no longer be described by a vector in the state space, a pure state.

The description requires ensembles that represent mixed states.

The essence of ensembles is encoded in the density matrix, a Hermitian, positive semidefinite operator of unit trace.

For quantum systems with two interacting subsystems, also called bipartite systems, the state of any subsystem is generally a mixed state which requires a density matrix for its description, even when the total system is in a pure state.

The structure of pure, entangled states of a bipartite system is captured by the Schmidt decomposition, which relates it to the density matrices of the subsystems.

We look at decoherence, the process in which the pure state of a subsystem becomes mixed, and consider a phenomenological description of the process via the Lindblad equation.

We conclude with a look at measurements in quantum mechanics, contrasting the postulates of the Copenhagen interpretation with insights from decoherence and other interpretations.

Ensembles and Mixed States

We have seen that probabilities play a central and inescapable role in quantum mechanics.

This is quite striking, given that in classical physics probabilities arise *only* due to lack of knowledge about the system.

If we toss dice and are unable or unwilling to investigate the myriad factors that in principle determine the outcome, we have to consider probabilities for the possible results.

In quantum mechanics, however, perfect knowledge still does not do away with probabilities.

Consider a state $|\psi\rangle \in V$, with V an N-dimensional complex vector space.

Even if the state is known exactly, its properties, as defined by the observables in the theory, are only determined probabilistically.

This is not for lack of information, we believe.

Given the probabilistic interpretation of quantum mechanics, experiments are understood in the framework provided by an *ensemble*: multiple copies of the quantum system, all in the same state $|\psi\rangle$.

Measurements performed on each of the elements of the ensemble can be used to confirm the expected probabilities.

This is the *intrinsic* randomness of quantum mechanics.

Interestingly, the randomness that arises in classical mechanics due to lack of knowledge, which requires probabilities, has a counterpart in quantum mechanics and adds a *new layer of randomness* to the theory.

We will first consider how this new layer also arises in quantum mechanics due to incomplete knowledge.

As we will see, in this situation it is useful to consider more general kinds of ensembles.

At a more fundamental level, however, we will note that this new randomness arises naturally in quantum mechanics *even* with complete knowledge.

This happens in the description of a *subsystem* that happens to be entangled with the rest of the system.

This is a good reason to view this new layer of randomness as a general feature of quantum mechanics.

As we discuss the issues and complications associated with general ensembles, we will be led to the concept of a density matrix, an *operator* on the state space of the theory that encodes the quantum state of the system and includes this added layer of randomness.

A **pure state** is a familiar state $|\psi\rangle \in V$, a vector in the Hilbert space of the theory, a wave function.

On the other hand, if we have extra randomness and the state of the quantum system cannot be described by a vector in V, we have a **mixed state**.

To show how lack of knowledge introduces randomness in quantum mechanics, let us reconsider the Stern-Gerlach experiment.

In this experiment the beam of silver atoms that emerges from the hot oven is unpolarized: the spin one-half state of the atoms is random.

If we denote the spin state of an atom as $|\mathbf{n}\rangle$ with $\mathbf{n}$ a unit vector, the different atoms have vectors $\mathbf{n}$ pointing in random directions.

Can we find a quantum state $|\psi\rangle$ whose intrinsic randomness affords a description of the atoms in the beam as an ensemble of $|\psi\rangle$?

The answer is clearly no.

The general state is

$$|\psi\rangle = a_+|+\rangle + a_-|-\rangle, \quad a_+, a_- \in \mathbb{C}, \tag{1}$$

with $|\pm\rangle$ the familiar $\hat{S}_z$ eigenstates.

The state $|\psi\rangle$, a pure state, is fixed when the coefficients a_+ and a_- are fixed, but this also fixes the direction $\mathbf{n}$ of the spin state.

Thus, a state $|\psi\rangle$ as above does not describe states $|\mathbf{n}\rangle$ with random $\mathbf{n}$.

While we will deal with the case of random $\mathbf{n}$ later, let us consider a simpler situation.

Assume you have an oven in which 50% of the atoms come out polarized as $|+\rangle$ and the other 50% come out polarized as $|-\rangle$.

We can describe the beam by writing the pairs $(p_i, |\psi_i\rangle)$ in which we give the probability p_i of a given atom to be in the quantum state $|\psi_i\rangle$.

For the situation we just described, we would write

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

We used the label E_z for the *ensemble* of z-polarized states.

We say that this ensemble has two *entries*, each entry consisting of a state and its probability.

The ensemble here is providing a representation of the mixed state of our system.

We can visualize the collection of atoms as a very large ensemble built by joining two equal-size ensembles, one built solely from states that are all $|+\rangle$, and the other built solely from states that are all $|-\rangle$.

This is a more general ensemble than one in which all copies of the system are in the same quantum state.

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

$$E = \left\{ (p_1, |\psi_1\rangle), \ \ldots, (p_n, |\psi_n\rangle) \right\}, \quad p_1, \ldots, p_n > 0, \quad p_1 + \cdots + p_n = 1. \tag{3}$$

Here $n \geq 1$ is an integer denoting the number of entries in the ensemble.

The ensemble provides a description of a general mixed state.

The states $|\psi_a\rangle \in V$ above are all normalized:

$$\langle \psi_a | \psi_a \rangle = 1 \quad \text{for all} \quad a = 1, \ldots, n. \tag{4}$$

However, they are *not* required to be orthogonal to each other.

We can imagine the ensemble E containing a large number M of copies of the system, with $p_a \cdot M$ copies in the state $|\psi_a\rangle$, for each $a = 1, ..., n$.

The number n need not be related to the dimensionality dim V of the state space.

We can have $n = 1$, in which case $p_1 = 1$, and the ensemble represents a pure state $|\psi_1\rangle$; all elements of the ensemble are in this state.

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.

In fact, nothing goes wrong if $n = \infty$, and the ensemble contains an infinite set of entries.

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

$$\langle \hat{Q} \rangle_E = \sum_{a=1}^{n} p_a \langle \psi_a | \hat{Q} | \psi_a \rangle = p_1 \langle \psi_1 | \hat{Q} | \psi_1 \rangle + \cdots + p_n \langle \psi_n | \hat{Q} | \psi_n \rangle. \tag{5}$$

This is 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 that gives the fraction of all states in E that are in the subensemble.

Then we must add the contributions from all values of a.

In our example above, where silver atoms emerge as described by the ensemble E_z in Eq. (2), we would see that

$$\langle \hat{Q} \rangle_{E_Z} = \tfrac{1}{2}\langle +|\hat{Q}|+\rangle + \tfrac{1}{2}\langle -|\hat{Q}|-\rangle. \tag{6}$$

Suppose, however, that you are now in possession of an oven that produces 50% of atoms in the state $|x; +\rangle$ and the other 50% in the state $|x; -\rangle$.

The ensemble E_x here would be

$$E_x = \left\{ \left(\tfrac{1}{2}, |x; +\rangle \right), \quad \left(\tfrac{1}{2}, |x; -\rangle \right) \right\}. \tag{7}$$

The expectation value of $\hat{Q}$ in this ensemble is

$$\langle \hat{Q} \rangle_{E_x} = \tfrac{1}{2}\langle x; +|\hat{Q}|x; +\rangle + \tfrac{1}{2}\langle x; -|\hat{Q}|x; -\rangle. \tag{8}$$

A curious result emerges if we use $|x; \pm\rangle = \tfrac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle)$ to rewrite $\langle \hat{Q} \rangle_{E_x}$:

$$\langle \hat{Q} \rangle_{E_x} = \tfrac{1}{4}((\langle +| + \langle -|)\hat{Q}(|+\rangle + |-\rangle)) + \tfrac{1}{4}((\langle +| - \langle -|)\hat{Q}(|+\rangle - |-\rangle)). \tag{9}$$

The off-diagonal matrix elements of $\hat{Q}$ cancel out, and we are left with

$$\langle \hat{Q} \rangle_{E_x} = \tfrac{1}{2}\langle +|\hat{Q}|+\rangle + \tfrac{1}{2}\langle -|\hat{Q}|-\rangle = \langle \hat{Q} \rangle_{E_Z}. \tag{10}$$

The expectation values are identical in the two ensembles E_z and E_x.

Since this is true for arbitrary observables, we must conclude that no matter how different the ensembles are they are indistinguishable and thus physically equivalent.

Both ensembles in fact represent the same beam coming out of the oven; they represent the same mixed state.

With rather different ensembles turning out to be equivalent, we are led to find a better way to represent the mixed quantum state of a particle in the beam.

This will be done with density matrices.

Example 1. *Unpolarized ensemble*.

The oven in the Stern-Gerlach experiment produces unpolarized silver atoms.

We wish to write the expectation value of $\hat{Q}$ in this ensemble and compare it with the result for the E_z ensemble.

In an unpolarized state, the values of **n** are uniformly distributed over solid angle.

Since the total solid angle is 4π, the probability that the vector **n** is within a solid angle $d\Omega$ is $d\Omega/(4\pi)$.

The unpolarized ensemble E_{unp} is defined with an infinite number of entries composed by probabilities and states for all possible $d\Omega$:

$$E_{\text{unp}} = \bigcup_{d\Omega} \left(\tfrac{d\Omega}{4\pi},\ |\mathbf{n}(\theta,\phi)\rangle \right), \quad |\mathbf{n}(\theta,\phi)\rangle = \cos\tfrac{\theta}{2}|+\rangle + \sin\tfrac{\theta}{2}e^{i\phi}|-\rangle. \tag{11}$$

The expectation value of any observable $\hat{Q}$ in this ensemble is obtained by integration:

$$\begin{aligned}
\langle\hat{Q}\rangle_{E_{\text{unp}}} &= \int \frac{d\Omega}{4\pi}\, \langle\mathbf{n}(\theta,\phi)|\,\hat{Q}\,|\mathbf{n}(\theta,\phi)\rangle \\
&= \frac{1}{4\pi} \int \sin\theta\, d\theta\, d\phi \left(\cos\tfrac{\theta}{2}\langle+| + \sin\tfrac{\theta}{2}e^{-i\phi}\langle-|\right)\hat{Q}\left(\cos\tfrac{\theta}{2}|+\rangle + \sin\tfrac{\theta}{2}e^{i\phi}|-\rangle\right).
\end{aligned} \tag{12}$$

The integral over ϕ kills the off-diagonal matrix elements of $\hat{Q}$, and we find that

$$\langle\hat{Q}\rangle_{E_{\text{unp}}} = \tfrac{1}{2}\int_0^\pi \sin\theta\, d\theta \left(\cos^2\tfrac{\theta}{2}\langle+|\hat{Q}|+\rangle + \sin^2\tfrac{\theta}{2}\langle-|\hat{Q}|-\rangle\right). \tag{13}$$

Both integrals evaluate to one, and the result is

$$\langle \hat{Q} \rangle_{E_{\text{unp}}} = \tfrac{1}{2}\langle +|\hat{Q}|+\rangle + \tfrac{1}{2}\langle -|\hat{Q}|-\rangle. \tag{14}$$

This is once more the same expectation value we found in the ensembles E_z and E_x.

This shows that the unpolarized ensemble E_{unp} is in fact physically equivalent to the ensembles where half the states are polarized in one direction and the other half in the opposite direction.

We checked this for states along z and along x.

If one now checks it for arbitrary direction, i.e., the ensemble where 50% of the states are $|\mathbf{n}; +\rangle$ and the other 50% are $|\mathbf{n}; -\rangle$, for arbitrary but fixed unit vector $\mathbf{n}$, it is physically equivalent to the unpolarized ensemble.

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:

$$|\psi_{AB}\rangle = \tfrac{1}{\sqrt{2}}\left(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\right). \tag{15}$$

Assume 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 $|-\rangle$, the state of Bob is $|+\rangle$.

The state of Bob is known if we know the measurement Alice did *and* the result she found.

If we do not know the result of her measurement, the situation for Bob is less clear.

Suppose all we know is that Alice measured along the z-direction.

What then is the state of Bob's particle?

To answer this we can again think in terms of an ensemble in which each element contains the entangled pair $|\psi_{AB}\rangle$.

If Alice measures along z, about half of the time she will get $|+\rangle$, and the other half of the time she will get $|-\rangle$.

As a consequence, in half of the elements of the ensemble the state of Bob will be $|-\rangle$, and in the other half, the state of Bob will be $|+\rangle$.

The state of Bob can be described by the ensemble E_{Bob} that reads

$$E_{\text{Bob}} = \left\{ \left(\tfrac{1}{2}, |+\rangle\right), \left(\tfrac{1}{2}, |-\rangle\right) \right\}. \tag{16}$$

Suppose, instead, that Alice decides to measure in an arbitrary direction $\mathbf{n}$.

To analyze this, it is convenient to use the rotational invariance of the singlet state to rewrite it as follows:

$$|\psi_{AB}\rangle = \tfrac{1}{\sqrt{2}} \left(|\mathbf{n}; +\rangle_A |\mathbf{n}; -\rangle_B - |\mathbf{n}; -\rangle_A |\mathbf{n}; +\rangle_B \right). \tag{17}$$

If Alice measures and the result is not known, the state of Bob is again an ensemble.

