Chapter 3: Quantum Entanglement

They don't think it be like it is,
but it do.

Oscar Gamble

3.1. QUANTUM STATES OF MULTI-PARTICLE SYSTEMS

So far, we have studied quantum mechanical systems consisting of single particles; the next important step is to consider systems of multiple particles. As we shall see, applying the postulates of quantum mechanics to multi-particle systems leads to many important and counterintuitive phenomena, such as **quantum entanglement**.

3.1.1. Tensor products

Suppose we have two quantum objects, A and B. According to quantum mechanics, A is associated with some Hilbert space $\mathscr{H}_A$ (i.e., every state of A is a vector in that space), and B is similarly associated with a Hilbert space $\mathscr{H}_B$. The two spaces $\mathscr{H}_A$ and $\mathscr{H}_B$ may be mathematically distinct; for example, they may have different dimensions. Obviously, the combined system of A and B should also be describable by quantum mechanics. What is its Hilbert space?

In linear algebra, there is an concept called the **tensor product** that happens to be exactly what we need. Given $|a\rangle \in \mathscr{H}_A$ and $|b\rangle \in \mathscr{H}_B$, consider an ordered pair of these two vectors, which we call "the tensor product of $|a\rangle$ and $|b\rangle$". We denote this by

$$|a\rangle \otimes |b\rangle.$$

Note that this is an *ordered* pair, i.e., $|a\rangle \otimes |b\rangle$ and $|b\rangle \otimes |a\rangle$ are not identical.

It turns out that tensor products can act as vectors: we can form linear combinations by adding them to each other and/or multiplying them by scalars (complex numbers). These vector operations are compatible with the original vector operations for $\mathscr{H}_A$ and $\mathscr{H}_B$, in the sense that they obey the "factorization rules"

$$\Big(\lambda|a\rangle + \lambda'|a'\rangle\Big) \otimes |b\rangle = \lambda|a\rangle \otimes |b\rangle \;+\; \lambda'|a'\rangle \otimes |b\rangle, \tag{3.1}$$

$$|a\rangle \otimes \Big(\lambda|b\rangle + \lambda'|b'\rangle\Big) = \lambda|a\rangle \otimes |b\rangle \;+\; \lambda'|a\rangle \otimes |b'\rangle. \tag{3.2}$$

(Note that the expressions inside the parentheses are vector operations in $\mathscr{H}_A$ and $\mathscr{H}_B$ respectively.) These are reminiscent of the rules of algebra, with $\otimes$ acting like multiplication, except that $|a\rangle \otimes |b\rangle$ is not considered equivalent to $|b\rangle \otimes |a\rangle$.

We will be dealing with tensor products a lot, and it can be cumbersome to keep writing the $\otimes$. For convenience, it is customary to omit the $\otimes$ in bra-ket notation:

$$|a\rangle \otimes |b\rangle \;\;\equiv\;\; |a\rangle|b\rangle. \tag{3.3}$$

But even as we write the tensor product this way, as a "product of two kets", the ordering remains important. The left slot is implicitly understood to contain the A-type ket, while the right slot contains the B-type ket.

The space of all tensor products, *and linear combinations thereof*, forms a Hilbert space. We call this the **tensor product space** of $\mathscr{H}_A$ and $\mathscr{H}_B$, which is denoted by

$$\mathscr{H}_A \otimes \mathscr{H}_B.$$

(For denoting tensor product spaces, we will not omit the $\otimes$ symbol.) The tensor product thus provides a natural way to combine two Hilbert spaces into a larger Hilbert space.