Since the probabilities that she finds $|\mathbf{n}; -\rangle$ and $|\mathbf{n}; +\rangle$ are the same, the correlations in the entangled state imply that this time the ensemble for Bob's state is

$$E_{\text{Bob}} = \left\{ \left(\tfrac{1}{2}, |\mathbf{n}; +\rangle\right), \left(\tfrac{1}{2}, |\mathbf{n}; -\rangle\right) \right\}. \tag{18}$$

The two ensembles that we get, from Alice measuring along z and along $\mathbf{n}$, are equivalent, as we demonstrated before by considering expectation values.

Again, we wish to have a better understanding of why the state of Bob's particle did not depend on the direction Alice used to make her measurement.

Example 2. *Absence of a pure-state description of an entangled particle.*

Let us now consider again the same entangled state of two particles, one held by Alice and the other by Bob:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\right). \tag{19}$$

Is there a state $|\psi_A\rangle$ of Alice's particle that summarizes all we know about this particle?

If such a state existed, we would require the expectation value of any observable in $|\psi_A\rangle$ to be equal to the expectation value of $\hat{Q} \otimes \mathbb{1}$ in $|\psi_{AB}\rangle$:

$$\langle\psi_A|\hat{Q}|\psi_A\rangle = \langle\psi_{AB}|\hat{Q} \otimes \mathbb{1}|\psi_{AB}\rangle? \tag{20}$$

We will see that there is *no* such state $|\psi_A\rangle$.

No pure state can represent Alice's state if it is entangled with another state.

To see this we examine the cases when $\hat{Q}$ is σ_x, σ_y, and σ_z.

Note that

$$\sigma_x \otimes \mathbb{1}|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|-\rangle_A|-\rangle_B - |+\rangle_A|+\rangle_B\right),$$

$$\sigma_y \otimes \mathbb{1}|\psi_{AB}\rangle = i\frac{1}{\sqrt{2}}\left(|-\rangle_A|-\rangle_B + |+\rangle_A|+\rangle_B\right), \tag{21}$$

$$\sigma_z \otimes \mathbb{1}|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle_A|-\rangle_B + |-\rangle_A|+\rangle_B\right).$$

It follows quickly that all three expectation values vanish:

$$\langle \psi_{AB} | \sigma_x \otimes \mathbb{1} | \psi_{AB} \rangle = \langle \psi_{AB} | \sigma_y \otimes \mathbb{1} | \psi_{AB} \rangle = \langle \psi_{AB} | \sigma_z \otimes \mathbb{1} | \psi_{AB} \rangle = 0. \tag{22}$$

If a pure-state representative $|\psi_A\rangle$ of Alice's particle exists, then it must then satisfy

$$\langle \psi_A | \sigma_x | \psi_A \rangle = \langle \psi_A | \sigma_y | \psi_A \rangle = \langle \psi_A | \sigma_z | \psi_A \rangle = 0. \tag{23}$$

There is in fact a simple proof that the state $|\psi_A\rangle$ with vanishing expectation values for σ_x, σ_y, and σ_z does not exist.

Any spin state points somewhere, and therefore $|\psi_A\rangle = \gamma |\mathbf{n}\rangle$, for some constant $\gamma \neq 0$ and some direction $\mathbf{n}$.

But we also have $\langle \mathbf{n} | \mathbf{n} \cdot \boldsymbol{\sigma} | \mathbf{n} \rangle = 1$.

This means $\mathbf{n} \cdot \boldsymbol{\sigma}$ has a nonzero expectation value in $|\psi_A\rangle$, but this is impossible if all three Pauli matrices have zero expectation value in $|\psi_A\rangle$. □

We have thus shown that there is no pure state representing the quantum state of Alice's particle when entangled.

How do we describe such a quantum state?

By using a density matrix.

The description of the state of an entangled particle is given in all generality later.

The Density Matrix

We will now see how the information that defines a general ensemble can be used to construct an interesting operator ρ acting on the Hilbert space V of the theory.

The operator $\rho \in \mathcal{L}(V)$ is called a density matrix.

Our work begins with the general ensemble of equation Eq. (3):

$$E = \left\{ (p_1, |\psi_1\rangle), \ldots, (p_n, |\psi_n\rangle) \right\}, \quad p_1, \ldots, p_n > 0, \quad p_1 + \cdots + p_n = 1. \tag{24}$$

We recall that for this ensemble the expectation value of any observable is given by

$$\langle \hat{Q} \rangle_E = \sum_{a=1}^{n} p_a \langle \psi_a | \hat{Q} | \psi_a \rangle. \tag{25}$$

We now use the trace identity $\text{tr}(|u\rangle\langle w|) = \langle w|u\rangle$, derived below.

Consider two states $|u\rangle, |w\rangle \in V$, and use them to define the operator $|u\rangle\langle w|$.

Assume for this purpose that $|i\rangle$ with $i = 1, \cdots, N$ forms an orthonormal basis.

Earlier we defined that $\quad tr\,M = \sum_{i} \langle i| M |i\rangle \quad$, for any operator M so we see that

$$\text{tr}(|u\rangle\langle w|) = \sum_{i=1}^{N} \langle i|(|u\rangle\langle w|)|i\rangle = \sum_{i=1}^{N} \langle i|u\rangle\langle w|i\rangle.$$

With a reordering of the multiplicative factors in the last expression, we encounter a resolution of the identity:

$$\text{tr}(|u\rangle\langle w|) = \sum_{i=1}^{N} \langle w|i\rangle\langle i|u\rangle = \langle w|\left(\sum_{i=1}^{N} |i\rangle\langle i|\right)|u\rangle = \langle w|u\rangle,$$

We then rewrite the above expectation value in terms of the trace of $|\psi_a\rangle\langle\psi_a|$:

$$\langle\hat{Q}\rangle_E = \sum_{a=1}^{n} p_a \mathrm{tr}\left(\hat{Q}|\psi_a\rangle\langle\psi_a|\right). \tag{26}$$

For any constant p and any matrix A, we have $p\,\mathrm{tr}A = \mathrm{tr}(pA)$, and therefore

$$\langle\hat{Q}\rangle_E = \sum_{a=1}^{n} \mathrm{tr}\left(\hat{Q}\,p_a|\psi_a\rangle\langle\psi_a|\right) = \mathrm{tr}\left(\hat{Q}\sum_{a=1}^{n} p_a|\psi_a\rangle\langle\psi_a|\right), \tag{27}$$

where we also recalled the linearity property   .

This result shows that *all* the relevant information about the ensemble E is encoded in the operator inside the trace, to the right of $\hat{Q}$.

This operator will be called the density matrix operator $\rho_E \in \mathcal{L}(V)$ associated to the ensemble or mixed state E:

$$\text{Density matrix for } E: \quad \rho_E \equiv \sum_{a=1}^{n} p_a|\psi_a\rangle\langle\psi_a|. \tag{28}$$

Indeed, all the information about E is encoded in ρ_E because all we compute are expectation values of observables, and for them we now find that

$$\langle\hat{Q}\rangle_E = \mathrm{tr}\left(\hat{Q}\rho_E\right). \tag{29}$$

The expectation value of $\hat{Q}$ is obtained by multiplying $\hat{Q}$ by ρ_E and taking the trace.

The density matrix makes immediately clear some of the results we discussed before.

For the E_z and E_x ensembles introduced in Eq. (2) and Eq. (7),

$$\rho_{E_Z} = \tfrac{1}{2}|+\rangle\langle+| + \tfrac{1}{2}|-\rangle\langle-| = \tfrac{1}{2}\mathbb{1},$$

$$\rho_{E_X} = \tfrac{1}{2}|x;+\rangle\langle x;+| + \tfrac{1}{2}|x;-\rangle\langle x;-| = \tfrac{1}{2}\mathbb{1},$$

(30)

where we simply used two different resolutions of the identity $\mathbb{1}$, one for the $|\pm\rangle$ basis states (*first line*) and one for the $|x;\pm\rangle$ basis states (*second line*).

The two density matrices are identical, explaining why all observables in the two ensembles are the same.

Recall that these ensembles represented unpolarized beams, which are, arguably, maximally random beams.

We now see that for such a random state the density matrix is a multiple of the identity matrix.

While a detailed computation would confirm it, the density matrix for the unpolarized ensemble E_{unp} is also $\mathbb{1}/2$.

We know this is true because we showed that the expectation values in this ensemble are the same as in the E_z ensemble.

Remarks:

1. The density matrix is a Hermitian operator.

   This is manifest because the p_i are real, and $(|\chi\rangle\langle\eta|)^\dagger = |\eta\rangle\langle\chi|$, implying that $(|\psi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\psi|$.

   It follows that ρ can always be diagonalized and has real eigenvalues.

2. The density matrix is a positive semidefinite operator.

All its eigenvalues are nonnegative.

In a complex vector space with inner product $\langle \cdot, \cdot \rangle$, an operator M is said to be positive semidefinite if for any vector v we have $\langle v, Mv \rangle \geq 0$.

Using bra-ket notation, the condition that the density matrix ρ be positive semidefinite is

$$\langle \psi | \rho | \psi \rangle \geq 0 \quad \text{for all } |\psi\rangle. \tag{31}$$

Using the expression for ρ, we have

$$\langle \psi | \rho | \psi \rangle = \sum_{a=1}^{n} p_a \langle \psi | \psi_a \rangle \langle \psi_a | \psi \rangle = \sum_{a=1}^{n} p_a |\langle \psi_a | \psi \rangle|^2 \geq 0, \tag{32}$$

since we are adding the products of nonnegative numbers.

It now follows that the eigenvalues of ρ cannot be negative.

Indeed, a matrix M with a negative eigenvalue cannot be positive semidefinite because $\langle v, Mv \rangle < 0$ when v is the corresponding eigenvector.

3. The trace of ρ is equal to one:

$$\text{tr}\,\rho = 1. \tag{33}$$

This property also follows from direct computation:

$$\text{tr}\,\rho = \text{tr}\left(\sum_{a=1}^{n} p_a |\psi_a\rangle \langle \psi_a|\right) = \sum_{a=1}^{n} p_a \text{tr}(|\psi_a\rangle \langle \psi_a|), \tag{34}$$

by linearity of the trace.

It then follows that

$$\text{tr}\,\rho = \sum_{a=1}^{n} p_a \langle \psi_a | \psi_a \rangle = \sum_{a=1}^{n} p_a = 1. \tag{35}$$

4. The density matrix removes redundancies from the ensemble description of mixed states.

We have seen that different ensembles E and E' sometimes give the same density matrices: $\rho_E = \rho'_E$.

Since ρ is a Hermitian operator, we can use an orthonormal basis of V to write it as

$$\rho = \sum_{i,j=1}^{N} \rho_{ij} |i\rangle \langle j|, \tag{36}$$

where the ρ_{ij} are the entries of a Hermitian $N \times N$ matrix, with N the dimension of the vector space V of the theory.

Such a matrix is specified by N^2 real numbers.

Since the trace of this matrix is one, ρ is specified by $N^2 - 1$ real numbers if there are no additional constraints (in fact there are none!).

On the other hand, ensembles can require arbitrarily large amounts of data, especially when the number of entries $(p_a, |\psi_a\rangle)$ is large.

Thus, the density matrix removes redundant data in the ensemble description of the mixed state.

5. The phases in the states $|\psi_a\rangle$ of the ensemble are irrelevant to the density matrix.

Since the states $|\psi_a\rangle$ entering the description of the ensemble are normalized, they are only ambiguous up to a phase.

That phase cancels out in the density matrix, so they have no physical import. Indeed, if $\rho_E = \rho'_E$, we have

$$|\psi'_a\rangle\langle\psi'_a| = e^{i\theta_a}|\psi_a\rangle\langle\psi_a|e^{-i\theta_a} = |\psi_a\rangle\langle\psi_a|. \tag{37}$$

6. With a little abuse of terminology, physicists sometimes speak of the density matrix as the "state" or the "state operator" of the quantum system.

The density matrix can describe pure states and mixed states.

If the system is described by a pure state $|\psi\rangle$, the ensemble collapses to one entry, $E = \{(1, |\psi\rangle)\}$, and the associated density matrix is the

$$\text{pure state:} \quad \rho = |\psi\rangle\langle\psi|. \tag{38}$$

In this case ρ is in fact a *rank-one orthogonal projector* to the subspace of V generated by $|\psi\rangle$.

It is an orthogonal projector because ρ is Hermitian and satisfies

$$\rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \rho. \tag{39}$$

It is rank one because it has unit trace or, equivalently, because it projects to a one-dimensional subspace of V.

Note that given the density matrix ρ of a pure state we can easily recover the state $|\psi\rangle$: we simply let ρ act on any vector in V that is not in the kernel of ρ, the result being a vector along $|\psi\rangle$.

Because of the projector property and the trace property of ρ, we see that

$$\text{tr}\,\rho^2 = \text{tr}\rho = 1, \quad \text{for a pure state.} \tag{40}$$

Interestingly, the value of $\text{tr}\,\rho^2$ allows us to decide if we have a pure state or a mixed state:

Theorem 1. *$\text{tr}\,\varrho^2 \leq 1$, with the inequality saturated only for pure states.*

In summary, the various traces of the density matrix satisfy

$$\text{tr}\rho^2 \leq \text{tr}\,\rho = 1. \tag{41}$$

The value of $\text{tr}\,\rho^2$ can be used to characterize quantum states.

We define the **purity** $\zeta(\rho)$ of a density matrix ρ using this value:

When $\zeta = 1$, the state is pure.

As the value of the purity ζ goes below one, the state becomes mixed.

We declare that the lower the value of ζ, the less pure or more mixed the state.

Thus, a *maximally mixed* state is a state with the lowest possible value of ζ.

One can show that for a maximally mixed state the density matrix is actually a multiple of the identity matrix.

This fixes the density matrix, as the trace must be equal to one.

The unpolarized spin density matrix discussed in Eq. (30) is in fact maximally mixed.

Example 3. *Density matrix for spin one-half pure states.*

Here the density matrix is very simple: $|\mathbf{n}\rangle\langle\mathbf{n}|$ for a pure state $|\mathbf{n}\rangle$ pointing along the direction of the unit vector $\mathbf{n}$.

Since the density matrix is a Hermitian operator and the set of 2×2 Hermitian matrices is spanned by the identity and the Pauli matrices, we should be able to write

$$|\mathbf{n}\rangle\langle\mathbf{n}| = \tfrac{1}{2}a_0\, \mathbb{1} + \tfrac{1}{2}\sum_{i=1}^{3} a_i\sigma_i, \tag{42}$$

where the factors of have been included for convenience, and a_0 as well as a_1, a_2, a_3 are real constants.

This turns out to be:

$$|\mathbf{n}\rangle\langle\mathbf{n}| = \tfrac{1}{2}\left(\mathbb{1} + \mathbf{n}\cdot\boldsymbol{\sigma}\right). \tag{43}$$

So, starting from an ensemble, the associated density matrix is a positive semidefinite matrix with unit trace.

There are no extra conditions on the density matrix.

Example 4. *Density matrix for general spin one-half states.*

We again begin by writing the density matrix ρ as a general 2×2 Hermitian matrix:

$$\rho = \tfrac{1}{2}a_0\, \mathbb{1} + \tfrac{1}{2}\mathbf{a}\cdot\boldsymbol{\sigma}, \quad a_0, a_1, a_2, a_3 \in \mathbb{R}. \tag{44}$$

$\mathrm{tr}\,\rho = 1$ fixes $a_0 = 1$.

The only remaining condition on ρ is that of positivity: none of its eigenvalues can be negative.

The eigenvalues of $\mathbf{a} \cdot \boldsymbol{\sigma}$ are $\pm |\mathbf{a}|$, and therefore the eigenvalues of ϱ are

$$\tfrac{1}{2}(1 \pm |\mathbf{a}|) \geq 0. \tag{45}$$

Positivity requires $1 - |\mathbf{a}| \geq 0$ or, equivalently, $|\mathbf{a}| \leq 1$.

All in all, the density matrix for a general mixed or pure state is as follows:

$$\text{Spin one-half density matrix:} \quad \rho = \tfrac{1}{2}(\mathbb{1} + \mathbf{a} \cdot \boldsymbol{\sigma}), \quad |\mathbf{a}| \leq 1. \tag{46}$$

Measurement along an orthonormal basis

Recall that we can measure a pure state $|\psi\rangle$ along an orthonormal basis $|1\rangle$, ..., $|N\rangle$ of a dimension N vector space V, and the probability $p(i)$ of being in the state $|i\rangle$ is $|\langle i|\psi\rangle|^2$.

After measurement, the state will be in one of the states $|i\rangle$.

This is readily extended to cases in which the measurement is conducted on a mixed-state ensemble Eq. (3).

This time the probability $p(i)$ of finding $|i\rangle$ is obtained by weighting, with probability p_a, the probability $|\langle i|\psi_a\rangle|^2$ of finding the state $|\psi_a\rangle$ in $|i\rangle$:

$$p(i) = \sum_{a=1}^{n} p_a |\langle i|\psi_a\rangle|^2 = \sum_{a=1}^{n} p_a \langle i|\psi_a\rangle \langle \psi_a|i\rangle = \langle i| \sum_{a=1}^{n} p_a |\psi_a\rangle \langle \psi_a|i\rangle. \tag{47}$$

From this we get the simple expression

$$p(i) = \langle i|\rho|i\rangle. \tag{48}$$

As it should, this probability depends only on ρ and not on the ensemble that defines ρ.

After this measurement the system will be in one of the basis states.

If we obtain $|i\rangle$, the density matrix ρ becomes $|i\rangle\langle i|$.

This state is in fact the orthogonal projector $M_i \equiv |i\rangle\langle i|$ where

$$M_i^\dagger = M_i, \quad M_i M_i = M_i, \quad \sum_i M_i = \mathbb{1}. \tag{49}$$

The collection $\{M_i\}$ forms a complete set of orthogonal projectors.

Assume that a measurement along the basis has been performed, but the result is not available to us.

What becomes of the density matrix?

We know that after measurement we have, for each i, the probability $p(i)$ for the system to be in the state $|i\rangle$.

The new ensemble $\tilde{E}$ is therefore

$$\tilde{E} = \left\{ (p(1), |1\rangle), \ldots, (p(N), |N\rangle) \right\}. \tag{50}$$

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

$$\tilde{\rho} = \sum_i p(i)|i\rangle\langle i| = \sum_i |i\rangle \langle i|\rho|i\rangle \langle i|, \tag{51}$$

where we used our result for $p(i)$.

This can now be rewritten in a suggestive way:
$$\tilde{\rho} = \sum_i M_i \rho M_i. \tag{52}$$

This passage from ϱ to   gives us the effect of measurement along a basis on a quantum system when the result is not available.

We quickly check that, as required, the trace of the new density matrix remains equal to one:

$$\operatorname{tr}\tilde{\rho}=\sum_i\operatorname{tr}(M_i\,\rho\,M_i)=\sum_i\operatorname{tr}(\rho\,M_iM_i)=\sum_i\operatorname{tr}(\rho\,M_i)=\operatorname{tr}\left(\rho\sum_i M_i\right)=\operatorname{tr}\rho=1.\tag{53}$$

In the various steps, we used the cyclicity of the trace as well as the second and third properties in Eq. (49).

Dynamics of Density Matrices

Since the density matrix describes in all generality the possible quantum states of a system, it is of interest to see how it evolves in time.

To this end we need the Schrödinger equation written for a ket $|\psi\rangle$ as well as for a bra $\langle\psi|$:

$$\frac{\partial}{\partial t}|\psi\rangle=-\frac{i}{\hbar}\hat{H}|\psi\rangle,\qquad\frac{\partial}{\partial t}\langle\psi|=\frac{i}{\hbar}\langle\psi|\hat{H}.\tag{54}$$

Here $\hat{H}$ is the Hamiltonian.

We can now compute the rate of change of the projector $|\psi\rangle\langle\psi|$:

$$\frac{\partial}{\partial t}|\psi\rangle\langle\psi|=-\frac{i}{\hbar}\hat{H}|\psi\rangle\langle\psi|+\frac{i}{\hbar}|\psi\rangle\langle\psi|\hat{H}=-\frac{i}{\hbar}\,[\hat{H},|\psi\rangle\langle\psi|].\tag{55}$$

Using the ensemble definition of the density matrix, we then get

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t} \sum_{a=1}^{n} p_a |\psi_a\rangle \langle \psi_a| = \sum_{a=1}^{n} p_a \frac{\partial}{\partial t} |\psi_a\rangle \langle \psi_a| = -\frac{i}{\hbar} \sum_{a=1}^{n} p_a [\hat{H}, |\psi_a\rangle \langle \psi_a|]$$

$$= -\frac{i}{\hbar} \left[\hat{H}, \sum_{a=1}^{n} p_a |\psi_a\rangle \langle \psi_a| \right].$$

(56)

This implies the simple result

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

(57)

This equation determines the time evolution of the density matrix of a quantum system.

It manifestly preserves the Hermiticity of ρ because it sets its derivative $\frac{\partial \rho}{\partial t}$ equal to a Hermitian operator.

Indeed, $\frac{1}{i\hbar}[\hat{H}, \rho]$ is Hermitian because the commutator of Hermitian operators is anti-Hermitian, and the factor of i makes it Hermitian.

Moreover, the trace of ρ is unchanged:

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

(58)

since the trace of a commutator vanishes due to cyclicity.

This is automatic in finite-dimensional vector spaces but must be checked carefully when working in infinite-dimensional vector spaces.

Suppose we solve for the time evolution of states by constructing the unitary operator $\square(t)$ that evolves states as follows:

$$|\psi(t)\rangle = \mathcal{U}(t)|\psi(0)\rangle. \tag{59}$$

It is then clear that the density matrix, which at any time is a sum of terms of the form $|\psi_a(t)\rangle\langle\psi_a(t)|$, evolves as

$$\rho(t) = \mathcal{U}(t)\rho(0)\mathcal{U}^\dagger(t). \tag{60}$$

This evolution, of course, is consistent with the differential equation Eq. (57).

The above expression for $\rho(t)$ makes it manifest that if $\rho(0)$ is positive semidefinite, so is $\rho(t)$ for all times t.

Indeed, for any vector v in the state space we see that

$$\langle v|\rho(t)|v\rangle = \langle v|\mathcal{U}\rho(0)\mathcal{U}^\dagger|v\rangle = \langle \mathcal{U}^\dagger v|\rho(0)|\mathcal{U}^\dagger v\rangle \geq 0. \tag{61}$$

We know from the Schrödinger equation that a pure state $|\psi\rangle$ remains pure under time evolution.

This is also visible from the density matrix $\rho(t) = \mathcal{U}(t)|\psi\rangle\langle\psi|\mathcal{U}^\dagger(t)$.

In fact, a more general result holds.

We can quickly see that the purity $\zeta = \mathrm{tr}\,\rho^2$ does not change over time:

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

$$= \tfrac{2}{i\hbar}\mathrm{tr}(\rho[\hat{H}, \rho]) = \tfrac{2}{i\hbar}\mathrm{tr}(\rho\hat{H}\rho - \rho\rho\hat{H}) = 0, \tag{62}$$

by repeated use of the cyclicity of the trace.

Since the purity does not change under unitary time evolution and a pure state has purity equal to one, a pure state will remain pure.

The considerations of time evolution in this section apply to isolated systems.

They change in an interesting way when we consider the density matrix of a *subsystem* of an isolated system, as we will begin exploring next.

Subsystems and Schmidt Decomposition

Let us consider the physics of a quantum system A that is a part, or a subsystem, of a composite system AB.

The composite system is isolated from the rest of the world and is defined on a state space $\mathcal{H}_A \otimes \mathcal{H}_B$, with $\mathcal{H}_A$ and $\mathcal{H}_B$ the state spaces for A and B subsystems, respectively.

Typically, one has interactions that couple the two systems A and B, and the systems are entangled.

The system AB is a **bipartite** system, which just means it is composed of two parts.

In example 2 we considered a composite system AB in a pure entangled state and demonstrated that there is no pure state that represents the system A.

We need a density matrix.

This is truly the only option if AB is not in a pure state.

To fix notation, assume the spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ have dimensions d_A and d_B, respectively, and have orthonormal bases given by

$$\dim \mathcal{H}_A = d_A, \quad (e_1^A, \ldots, e_{d_A}^A) \text{ orthonormal basis,}$$

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

(63)

Let there be a density matrix ρ_{AB} for the full AB system.

We then ask: What is the relevant density matrix ρ_A that can be used to compute the results of measurements on A?

The answer turns out to be quite simple.

Since the system B plays no role here, ρ_A, sometimes called the *reduced density matrix*, is obtained by taking the partial trace over $\mathcal{H}_B$ of the full density matrix:

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

(64)

This proposal passes a basic consistency check: if ρ_{AB} is a density matrix, so is ρ_A.

To see this first note that the trace works out correctly:

$$\mathrm{tr}_A\, \rho_A = \mathrm{tr}_A\, \mathrm{tr}_B\, \rho_{AB} = \mathrm{tr}\, \rho_{AB} = 1,$$

(65)

where tr is the full trace in the tensor product space.

Moreover, ρ_A is a positive semidefinite operator.

To prove this we must show that $\langle v_A | \rho_A | v_A \rangle \geq 0$ for any $|v_A\rangle \in \mathcal{H}_A$. This is not complicated:

$$\langle v_A | \rho_A | v_A \rangle = \langle v_A | \sum_k \langle e_k^B | \rho_{AB} | e_k^B \rangle | v_A \rangle = \sum_k \langle v_A | \langle e_k^B | \, \rho_{AB} \, | v_A \rangle | e_k^B \rangle \geq 0,$$

(66)

since every term in the sum is nonnegative because ρ_{AB} is positive semidefinite.
Being a positive semidefinite operator of unit trace, ρ_A can represent a density matrix.

The formula Eq. (64) is justified by showing that for an arbitrary operator $\mathcal{O}_A \in \mathcal{L}(\mathcal{H}_A)$ the expectation value obtained using ρ_A equals the expectation value of $\mathcal{O}_A \otimes \mathbb{1}_B$ using the full density matrix ρ_{AB}:

$$\text{tr}_A\left(\rho_A \mathcal{O}_A\right) = \text{tr}\left(\rho_{AB} \mathcal{O}_A \otimes \mathbb{1}_B\right). \tag{67}$$

To see this let us write a general density matrix ρ_{AB} as the most general operator on $\mathcal{H}_A \otimes \mathcal{H}_B$.

Recalling that $\mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B) = \mathcal{L}(\mathcal{H}_A) \otimes \mathcal{L}(\mathcal{H}_B)$, we use basis operators $|e_i^A\rangle\langle e_j^A| \in \mathcal{L}(\mathcal{H}A)$ and $|e_k^B\rangle\langle e_l^B| \in \mathcal{L}(\mathcal{H}_B)$ to write the most general linear superposition of tensor products:

$$\rho_{AB} = \sum_{i,j,k,l} \rho_{ij,kl} \, |e_i^A\rangle\langle e_j^A| \otimes |e_k^B\rangle\langle e_l^B|. \tag{68}$$

It follows that

$$\rho_A = \text{tr}_B \rho_{AB} = \sum_{i,j,k,l} \rho_{ij,kl} \, |e_i^A\rangle\langle e_j^A| \otimes \langle e_l^B|e_k^B\rangle = \sum_{i,j,k} \rho_{ij,kk} \, |e_i^A\rangle\langle e_j^A|, \tag{69}$$

and as a result, the left-hand side of Eq. (67) is

$$\text{tr}_A\left(\rho_A \, \mathcal{O}_A\right) = \sum_{i,j,k} \rho_{ij,kk} \, \langle e_j^A|\mathcal{O}_A|e_i^A\rangle. \tag{70}$$

Similarly, we compute the right-hand side of Eq. (67):

$$\text{tr}(\rho_{AB} \, \mathcal{O}_A \otimes \mathbb{1}_B) = \text{tr}_A \text{tr}_B \sum_{i,j,k,l} \rho_{ij,kl} \, |e_i^A\rangle\langle e_j^A| \mathcal{O}_A \otimes |e_k^B\rangle\langle e_l^B|$$

$$= \sum_{i,j,k} \rho_{ij,kk} \, \langle e_j^A|\mathcal{O}_A|e_i^A\rangle, \tag{71}$$

making it clear that Eq. (67) holds and thus justifying the claimed formula for the density matrix ρ_A of the subsystem A.

Note that nowhere in the proof of Eq. (67) have we used any particular property of the density operator ρ_{AB}.

This means that this identity is true for arbitrary operators:

Theorem 2. *Let $S_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ be an arbitrary operator, and $S_A = tr_B \, S_{AB}$.*

Then for any $\mathcal{O}_A \in \mathcal{L}(\mathcal{H}_A)$ we find that

$$tr_A\left(S_A \mathcal{O}_A\right) = tr\left(S_{AB} \mathcal{O}_A \otimes \mathbb{1}_B\right). \tag{72}$$

Example 5. *A pure state of two entangled spins and density matrix of a subsystem.*

Consider the pure-state system AB of two spins examined before:

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\right). \tag{73}$$

Alice has particle A, and Bob has particle B.

We aim to find the density matrix ρ_B for subsystem B, Bob's particle.

The density matrix for the full system is just $\varrho_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}|$, which we can write out conveniently as sums of tensor products of operators

$$
\begin{aligned}
\rho_{AB} &= \tfrac{1}{\sqrt{2}}\left(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\right)\tfrac{1}{\sqrt{2}}\left(\langle+|_A\langle-|_B - \langle-|_A\langle+|_B\right)\\[4pt]
&= \quad \tfrac{1}{2}\left(|+\rangle\langle+|\right)_A \otimes \left(|-\rangle\langle-|\right)_B\\[4pt]
&\quad - \tfrac{1}{2}\left(|+\rangle\langle-|\right)_A \otimes \left(|-\rangle\langle+|\right)_B\\[4pt]
&\quad - \tfrac{1}{2}\left(|-\rangle\langle+|\right)_A \otimes \left(|+\rangle\langle-|\right)_B\\[4pt]
&\quad + \tfrac{1}{2}\left(|-\rangle\langle-|\right)_A \otimes \left(|+\rangle\langle+|\right)_B.
\end{aligned}
\tag{74}
$$

We can now take the trace over A to find the density matrix for B.

From the four terms displayed on the last right-hand side, the second and third have zero tr_A.

The nonvanishing contributions give

$$
\rho_B = \text{tr}_A\,\rho_{AB} = \tfrac{1}{2}|-\rangle\langle-| + \tfrac{1}{2}|+\rangle\langle+|.
\tag{75}
$$

The state of B is maximally mixed. This was probably expected, as the original pure state $|\psi_{AB}\rangle$ seems as entangled as can be.

Another curious fact emerges when we recall that in Eq.(11) we obtained the ensemble that Bob gets when Alice does a measurement of her particle but does not communicate the result.

The ensemble is exactly the same as that described by the above ρ_B.

Thus, whether or not Alice measures, the state of B is the same, in this case the maximally mixed state.

We will understand this remarkable coincidence more generally shortly.

Schmidt decomposition The *pure* states $|\psi_{AB}\rangle$ of a bipartite system AB can be written in an insightful way by using as a guide the associated density matrices ρ_A and ρ_B of the subsystems.

The result is the *Schmidt decomposition* of the pure state $|\psi_{AB}\rangle$, named in honor of Erhard Schmidt (1876–1959), also known for the Gram-Schmidt procedure that yields orthonormal basis vectors from a set of nonorthonormal ones.

The decomposition displays a simple structure—simpler than the general structure allowed from the tensor product:

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.

Suppose we have a bipartite system AB and a pure state $|\Psi_{AB}\rangle$ in which A is entangled with B:

$$|\Psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B. \tag{76}$$

The dimensions and basis states for $\mathcal{H}_A$ and $\mathcal{H}_B$ are as in Eq. (63).

Assume that we choose to label the systems so that

$$d_A \leq d_B. \tag{77}$$

A state $|\Psi_{AB}\rangle$ is typically written as an expansion over the obvious basis states $|e_i^A\rangle \otimes |e_j^B\rangle$ of $\mathcal{H}_A \otimes \mathcal{H}_B$:

$$|\Psi_{AB}\rangle = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} \psi_{ij} |e_i^A\rangle \otimes |e_j^B\rangle. \tag{78}$$

Here the ψ_{ij} are $d_A \cdot d_B$ expansion coefficients.

In the Schmidt decomposition, we will do much better than this.

Actually, the above expression can be rewritten as

$$|\Psi_{AB}\rangle = \sum_{i=1}^{d_A} |e_i^A\rangle \otimes |\psi_i^B\rangle, \quad \text{with} \quad |\psi_i^B\rangle = \sum_{j=1}^{d_B} \psi_{ij}|e_j^B\rangle. \tag{79}$$

While this is nicer, not much can be said about the $|\psi_i^B\rangle$ states; in particular, they need not be orthonormal.

In the Schmidt decomposition, the sum analogous to the sum over i runs up to an integer r called the Schmidt index, which can be smaller than d_A. Moreover, the states from $\mathcal{H}_B$ as well as those from $\mathcal{H}_A$ are orthonormal.

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

$$\rho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}|, \quad \rho_A = \text{tr}_B \rho_{AB} = \text{tr}_B \left(|\Psi_{AB}\rangle\langle\Psi_{AB}|\right). \tag{80}$$

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 $k = 1, ..., d_A$ be the eigenvalues and eigenvectors of ρ_A, with the eigenvectors $|k_A\rangle$ chosen to be an orthonormal basis for $\mathcal{H}_A$ and the eigenvalues p_k nonnegative.

We see that the density matrix ρ_A has furnished us with a second orthonormal basis of states for $\mathcal{H}_A$.

The density matrix ρ_A can then be written as

$$\rho_A = \sum_{k=1}^{r} p_k |k_A\rangle\langle k_A|, \quad r \le d_A, \text{ and } p_{k>r} = 0. \tag{81}$$

It may happen, for example, that ρ_A is a pure state, in which case the above sum has just one term, and only one p_k is nonzero.

In general, the sum defining ρ_A has $r \le d_A$ terms.

Let us assume this and order the list of eigenvectors and eigenvalues so that the first r eigenvalues are nonzero and the rest vanish.

Then we will write

$$\rho_A = \sum_{k=1}^{r} p_k |k_A\rangle\langle k_A|, \quad r \le d_A, \text{ and } p_{k>r} = 0. \tag{82}$$

Let us now consider $|\psi_{AB}\rangle$.

Since the $|k_A\rangle$ span $\mathscr{H}_A$, we can write

$$|\psi_{AB}\rangle = \sum_{k=1}^{d_A} |k_A\rangle \otimes |\psi_k^B\rangle, \qquad |\psi_k^B\rangle \tag{83}$$

with $|\psi_k^B\rangle$ some collection of states in H_B.

Note that we have at most d_A terms, not the $d_A \cdot d_B$ terms that would arise if we used the basis states of H_B to expand the $|\psi_k^B\rangle$ states.

Forming the density matrix associated with $|\psi_{AB}\rangle$, we find that

$$\rho_{AB} = \sum_{k,\tilde{k}=1}^{d_A} |k_A\rangle \otimes |\psi_k^B\rangle \langle \tilde{k}_A| \otimes \langle \psi_{\tilde{k}}^B|. \tag{84}$$

Taking the trace over B, we now get

$$\rho_A = \mathrm{tr}_B \rho_{AB} = \sum_{k,\tilde{k}=1}^{d_A} |k_A\rangle\langle \tilde{k}_A| \langle \psi_{\tilde{k}}^B|\psi_k^B\rangle. \tag{85}$$

Compare now with our previous expression for ρ_A in Eq. (82), where no state $|k_A\rangle$ with $k > r$ appears.

This means that we should reconsider our ansatz for $|\psi_{AB}\rangle$: no state $|k_A\rangle$ with $k > r$ can appear there either.

If they did, there would be some nonvanishing terms in ρ_A that are not included in Eq. (82).

We therefore rewrite
$$|\psi_{AB}\rangle = \sum_{k=1}^{r} |k_A\rangle \otimes |\psi_k^B\rangle, \tag{86}$$

which leads to

$$\rho_{AB} = \sum_{k,\tilde{k}=1}^{r} |k_A\rangle \otimes |\psi_k^B\rangle \langle \tilde{k}_A| \otimes \langle \psi_{\tilde{k}}^B| \quad \Rightarrow \quad \rho_A = \sum_{k,\tilde{k}=1}^{r} |k_A\rangle\langle \tilde{k}_A| \langle \psi_{\tilde{k}}^B|\psi_k^B\rangle. \tag{87}$$

Once again comparing with ρ_A in Eq. (82), we see there should be no terms with $k \neq \tilde{k}$.

Full agreement then requires that

$$\langle \psi_{\tilde{k}}^B | \psi_k^B \rangle = p_k \, \delta_{k\tilde{k}}, \quad k, \tilde{k} = 1, \ldots, r. \tag{88}$$

In other words, states $|\psi_k^B\rangle$ with different values of k must be orthogonal.

It is therefore useful to introduce normalized versions $|k_B\rangle$ of the states as follows:

$$|k_B\rangle \equiv \frac{|\psi_k^B\rangle}{\sqrt{p_k}}, \quad k = 1, \ldots, r. \tag{89}$$

These states satisfy

$$\langle k_B | k_B' \rangle = \delta_{k,k'}, \quad k, k' = 1, \ldots, r. \tag{90}$$

If $r < d_B$, one can define additional orthonormal vectors to have a full basis for $\mathscr{H}_B$.

These extra vectors will not feature below.

We have already shown that the pure state $|\psi_{AB}\rangle$ of the bipartite system AB can always be written as a sum of r terms.

From Eq. (86) and Eq. (89), we now get the Schmidt decomposition of the pure state $|\psi_{AB}\rangle$:

$$|\psi_{AB}\rangle = \sum_{k=1}^{r} \sqrt{p_k} \, |k_A\rangle \otimes |k_B\rangle, \quad r \leq d_A \leq d_B. \tag{91}$$

In here,

$$\sum_{k=1}^{r} p_k = 1, \quad p_k > 0, \quad k = 1, \ldots, r, \tag{92}$$

and the states $|k_A\rangle \in \mathscr{H}_A$ and $|k_B\rangle \in \mathscr{H}_B$, with $k = 1, ..., r$, form orthonormal sets:

$$\langle k_A | k_A' \rangle = \delta_{k,k'}, \quad \langle k_B | k_B' \rangle = \delta_{k,k'}. \tag{93}$$

Despite the similar notation, the $|k_A\rangle$ and $|k_B\rangle$ states have nothing to do with each other; they live in different spaces.

The Schmidt decomposition Eq. (91) has the properties we anticipated before.

It involves the sum of $r \leq d_A$ terms, each a basis state of $\mathcal{H}_A$ multiplied by some state in $\mathcal{H}_B$.

Moreover, the $\mathcal{H}_B$ states $|k_B\rangle$ multiplying the $|k_A\rangle$ basis states also form an orthonormal set.

Finally, since the construction is inspired by density matrices, the reduced density matrix ρ_A, and in fact $\rho_B = \text{tr}_A \rho_{AB}$ as well, are nicely written in the above language.

We already had ρ_A from Eq. (82), and ρ_B follows from a very brief calculation:

$$\rho_A = \sum_{k=1}^{r} p_k |k_A\rangle\langle k_A|, \qquad \rho_B = \sum_{k=1}^{r} p_k |k_B\rangle\langle k_B|. \tag{94}$$

The $\mathcal{H}_A$ and $\mathcal{H}_B$ basis vectors used in the Schmidt decomposition make the density matrices ρ_A and ρ_B diagonal.

Moreover, ρ_A and ρ_B have exactly the same nonzero eigenvalues!

This is an important result for any bipartite system in a pure state.

Since any pure state of a bipartite system AB has a Schmidt decomposition, the value of r is unambiguously determined.

This value is called the **Schmidt number** of the state.

If a state of *AB* has Schmidt number one, the *A* and *B* subsystems are not entangled: the Schmidt decomposition provides a manifest description of the *AB* state as the tensor product of a state in $\mathcal{H}_A$ and a state in $\mathcal{H}_B$.

Moreover, if the Schmidt number *r* is greater than one, the subsystems are definitely entangled.

This is clear because the reduced density matrices ρ_A and ρ_B are mixed (they have $r > 1$ terms), and a state of *AB* where *A* and *B* are not entangled always leads to density matrices ρ_A and ρ_B that represent pure states.

One can prove that for any pure entangled state of AB the purity of ρ_A equals the purity of ρ_B with value:

$$\zeta(\rho_A) = \zeta(\rho_B) = \sum_{k=1}^{r} p_k^2. \tag{95}$$

Consider a bipartite system *AB* where *A* and *B* have state spaces of the same dimensionality, and the state of *AB* is pure.

The result of the above exercise shows that when ρ_A is maximally mixed, so is ρ_B.

In such a case, we say that *A* and *B* are *maximally entangled*.

For the following state $\left| \hat{\psi}_{AB} \right\rangle$ of two spin one-half particles A and B:

$$|\hat{\psi}_{AB}\rangle = \tfrac{1}{\sqrt{2}}|+\rangle_A|+\rangle_B + \tfrac{1}{2}|-\rangle_A|+\rangle_B - \tfrac{1}{2}|-\rangle_A|-\rangle_B,$$

$$= \tfrac{1}{\sqrt{2}}|+\rangle_A|+\rangle_B + \tfrac{1}{\sqrt{2}}|-\rangle_A|x;-\rangle_B. \tag{96}$$

it can be shown that the density matrix ρ_A for particle A is

$$\rho_A = \tfrac{1}{2}|+\rangle\langle+| \ + \ \tfrac{1}{2\sqrt{2}}|+\rangle\langle-| \ + \ \tfrac{1}{2\sqrt{2}}|-\rangle\langle+| \ + \ \tfrac{1}{2}|-\rangle\langle-|. \tag{97}$$

Let us now find the Schmidt decomposition for $\left|\hat{\psi}_{AB}\right\rangle$.

First, one diagonalizes the reduced density matrix ρ_A

$$\rho_A = \tfrac{1}{2}\left(1+\tfrac{1}{\sqrt{2}}\right)|x;+\rangle\langle x;+| \ + \ \tfrac{1}{2}\left(1-\tfrac{1}{\sqrt{2}}\right)|x;-\rangle\langle x;-|. \tag{98}$$

On account of the relation between ϱ_A and the state $|\psi_{AB}\rangle$ it arises from, exemplified in equations Eq. (94) and Eq. (91), we have a simple ansatz for the state $\left|\hat{\psi}_{AB}\right\rangle$:

$$|\hat{\psi}_{AB}\rangle = \tfrac{1}{\sqrt{2}}\sqrt{1+\tfrac{1}{\sqrt{2}}}\,|x;+\rangle_A|1_B\rangle + \tfrac{1}{\sqrt{2}}\sqrt{1-\tfrac{1}{\sqrt{2}}}\,|x;-\rangle_A|2_B\rangle, \tag{99}$$

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

Writing the $|\pm\rangle_A$ states in the expression (96) for $\left|\hat{\psi}_{AB}\right\rangle$ in terms of $|x;\pm\rangle_A$, a short calculation gives

$$\begin{aligned}
|\hat{\psi}_{AB}\rangle = \ &\tfrac{1}{2}|x;+\rangle_A \otimes \left((1+\tfrac{1}{\sqrt{2}})|+\rangle_B - \tfrac{1}{\sqrt{2}}|-\rangle_B\right) \\
&+ \tfrac{1}{2}|x;-\rangle_A \otimes \left((1-\tfrac{1}{\sqrt{2}})|+\rangle_B + \tfrac{1}{\sqrt{2}}|-\rangle_B\right).
\end{aligned} \tag{100}$$

The earlier result (99) tells us how to rewrite this in a way that orthonormality is manifest.
We find that

$$|\hat{\psi}_{AB}\rangle = \frac{1}{\sqrt{2}}\sqrt{1+\frac{1}{\sqrt{2}}}\,|x;+\rangle_A \otimes \sqrt{1-\frac{1}{\sqrt{2}}}\left((1+\frac{1}{\sqrt{2}})|+\rangle_B - \frac{1}{\sqrt{2}}|-\rangle_B\right)$$

$$+ \frac{1}{\sqrt{2}}\sqrt{1-\frac{1}{\sqrt{2}}}\,|x;-\rangle_A \otimes \sqrt{1+\frac{1}{\sqrt{2}}}\left((1-\frac{1}{\sqrt{2}})|+\rangle_B + \frac{1}{\sqrt{2}}|-\rangle_B\right).$$

$$(101)$$

This is the Schmidt decomposition of $\left|\hat{\psi}_{AB}\right\rangle$.

You can check that the states to the right of $|x;\pm\rangle_A$ are orthonormal.

The Schmidt number is two, and the subsystems A and B are entangled.

Measurement along a basis in a subsystem

We now want to extend to bipartite systems the result $\tilde{\rho} = \sum M_i \rho M_i$ (see Eq. (53)), giving the density matrix $\tilde{\rho}$ after measurement along an orthonormal basis $\{|i\rangle\}$ when the result of the measurement is not known, and the original density matrix is ϱ.

Here, $M_i = |i\rangle\langle i|$.

Consider therefore a bipartite system AB, and imagine that Alice measures the state of A along a basis $\{|i\rangle_A\}$ associated with projectors $M_i^A = |i\rangle_A\,{}_A\langle i|$, satisfying

$$M_i^{A\dagger} = M_i^A, \quad M_i^A M_i^A = M_i^A, \quad \sum_i M_i^A = \mathbb{1}_A.$$

$$(102)$$

Assume that we start with a density matrix ρ_{AB}, and we do not know the result of Alice's measurement. In analogy to the previous result, the density matrix $\tilde{\rho}_{AB}$ after measurement is

$$\tilde{\rho}_{AB} = \sum_i (M_i^A \otimes \mathbb{1}_B)\, \rho_{AB}\, (M_i^A \otimes \mathbb{1}_B).$$

$$(103)$$

While clearly very plausible, this claim can be proven explicitly.

With this result we can learn something important about entanglement.

We now look for the reduced density matrix B of B following from $\tilde{\rho}_B$ to see the effect on Bob due to Alice's measurement on A.

Can Bob tell that Alice did a measurement?

We have already seen in some particular case (example 5) that Bob cannot.

We begin our work with the density matrix of B *after* measurement:

$$\tilde{\rho}_B = \text{tr}_A \tilde{\rho}_{AB} = \text{tr}_A \sum_i (M_i^A \otimes \mathbb{1}_B)\, \rho_{AB}\, (M_i^A \otimes \mathbb{1}_B). \tag{104}$$

We wish to compare $\tilde{\rho}_B$ with the density matrix $\rho_B = \text{tr}_A \rho_{AB}$ of B *before* measurement.

To analyze this we use a general representation of the original bipartite density matrix in terms of a collection of operators $\mathcal{O}_k^A$ and $\mathcal{O}_k^B$ indexed by some label k:

$$\rho_{AB} = \sum_k \mathcal{O}_k^A \otimes \mathcal{O}_k^B, \quad \mathcal{O}_k^A \in \mathcal{L}(H_A), \quad \mathcal{O}_k^B \in \mathcal{L}(H_B), \quad \forall k. \tag{105}$$

Then we have

$$\tilde{\rho}_B = \text{tr}_A \sum_{i,k} (M_i^A \otimes \mathbb{1}_B)\, \mathcal{O}_k^A \otimes \mathcal{O}_k^B\, (M_i^A \otimes \mathbb{1}_B)$$

$$= \text{tr}_A \sum_{i,k} M_i^A \mathcal{O}_k^A M_i^A \otimes \mathcal{O}_k^B = \sum_{i,k} \text{tr}_A (M_i^A \mathcal{O}_k^A M_i^A)\, \mathcal{O}_k^B. \tag{106}$$

Recalling the cyclicity of the trace and the projector properties of M_i^A listed above, we have

$$\mathrm{tr}_A(M_i^A \mathcal{O}_k^A M_i^A) = \mathrm{tr}_A(M_i^A \mathcal{O}_k^A)..$$

Since the sum of M_i^A's over i gives the identity matrix, we get

$$\tilde{\rho}_B = \sum_k \sum_i \mathrm{tr}_A(M_i^A \mathcal{O}_k^A)\, \mathcal{O}_k^B = \sum_k \mathrm{tr}_A(\mathcal{O}_k^A)\, \mathcal{O}_k^B = \mathrm{tr}_A \rho_{AB} = \rho_B. \tag{107}$$

Alice's measurement, with results unknown to Bob, does *not* change Bob's density matrix.

This means that Alice cannot use a measurement to communicate information instantaneously to Bob.

Since the particles in entangled pairs can be very far away, this prevents superluminal transfer of information, thus avoiding conflict with special relativity.

Note that the result did not depend on using the density matrix of *AB*.

The result holds for an arbitrary operator S_{AB} on *AB*:

No-signaling theorem.

Let $S_{AB} \in \mathrm{L}(\mathrm{H}_A \otimes \mathrm{H}B)$ be an arbitrary operator and $\tilde{S}_{AB}$ be defined by

$$\tilde{S}_{AB} = \sum_i (M_i^A \otimes \mathbb{1}_B)\, S_{AB}\, (M_i^A \otimes \mathbb{1}_B), \tag{108}$$

with M_i^A orthogonal projectors satisfying Eq. (102).

Then, $\mathrm{tr}_A\, \tilde{S}_{AB} = \mathrm{tr}_A S_{AB}$.

If Alice and Bob share an entangled pair of quantum systems, this theorem prevents Alice from sending a message or a signal to Bob instantaneously by performing measurements.

Thus the name *no-signaling theorem*.

We can also imagine that Alice, instead of measuring, applies some Hamiltonian to her system, causing some unitary evolution represented by the operator $\mathcal{U}_A$.

In this case the evolved density matrix $\tilde{\rho}_{AB}$ of the bipartite system whose initial density matrix is ρ_{AB} takes the form

$$\hat{\rho}_{AB} = (\mathcal{U}_A \otimes \mathbb{1}_B)\, \rho_{AB}\, (\mathcal{U}_A^\dagger \otimes \mathbb{1}_B). \tag{109}$$

It is now simple to show, just as above, that the density matrix for Bob is not affected:

$$\hat{\rho}_B \equiv \mathrm{tr}_A\, \hat{\rho}_{AB} = \rho_B \tag{110}$$

where $\rho_B = \mathrm{tr}_A\, \rho_{AB}$ is the density matrix of B before Alice subjected her particle to unitary evolution.

Alice cannot signal Bob by acting on her system with arbitrary unitary evolution.

Open Systems and Decoherence

We now consider an isolated quantum system AE, which we will view as a bipartite system composed of a subsystem A, the focus of our interest, and a subsystem E called the *environment*.

In practice A could be a small quantum system, perhaps the spin state of a single nucleus in an NMR experiment, with E the thousands of nearby spin states that interact with our selected spin.

Or, in principle, the AE system could consist of two spin one-half particles, one comprising the A system and the other the E system.

We call A an **open system** because it is not isolated; it interacts with another quantum system, the environment E.

Starting from the density matrix ρ_{AE} for a system AE, we can define a reduced density matrix ρ_A for A by tracing over the environment E.

We are interested in this reduced density matrix; we do not aim to describe the environment.

Our main question is: How does ρ_A evolve in time?

The full AE density matrix represents an isolated system, so it must have unitary time evolution, as in Eq. (60), with $\mathcal{U}$ the evolution operator associated to the complete Hamiltonian of the AE system.

The time evolution of ρ_A, however, is *not* unitary.

This is easily seen in an example to be discussed in detail below: if we have two spins, one A and one E, and the initial AE state is a pure nonentangled state, the density ρ_A begins as that of a pure state.

The interactions, however, entangle the two spins, and as we have seen before, this means that ρ_A becomes a mixed state.

Under unitary evolution a pure state remains a pure state, and thus ϱ_A does *not* experience unitary evolution.

For the AE system, the open subsystem A can experience **decoherence**, the process where ρ_A begins as a pure state but turns into a mixed state.

At time equal zero, A may be in a pure state $|\psi_A\rangle$, a superposition of $\mathcal{H}_A$ basis states.

But then, by interacting with the environment E, the state of A becomes mixed.

The data defining the original superposition is no longer available on subsystem A, having migrated at least partially into correlations of A with the environment.

Decoherence is a problem for a quantum computer: the quantum circuit is expected to be in a pure state during any computation (see example 7 below).

In this section we first discuss the time evolution of the reduced density matrix ρ_A of an AE system.

We then consider an example illustrating the evolution of the density matrix of a spin one-half particle coupled to another one.

Consider the isolated system AE.

The operation tr_E, trace over the environment, maps a density matrix ρ_{AE} of AE into a density matrix ρ_A that describes subsystem A:

$$\text{tr}_E \colon \rho_{AE} \rightarrow \rho_A. \tag{111}$$

The time evolution of ρ_A is controlled by this map: we must find the time evolution of ρ_{AE} and then take the environment trace to find the time evolution of ρ_A:

$$\text{tr}_E \colon \rho_{AE}(t) \rightarrow \rho_A(t). \tag{112}$$

This is the strategy we follow.

Assume the Hamiltonian $\hat{H}$ of the full AE system is known so that we also have the unitary operator $\mathcal{U}$ that evolves states of AE.

Let $\mathcal{U} = \mathcal{U}(t)$ denote the operator that turns states at $t = 0$ into states at t.

We then have

$$\rho_{AE}(t) = \mathcal{U}\rho_{AE}(0)\mathcal{U}^\dagger. \tag{113}$$

As a result, the time-dependent density matrix for subsystem A is given by

$$\rho_A(t) = \text{tr}_E\left[\mathcal{U}\rho_{AE}(0)\mathcal{U}^\dagger\right]. \tag{114}$$

Note that the partial trace does not satisfy cyclicity when acting on operators in the full space, and therefore the $\mathcal{U}$ and $\mathcal{U}^\dagger$ cannot be brought together to cancel each other.

The above formula satisfies the consistency conditions that make ρ_A into a density matrix.

Indeed, recalling that $\text{tr} = \text{tr}_A\text{tr}_E$ we show that

$$\text{tr}_A\rho_A(t) = \text{tr}_A\text{tr}_E[\mathcal{U}\rho_{AE}(0)\mathcal{U}^\dagger] = \text{tr}[\mathcal{U}\rho_{AE}(0)\mathcal{U}^\dagger]$$

$$= \text{tr}[\rho_{AE}(0)\mathcal{U}^\dagger\mathcal{U}] = \text{tr}\,\rho_{AE}(0) = 1. \tag{115}$$

It is easy to show that $\rho_A(t)$, as defined, is positive semidefinite if $\rho_{AE}(0)$ is.

A reasonable assumption is to take the state of the environment at the initial time $t = 0$ to be pure and equal to some fixed state $|\psi_E\rangle$.

We could also take the state of A to be pure, but let us first consider the possibility that it is a density matrix $\rho_A(t_0)$.

In this case the initial density matrix of AE is

$$\rho_{AE}(0) = \rho_A(0) \otimes |\psi_E\rangle\langle\psi_E|. \tag{116}$$

The time evolution equation Eq. (114) then gives

$$\rho_A(t) = \text{tr}_E\left[\mathcal{U}(\rho_A(0) \otimes |\psi_E\rangle\langle\psi_E|)\mathcal{U}^\dagger\right], \quad \mathcal{U} = \mathcal{U}(t). \tag{117}$$

This shows how the density matrix of the subsystem evolves in time.

Keeping the time t and the state $|\psi_E\rangle$ fixed, the right-hand side defines a linear map from density matrices to density matrices, taking $\rho_A(0)$ to $\rho_A(t)$.

If at $t = 0$ system A is a pure state $|\phi_A\rangle$, we find that

$$\rho_A(t) = \text{tr}_E\left[\mathcal{U}(|\phi_A\rangle\langle\phi_A| \otimes |\psi_E\rangle\langle\psi_E|)\mathcal{U}^\dagger\right]. \tag{118}$$

Example 7. *Decoherence of a qubit.*

Consider a spin one-half particle representing a qubit or quantum bit in a quantum computer; a qubit being just a quantum two-state system.

The qubit is in the state

$$|\psi_A\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle, \quad |\alpha|^2 + |\beta|^2 = 1. \tag{119}$$

This qubit is coupled to a state $|0_E\rangle$ of the environment so that the total state $|\psi_{AE}\rangle$ of the system is given by

$$|\psi_{AE}\rangle = |\psi_A\rangle \otimes |0_E\rangle = (\alpha|\uparrow\rangle + \beta|\downarrow\rangle) \otimes |0_E\rangle = \alpha|\uparrow\rangle \otimes |0_E\rangle + \beta|\downarrow\rangle \otimes |0_E\rangle. \tag{120}$$

The qubit density matrix ρ_A from this state takes the form given by

$$\rho_A = |\psi_A\rangle\langle\psi_A| = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \beta\alpha^* & |\beta|^2 \end{pmatrix}, \tag{121}$$

using basis vectors $|1\rangle = |\uparrow\rangle$, $|2\rangle = |\downarrow\rangle$.

This is, of course, the density matrix of a pure state.

Now assume that an interaction of the qubit with the environment changes the state of the environment for the term where the qubit is down:

$$|\psi_{AE}\rangle = \alpha|\uparrow\rangle \otimes |0_E\rangle + \beta|\downarrow\rangle \otimes |0_E\rangle \quad \rightarrow \quad |\psi'_{AE}\rangle = \alpha|\uparrow\rangle \otimes |0_E\rangle + \beta|\downarrow\rangle \otimes |1_E\rangle, \tag{122}$$

with $|1_E\rangle$ that other state of the environment.

The primed state has the qubit entangled with the environment.

Assuming the states $|0_E\rangle$ and $|1_E\rangle$ are normalized and orthogonal to each other, the density matrix ρ'_A is now

$$\rho'_A = \mathrm{tr}_E \rho'_{AE} = \mathrm{tr}_E |\psi'_{AE}\rangle\langle\psi'_{AE}|$$

$$= \mathrm{tr}_E \left(\alpha|\uparrow\rangle \otimes |0_E\rangle + \beta|\downarrow\rangle \otimes |1_E\rangle\right)\left(\alpha^*\langle\uparrow| \otimes \langle 0_E| + \beta^*\langle\downarrow| \otimes \langle 1_E|\right) \tag{123}$$

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

As a matrix, we have

$$\rho'_A = \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}. \tag{124}$$

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

Indeed, in this case the purity of the state is less than one:

$$\text{tr}(\rho'_A)^2 = |\alpha|^4 + |\beta|^4 = (|\alpha|^2 + |\beta|^2)^2 - 2|\alpha|^2|\beta|^2 = 1 - 2|\alpha|^2|\beta|^2 < 1. \tag{125}$$

The qubit experienced decoherence.

This is an insidious problem for a quantum computer.

You can imagine that we do not want the environment to change the state of a qubit, but this issue can be taken care of by redundancy or error correction.

The decoherence problem is more difficult: we do not want the qubit, or the qubits on a circuit, to affect the environment!

Preventing such decoherence becomes harder as the circuit becomes larger.

It is indeed hard to suppress thermal and other couplings to the environment.

It is worth comparing the density matrices ρ_A and ρ'_A.

The former, as you can see, has off-diagonal matrix elements, storing the information about the relative phases of the different components of the wave function.

The latter does not.

Decoherence reduces or deletes the off-diagonal matrix elements of the density matrix in the basis dictated by the coupling to the environment.

Example 8. *From pure to mixed: two coupled spin one-half particles*.

To illustrate some of the above ideas, we consider two spin one-half particles: particle one and particle two, interacting through an *Ising* Hamiltonian:

$$\hat{H} = -\hbar\omega\,\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}, \quad \omega > 0. \tag{126}$$

This interaction tends to align both spins along the *z*-axis, as such a configuration gives a minimum of the energy.

Our focus will be on particle one, and we will treat particle two as the environment.

We will determine the time evolution of the reduced density matrix ρ_1 for particle one.

The result will display how a pure state of particle one evolves into a mixed state.

This evolution is expected because the interaction can turn a nonentangled state of the two particles into an entangled state.

As usual, we assume that at time equal zero the state of the two particles is a pure state.

The most general such state takes the form

$$|\psi_{12}(0)\rangle = \tfrac{1}{2}\left(a_+|\uparrow\uparrow\rangle + a_-|\uparrow\downarrow\rangle + b_+|\downarrow\uparrow\rangle + b_-|\downarrow\downarrow\rangle\right). \tag{127}$$

In here the kets contain two arrows.

The first corresponds to the state of particle one and the second to the state of particle two.

We will use the same convention for bras.

We have introduced a total of four coefficients, $a_\pm$, $b_\pm$, which are complex constants.

The normalization condition reads

$$\tfrac{1}{4}\left(|a_+|^2+|a_-|^2+|b_+|^2+|b_-|^2\right)=1. \tag{128}$$

For arbitrary coefficients the two particles are entangled at $t=0$, and the state of particle one is not pure.

The density matrix ρ_{12} of the whole system at $t=0$ is

$$\rho_{12}(0)=\tfrac{1}{4}\left(a_+|\uparrow\uparrow\rangle+a_-|\uparrow\downarrow\rangle+b_+|\downarrow\uparrow\rangle+b_-|\downarrow\downarrow\rangle\right)$$
$$\cdot\left(a_+^*\langle\uparrow\uparrow|+a_-^*\langle\uparrow\downarrow|+b_+^*\langle\downarrow\uparrow|+b_-^*\langle\downarrow\downarrow|\right). \tag{129}$$

The evolution operator $\mathcal{U}(t)=\exp(-i\hat{H}t/\hbar)$ is given by

$$\mathcal{U}=e^{i\omega t\,\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}},\quad \mathcal{U}^\dagger=e^{-i\omega t\,\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}}. \tag{130}$$

We then have $\rho_{12}(t)=\mathcal{U}\rho_{12}(0)\mathcal{U}^\dagger$, resulting in

$$\rho_{12}(t)=\tfrac{1}{4}\left(a_+e^{i\omega t}|\uparrow\uparrow\rangle+a_-e^{-i\omega t}|\uparrow\downarrow\rangle+b_+e^{-i\omega t}|\downarrow\uparrow\rangle+b_-e^{i\omega t}|\downarrow\downarrow\rangle\right)$$
$$\cdot\left(a_+^*e^{-i\omega t}\langle\uparrow\uparrow|+a_-^*e^{i\omega t}\langle\uparrow\downarrow|+b_+^*e^{i\omega t}\langle\downarrow\uparrow|+b_-^*e^{-i\omega t}\langle\downarrow\downarrow|\right). \tag{131}$$

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

$$\rho_1(t)=\mathrm{tr}_2\rho_{12}(t)=\tfrac{1}{4}\left(|a_+|^2+|a_-|^2\right)|\uparrow\rangle\langle\uparrow|$$
$$+\tfrac{1}{4}\left(a_+b_+^*e^{2i\omega t}+a_-b_-^*e^{-2i\omega t}\right)|\uparrow\rangle\langle\downarrow|$$
$$+\tfrac{1}{4}\left(a_+^*b_+e^{-2i\omega t}+a_-^*b_-e^{2i\omega t}\right)|\downarrow\rangle\langle\uparrow|$$
$$+\tfrac{1}{4}\left(|b_+|^2+|b_-|^2\right)|\downarrow\rangle\langle\downarrow|. \tag{132}$$

This is the general answer and can be applied to any initial condition.

Let us consider the case when $a_+ = a_- = b_+ = b_- = 1$, consistent with normalization.

Then the initial state is

$$|\psi_{12}(0)\rangle = \tfrac{1}{2}\left(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle\right)$$

$$= \tfrac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \otimes \tfrac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \tag{133}$$

$$= |x; +\rangle \otimes |x; +\rangle.$$

The two particles are not entangled at $t = 0$.

The density matrix for the first particle can be obtained from Eq. (122):

$$\rho_1(t) = \tfrac{1}{2}|\uparrow\rangle\langle\uparrow| + \tfrac{1}{2}\cos 2\omega t \left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right) + \tfrac{1}{2}|\downarrow\rangle\langle\downarrow|. \tag{134}$$

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.

But as time increases, the states became entangled, and the first particle experiences decoherence: its density matrix becomes that of a mixed state.

This is manifest at any time t^* when $\cos 2\omega t^* = 0$, making the off-diagonal terms of ρ_1 vanish.

At any such t^*, the state of the first particle is maximally mixed, and the density matrix is proportional to the identity matrix.

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

A short calculation gives

$$\mathrm{tr}\rho_1^2 = 1 - \tfrac{1}{2}\sin^2 2\omega t \le 1. \tag{135}$$

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 $\sin 2\omega t = 0$.

In this simple system, there is oscillatory behavior.

While an initially pure state decoheres, it becomes pure again at a later time.

A model of decoherence can be built by coupling the spin one-half particle we focus on — call it particle A — to all of the particles in a set of N interacting spin one-half particles.

For large N and for random couplings among the N particles, one would expect the dynamics to turn a pure, unentangled state of A into a maximally mixed state.

Decoherence would set in.

A Theory of Measurement?

Most textbooks follow the Copenhagen interpretation of quantum mechanics, largely devised by Niels Bohr and Werner Heisenberg from 1925 to 1927.

As we noted while discussing the axioms of quantum mechanics earlier, states evolve unitarily according to the (the time-development operator (or equivalently, the Schrödinger equation), except at measurements.

Measurements determine the values of observables, which are Hermitian operators.

For any observable $\mathcal{O}$, its eigenvalues are the possible results of measurements.

When we measure $\mathcal{O}$, the state collapses instantaneously into an $\mathcal{O}$ eigenstate, and the result of the measurement is the $\mathcal{O}$ eigenvalue of the eigenstate.

The various possible results of the measurement appear with probabilities governed by Born's rule.

We assume that for any Hermitian operator $\mathcal{O}$ there is some measuring device or apparatus, constructed with suitable ingenuity, that can carry out the measurement.

Moreover, the result of each measurement, while not predictable, is one of the eigenvalues, exactly.

One can elaborate on the idea of measurement, stating that one can measure along any orthonormal basis set of states in the state space, and one can also do partial measurements on a subsystem that is entangled with the rest of the quantum system.

Some questions arise, however, when one tries to understand the workings of the measurement apparatus and what happens during measurement such that, somehow, unitary evolution fails to hold.

These questions have stimulated much work, but surprisingly, no clear answers emerged for a long period of time.

In the "orthodox" Copenhagen interpretation, at least as explained by Bohr and Heisenberg, the measuring devices are classical, and thus classical physics has an inescapable role in quantum mechanics.

Landau and Lifshitz (1977), in their quantum mechanics monograph, also emphasize the need for a classical domain where the results of experiments are recorded and analyzed.

Some physicists speak of a "Heisenberg cut," a dividing line between a quantum domain and a classical domain.

Nowadays the perspective has changed somewhat.

Most physicists agree quantum mechanics should hold for all scales, and therefore there is no "cut" between a microscopic domain where quantum mechanics applies and a macroscopic domain where classical physics applies.

We believe that classical physics is what quantum physics looks like, to a good approximation, for wide classes of macroscopic systems.

Some large systems, however, can exhibit quantum, and thus nonclassical, behavior.

This perspective is supported by experiments in which larger and larger *mesoscopic* systems have been shown to exhibit quantum behavior.

SQUIDS, for example, are devices which support quantum superpositions of oppositely circulating currents, each with a billion electrons!

We will discuss below a plausible picture of measurement suggested by ideas of decoherence.

Before going into this, let us consider more explicitly how certain devices do measurements.

Measurements and collapse of the wave function

In the following we discuss measurements, paying particular attention to the moment when, within the Copenhagen interpretation, the wave function(quantum probability amplitude) collapses.

A simple example of measurement is provided by the detection of a single photon.

This can be done by a photomultiplier tube.

A single photon comes into the device and hits a photocathode, a surface with a thin conducting layer.

The photon then ejects an electron from a metal surface via the photoelectric effect.

The electron is directed by the focusing electrode toward the electron multiplier, a collection of metal plates where further electrons are released in a cascading effect.

This is a process of amplification, where the original photon to be detected eventually ends up producing a macroscopic electric current that is easily measured in the domain of classical electromagnetism.

The wave function of the photon, originally extending over a possibly large spatial domain, collapses, and the photon is found localized at the photodetector.

A similar principle is used to build a screen where we can detect the position of many incident photons, in this way creating an image.

Such a screen can use charge-coupled devices (CCDs).

The pixels on the screen are represented by capacitors constructed as doped metal-oxide semiconductors (MOS).

These capacitors transform an incoming photon into a macroscopic electric charge at the metal-oxide interface.

The data from these charges can then be read out and irreversibly placed in the classical domain, usually in digitized form.

We can also use photons to illustrate measurement along a basis.

For this purpose, consider a calcite crystal exhibiting birefringence: the index of refraction depends on the polarization and direction of the light beam.

The outputs of a suitably prepared crystal will then be two possible polarization states that we can call an $|H\rangle$-output, for horizontal polarization, and a $|V\rangle$-output, for vertical polarization (figure 1).
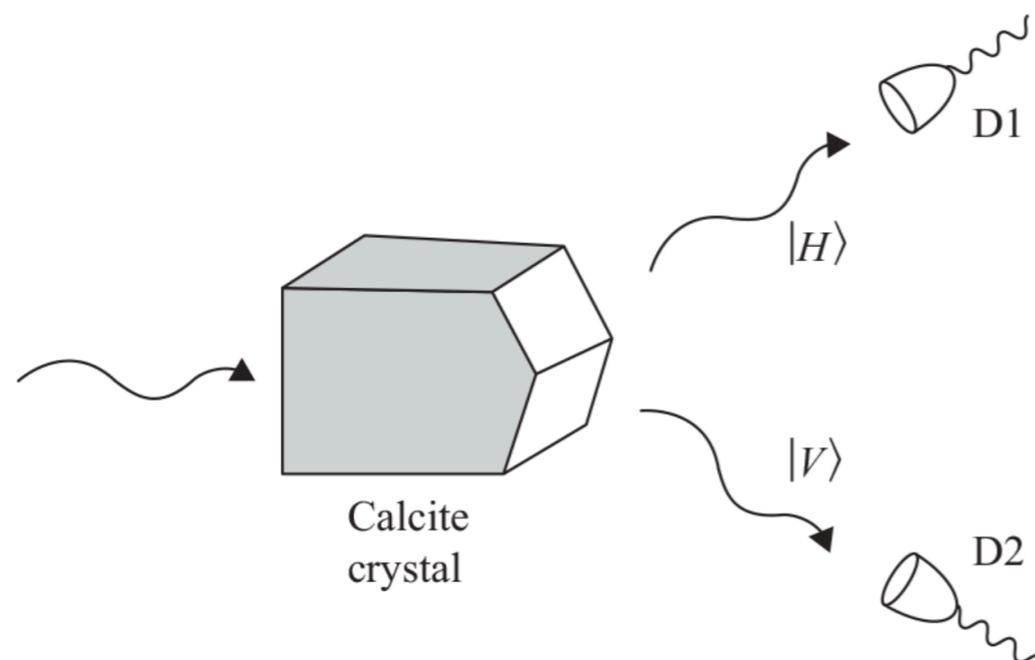
Figure 1

Measuring a photon along a basis of polarization states with a birefringent calcite crystal.

The incoming photon emerges from the crystal in a superposition of $|H\rangle$ and $|V\rangle$ states, for horizontal and vertical polarizations.

The photodetectors complete the measurement, forcing the photon wave function to collapse into a polarization state.

These are the basis states of the photon we are measuring along, with the help of the calcite crystal.

The crystal alone *does not* complete the measurement, however.

Suppose we send in a photon polarized at $45°$ relative to the $|H\rangle$ and $|V\rangle$ axes.

After hitting the calcite crystal, the photon will have some amplitude to emerge on $|H\rangle$ and some amplitude to emerge on $|V\rangle$.

The photon is now in a superposition of the two possible output states, and unitary evolution still holds.

The measurement can be completed by placing two photodetectors, one at each of the two outputs.

This forces the collapse of the wave function of the photon, and the photon is found in either the H photodetector, thus in the $|H\rangle$ state, or in the V photodetector, in the $|V\rangle$ state.

If you recall the Stern-Gerlach apparatus, the situation is in fact completely analogous: a spin one-half particle subject to a magnetic field gradient along z prepares the state in a superposition of up and down states, $|\uparrow\rangle$ and $|\downarrow\rangle$, appearing at the separate outputs of the apparatus.

The measurement is only **finalized** by having a screen placed at the outputs that records irreversibly the position of the detected particle, telling us which output the particle came from and thus its spin state.

An even simpler example, again with photons, is provided by a beam splitter, a device we discussed in the context of the Mach-Zehnder interferometer.

For an incident photon, a beam splitter puts the photon in the superposition state of two beams propagating in different directions.

Only after we put photodetectors on the paths does the wave function collapse, and the photon is detected in one and only one of the detectors.

We have often talked about measuring momentum.

One way to measure the momentum of a charged particle is to place it inside a uniform magnetic field, orthogonal to the velocity of the particle.

The particle will then move in a circle whose radius can be determined and used to calculate the value of the momentum.

If the particle is in a superposition state of various momenta, the introduction of the magnetic field will simply put the particle in a superposition of circular orbits of various radii.

The measurement has not happened yet.

If we now put a collection of detectors at locations corresponding to various radii (see figure 2), we will force the collapse of the wave function, and the particle will be observed at one of the detectors, again by some amplification effect.

This will tell us the radius of the orbit state the particle collapsed into and thus the value of the momentum the particle collapsed into, due to the measurement.
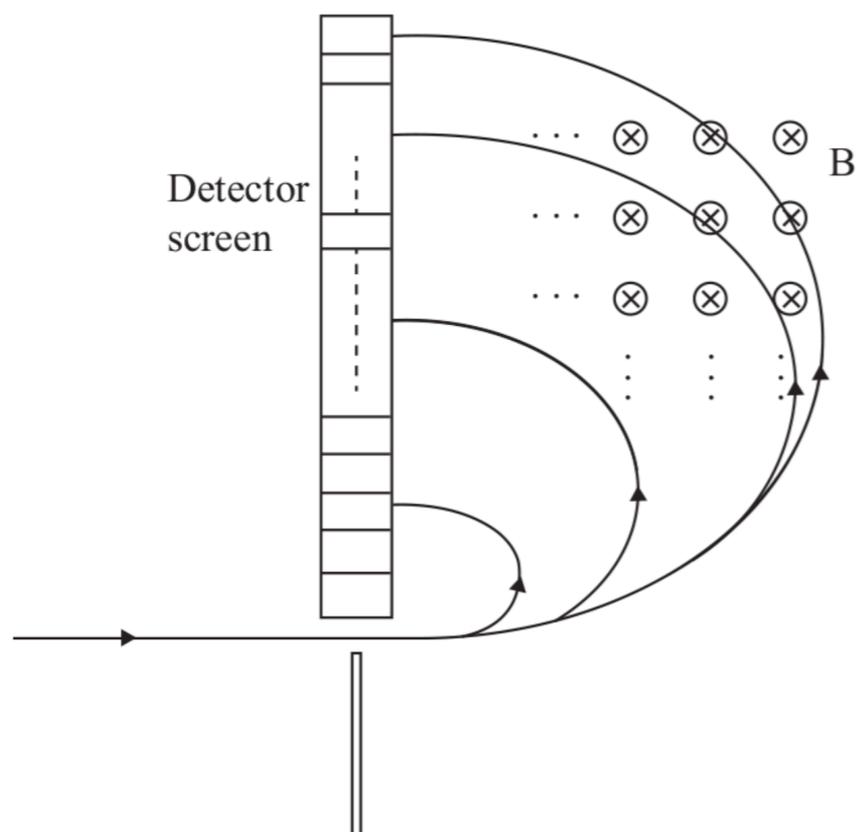
Figure 2

Measuring the momentum of a charged particle in a superposition of momentum eigenstates.

A magnetic field places the particle in a superposition of circular trajectories of various radii.

The detectors at the screen complete the measurement.

In all of the above measurements, the collapse happens by detection, in which a quantum state is amplified into a macroscopic signal that is well understood classically.

The above measurements do not display one aspect of idealized measurements: if we measure an observable $\mathcal{O}$ and we find an eigenstate, an immediate repeated measurement of $\mathcal{O}$ should give the *same* eigenstate.

Photon detection destroys the photon, preventing a repeated measurement.

When we measure the momentum of a particle, as explained above, the process leaves us without the particle.

Indeed, most measurements in quantum chemistry, quantum optics, and elementary particle physics involve single systems perturbed or destroyed by the measurement.

More delicate measurements must be designed in order to have wave function collapse while preserving the quantum state.

Quantum **nondemolition measurements** are a class of measurements in which the integrity of the quantum state is preserved.

They arise in the context of gravitational wave detection where small quantum mechanical amplitudes of the oscillation of large objects must be measured over and over with minimal perturbation to the quantum state.

The interaction-free measurements are an extreme example.

They show that it is possible to gain some information about a system, in this case the presence or absence of a detector, without having any interaction with the system.

Striking examples of quantum nondemolition measurements have been achieved using Rydberg atoms and resonant cavities.

The field, pioneered by Serge Haroche (Nobel Prize in Physics, 2012), is called cavity quantum electrodynamics.

Highly excited Rydberg atoms are useful because their energy levels are closely spaced, allowing transitions that emit or absorb photons with macroscopic wavelengths.

With a properly tuned cavity, one can produce atom-cavity oscillations in which a single atom, in an excited state, emits a photon that spends a little time in the cavity before being reabsorbed by the atom, which goes back to its original excited state to start the oscillation again.

The interactions of a moving Rydberg atom with photons within the cavity results in a tiny force felt by the atom.

The addition of more photons enhances this force, allowing for a remarkable measurement.

It becomes possible to infer the number of photons inside the cavity by measuring the time that an atom with known initial velocity takes to cross the cavity!

Before the atom goes in, the number of photons in the cavity is ambiguous, the cavity being in a quantum superposition of states with different numbers of photons.

At the moment the experimenter detects the outgoing Rydberg atom, the wave function of the cavity collapses to a state with a definite number of photons.

This is an ideal measurement!

Any subsequent Rydberg atom sent in to measure the number of photons will find the same value.

If the experiment is repeated, starting each time with the original field in the cavity, the statistics of the photon number distribution can be determined.

Premeasurement with a quantum apparatus

If quantum mechanics is the theory of the world at all scales, it is natural to try to understand the measurement process as a quantum interaction between a quantum system $\mathcal{S}$ and a quantum apparatus $\mathcal{A}$.

In our discussion of measurement above, the measuring apparatus combines a quantum element with an amplification that turns the signal into the classical domain.

In order to represent a purely quantum apparatus, we will consider a device with **pointer states**, states of a moving pointer that determine the value of the measurement.

Let the system $\mathcal{S}$ to be measured have an observable $\mathcal{O}_{\mathcal{S}}$ with eigenvectors $|s_i\rangle$ whose eigenvalues are s_i:

$$\mathcal{O}_{\mathcal{S}}|s_i\rangle = s_i|s_i\rangle, \quad i = 1, \ldots, n. \tag{135}$$

Here, we assume that i is an index that runs over a finite set of values.

Let us view the apparatus $\mathcal{A}$ as quantum.

We then have an observable $\mathcal{O}_{\mathcal{A}}$ acting on the state space of the apparatus with eigenstates $|a_i\rangle$, where a_i is the eigenvalue of $|a_i\rangle$:

$$\mathcal{O}_{\mathcal{A}}|a_j\rangle = a_j|a_j\rangle, \quad j = 1, \ldots, m, \ m \geq n. \tag{136}$$

The states $|a_j\rangle$ are pointer states that can be identified with the results of a measurement $\mathcal{O}_{\mathcal{A}}$ is designed to produce.

The idea is that we have a correspondence between the eigenstates of $\mathcal{O}_{\mathcal{S}}$ and those of $\mathcal{O}_{\mathcal{A}}$:

$$|s_j\rangle \longleftrightarrow |a_j\rangle. \tag{137}$$

We aim to arrange it so that when the system is in $|s_j\rangle$ and interacts with the apparatus, the pointer state becomes $|a_j\rangle$.

The pointer state tells us the value s_j of the system observable.

This is why one must assume $m \geq n$: the apparatus must have at least as many states as the system in order to be able to carry out a measurement.

Suppose that at $t = 0$ the system is in the state

$$|\psi(0)\rangle_S = \sum_{i=1}^{n} c_i|s_i\rangle, \tag{138}$$

a superposition of $\mathcal{O}_A$ eigenstates.

At time equal zero we can imagine the apparatus $\mathcal{A}$ in some definite state $|\phi(0)\rangle_A$ so that the complete state of the system and apparatus is

$$|\psi(0)\rangle_{SA} = \left(\sum_{i=1}^{n} c_i|s_i\rangle\right) \otimes |\varphi(0)\rangle_A. \tag{139}$$

At $t = 0$, an interaction between the system and the apparatus turns on; this interaction is governed by some Hamiltonian $\hat{H}_{SA}$.

The Hamiltonian is suitably designed such that the *premeasurement* that follows is carried out by time $t = \tau > 0$, for some value of τ.

The requirement is that at time τ the state of the combined system and apparatus becomes

$$|\psi(\tau)\rangle_{SA} = \sum_{i=1}^{n} c_i e^{\phi_i}|s_i\rangle \otimes |a_i\rangle, \tag{140}$$

where the ϕ_i are arbitrary phases.

The interaction has established the desired entanglement between the system $\mathcal{S}$ and the apparatus $\mathcal{A}$.

We call this premeasurement because the state of the whole system $\mathcal{SA}$ is still pure but is now a superposition of terms in which the $\mathcal{O}_\mathcal{S}$ and $\mathcal{O}_\mathcal{A}$ eigenstates are properly correlated.

There has been no wave function collapse, and therefore the measurement has not yet happened.

We can quickly illustrate that this kind of correlation is relatively easy to achieve.

Assume that both the system $\mathcal{S}$ and the apparatus $\mathcal{A}$ are two-level systems, so both can be described in the language of spin states.

We will take

$$\mathcal{O}_S = \sigma_z^S, \qquad \mathcal{O}_\mathcal{A} = \sigma_z^\mathcal{A}, \tag{141}$$

where the superscripts on the Pauli matrices tell us if we are dealing with the system or with the apparatus.

Let us also assume that the Hamiltonian $\hat{H}_{\mathcal{SA}}$ coupling S to $\mathcal{A}$ is

$$\hat{H}_{\mathcal{SA}} = \tfrac{1}{2}\hbar\omega(1 + \sigma_z^S) \otimes \sigma_x^\mathcal{A}, \tag{142}$$

with $\omega > 0$ a constant frequency.

Let the initial state of the system plus apparatus be

$$|\psi(0)\rangle_{\mathcal{SA}} = \left(c_+|+\rangle_S + c_-|-\rangle_S\right) \otimes |-\rangle_\mathcal{A}. \tag{143}$$

As indicated, at $t = 0$ the system is in a superposition of the two basis states $| \pm \rangle$ along the z-axis, while the apparatus is in a single state.

For the apparatus, it is convenient to work with σ_x eigenstates so that the Hamiltonian is diagonal.

Using $|-\rangle = \frac{1}{\sqrt{2}}(|x; +\rangle - |x; -\rangle)$ for the first term in the above wave function, we see that

$$|\psi(0)\rangle_{SA} = \frac{1}{\sqrt{2}}c_+|+\rangle_S \otimes (|x; +\rangle_A - |x; -\rangle_A) + c_-|-\rangle_S \otimes |-\rangle_A. \tag{144}$$

The unitary operator $\mathcal{U}$ that implements time evolution is

$$\mathcal{U}(t) = \exp(-i\hat{H}_{SA}t/\hbar) = \exp\left(-\tfrac{1}{2}i\omega t(1 + \sigma_z^S) \otimes \sigma_x^A)\right). \tag{145}$$

Note that

$$\mathcal{U}(t)|-\rangle_S \otimes |-\rangle_A = |-\rangle_S \otimes |-\rangle_A,$$

$$\mathcal{U}(t)|+\rangle_S \otimes |x; \pm\rangle_A = e^{\mp i\omega t}|+\rangle_S \otimes |x; \pm\rangle_A. \tag{146}$$

The time-evolved state is therefore

$$|\psi(t)\rangle_{SA} = \frac{1}{\sqrt{2}}c_+|+\rangle_S \otimes (e^{-i\omega t}|x; +\rangle_A - e^{i\omega t}|x; -\rangle_A) + c_-|-\rangle_S \otimes |-\rangle_A. \tag{147}$$

Passing back to the $| \pm \rangle$ basis for the apparatus, a short computation now gives

$$|\psi(t)\rangle_{SA} = -i(\sin \omega t)\,c_+|+\rangle_S \otimes |+\rangle_A + (\cos \omega t)c_+|+\rangle_S \otimes |-\rangle_A + c_-|-\rangle_S \otimes |-\rangle_A. \tag{148}$$

If we choose a time $t*$ such that $\omega t* = \pi/2$, then the second term vanishes, and we get

$$|\psi(t_*)\rangle_{SA} = = -i\,c_+|+\rangle_S \otimes |+\rangle_A + c_-|-\rangle_S \otimes |-\rangle_A. \tag{149}$$

This is of the form Eq. (140); the system and apparatus observables are correlated nicely, as we wanted to demonstrate.

This discussion so far follows the early work of von Neumann on measurement.

For him the apparatus is a large system, and along the lines we discussed, a correlation between the system $\mathcal{S}$ and the apparatus is established.

Von Neumann took the viewpoint that the large quantum system is "classical" and that the value of the apparatus observable can be read out as a classical variable.

Still, the mystery of collapse has not been resolved.

We get a picture of how a quantum system can interact with a quantum measuring device in a useful way, but the total system is still in a quantum superposition.

Measurement and decoherence

It seems clear that if we keep using the unitary evolution of quantum mechanics applied to a system, we are not going to see wave function collapse.

A picture that seems plausible in motivating the origin of probabilities, without speaking about collapse, uses the environment and decoherence.

Recall that we saw that for an open system time evolution is not unitary.

The idea in the picture we describe now is to establish that the density matrix of the open system $\mathcal{SA}$ describes an ensemble with probabilistic interpretation.

In realistic conditions, $\mathcal{S}$ and a macroscopic $\mathcal{A}$ are always in contact with the environment $\mathcal{E}$.

Interactions with $\mathcal{E}$ cause further entanglement, and in reality we have a state $|\psi\rangle_{\mathcal{SAE}}$ that takes the form

$$|\psi\rangle_{SAE} = \sum_i c_i |s_i\rangle \otimes |a_i\rangle \otimes |\mathcal{E}_i\rangle, \tag{150}$$

where $|\mathcal{E}_i\rangle$ are states of the environment $\mathcal{E}$.

We can now form the density matrix ρ_{SA} for SA by tracing over the environment:

$$\rho_{SA} = \mathrm{tr}_{\mathcal{E}}\, \rho_{SAE} = \mathrm{tr}_{\mathcal{E}}\, |\psi\rangle_{SAE}\langle\psi|_{SAE}$$

$$= \mathrm{tr}_{\mathcal{E}} \sum_{i,j=1}^{n} c_i c_j^* |s_i\rangle |a_i\rangle |\mathcal{E}_i\rangle \, \langle s_j| \langle a_j| \langle \mathcal{E}_j| \tag{151}$$

$$= \sum_{i,j=1}^{n} c_i c_j^* \langle \mathcal{E}_j | \mathcal{E}_i\rangle \, |s_i\rangle |a_i\rangle \langle s_j| \langle a_j|.$$

Given that the environment is described by a Hilbert space of extremely high dimensionality, it seems plausible that $\langle \mathcal{E}_j | \mathcal{E}_i\rangle \sim \delta_{ij}$: any two generic states of the environment are likely to have very small overlap.

But perhaps something more subtle is going on, and the "pointer" states $|a_i\rangle$ are such that they naturally get entangled with orthogonal states of the environment.

At any rate, under the assumption $\langle \mathcal{E}_j | \mathcal{E}_i\rangle = \delta_{ij}$ we see that

$$\rho_{SA} = \sum_{i=1}^{n} |c_i|^2 \cdot |s_i\rangle |a_i\rangle \langle s_i| \langle a_i|. \tag{152}$$

An observer focused on $\mathcal{SA}$ thus observes a density matrix, which can be interpreted as arising from the ensemble

$$E = \left\{ \left(|c_1|^2 |s_1\rangle |a_1\rangle \right), \ldots, \left(|c_n|^2 |s_n\rangle |a_n\rangle \right) \right\}. \tag{153}$$

In the ensemble there is a probability $|c_i|^2$ of finding the state $|s_i\rangle |a_i\rangle$ in which the pointer state is consistent with the state of the system.

One has to claim now that these are the states one observes when looking at $\mathcal{SA}$ after the measurement.

This kind of argument also suggests that we can never achieve a superposition of a cat-alive and a cat-dead state, as in the example proposed by Schrödinger:

$$\frac{1}{\sqrt{2}} \left(|\text{cat-alive}\rangle + |\text{cat-dead}\rangle \right). \tag{154}$$

In such a state, the cat is neither dead nor alive.

But certainly there is also an environment, and you could argue that at some time we have the state

$$\frac{1}{\sqrt{2}} \left(|\text{cat-alive}\rangle + |\text{cat-dead}\rangle \right) \otimes |\mathcal{E}_0\rangle. \tag{155}$$

But this situation is untenable: the cat, dead or alive, is interacting with the environment, even if contained in a box.

A living cat is breathing air.

A dead cat is lukewarm and still emits and absorbs blackbody photons.

The interactions imply that, almost instantaneously, the above state becomes

$$\frac{1}{\sqrt{2}} \left(|\text{cat-alive}\rangle \otimes |\mathcal{E}_1\rangle + |\text{cat-dead}\rangle \otimes |\mathcal{E}_2\rangle \right), \tag{156}$$

with two environment states $|\mathcal{E}_1\rangle$ and $|\mathcal{E}_2\rangle$ that are to great accuracy orthogonal: $\langle \mathcal{E}_1 | \mathcal{E}_2 \rangle \simeq 0$

As in the discussion above, if we trace over the environment, the result is then a density matrix ρ_{cat} given by

$$\rho_{\text{cat}} = \tfrac{1}{2}|\text{cat-alive}\rangle\langle\text{cat-alive}| + \tfrac{1}{2}|\text{cat-dead}\rangle\langle\text{cat-dead}| \tag{157}$$

that describes an ensemble of "cat systems" in which half of the cats are alive and half are dead.

We cannot observe any subtle superposition.

The above arguments leave a number of open questions.

We could get ensembles different from Eq. (153) if the coupling to the environment in Eq. (150) were different; for example, if each environment state were to couple to linear combinations of pointer states.

Additionally, the interpretation of the density matrix as an ensemble is not unique: we have seen that an unpolarized spin can be prepared with ensembles in infinitely many different ways.

In here, the resulting expression for the density matrix is taken as uniquely selected.

Common sense suggests that now is a good time to recommend the interested reader follow the current literature for further insight.