As an example, let A and B be distinct spin-1/2 degrees of freedom, so that $\mathscr{H}_A = \mathscr{H}_B = \mathbb{C}^2$ (the space of two-component complex vectors). For each spin-1/2 subsystem, we can adopt the orthonormal basis

$$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \tag{3.4}$$

representing (e.g.) a spin-up and spin-down state respectively. From these, we can construct four ordered pairs, $|\uparrow\rangle|\uparrow\rangle$, $|\uparrow\rangle|\downarrow\rangle$, $|\downarrow\rangle|\uparrow\rangle$, and $|\downarrow\rangle|\downarrow\rangle$, each of which can be interpreted as a state of the combined system of A and B; for instance, $|\uparrow\rangle|\downarrow\rangle$ represents a situation in which A has spin up and B has spin down. We assign to them the representation

$$\begin{aligned} |\uparrow\rangle|\uparrow\rangle &= \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad |\uparrow\rangle|\downarrow\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \\ |\downarrow\rangle|\uparrow\rangle &= \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad |\downarrow\rangle|\downarrow\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}. \end{aligned} \tag{3.5}$$

These constitute a basis for $\mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^4$, which serves as the state space for the combined system. Given any two vectors for A and B,

$$|a\rangle = a_1|\uparrow\rangle + a_2|\downarrow\rangle = \begin{pmatrix}a_1\\a_2\end{pmatrix} \in \mathbb{C}^2, \tag{3.6}$$

$$|b\rangle = b_1|\uparrow\rangle + b_2|\downarrow\rangle = \begin{pmatrix}b_1\\b_2\end{pmatrix} \in \mathbb{C}^2, \tag{3.7}$$

the factorization rules (3.1)–(3.2) imply that their tensor product is

$$|a\rangle|b\rangle = a_1b_1|\uparrow\rangle|\uparrow\rangle + a_1b_2|\uparrow\rangle|\downarrow\rangle + a_2b_1|\downarrow\rangle|\uparrow\rangle + a_2b_2|\downarrow\rangle|\downarrow\rangle = \begin{pmatrix}a_1b_1\\a_1b_2\\a_2b_1\\a_2b_2\end{pmatrix}. \tag{3.8}$$

Conversely, we can take Eq. (3.8) as the definition of the tensor product, which is consistent with the basis (3.5), and use it to derive the factorization rules (3.1)–(3.2). For instance,

$$\left[\begin{pmatrix}a_1\\a_2\end{pmatrix}+\begin{pmatrix}a_1'\\a_2'\end{pmatrix}\right]\otimes\begin{pmatrix}b_1\\b_2\end{pmatrix}=\begin{pmatrix}(a_1+a_1')b_1\\(a_1+a_1')b_2\\(a_2+a_2')b_1\\(a_2+a_2')b_2\end{pmatrix} \tag{3.9}$$

$$=\begin{pmatrix}a_1b_1\\a_1b_2\\a_2b_1\\a_2b_2\end{pmatrix}+\begin{pmatrix}a_1'b_1\\a_1'b_2\\a_2'b_1\\a_2'b_2\end{pmatrix} \tag{3.10}$$

$$=\begin{pmatrix}a_1\\a_2\end{pmatrix}\otimes\begin{pmatrix}b_1\\b_2\end{pmatrix}+\begin{pmatrix}a_1'\\a_2'\end{pmatrix}\otimes\begin{pmatrix}b_1\\b_2\end{pmatrix}. \tag{3.11}$$

The dual (or “bra”) of a tensor product $|a\rangle|b\rangle$ is denoted by $\langle a|\langle b|$. Note that taking the dual retains the ordering of the tensor product: the bra for A goes in the left slot, and the bra for B goes in the right slot. From Eq. (3.8), the dual of a $\mathbb{C}^2\otimes\mathbb{C}^2$ tensor product ket is

$$\langle a|\langle b| = \begin{pmatrix}a_1^*b_1^* & a_1^*b_2^* & a_2^*b_1^* & a_2^*b_2^*\end{pmatrix}. \tag{3.12}$$

Hence, the inner product between two tensor products is

$$\begin{aligned}\Big(\langle a|\langle b|\Big)\Big(|a'\rangle|b'\rangle\Big) &= \begin{pmatrix}a_1^*b_1^* & a_1^*b_2^* & a_2^*b_1^* & a_2^*b_2^*\end{pmatrix}\begin{pmatrix}a_1'b_1'\\a_1'b_2'\\a_2'b_1'\\a_2'b_2'\end{pmatrix}\\ &= (a_1^*a_1'+a_2^*a_2')(b_1^*b_1'+b_2^*b_2')\\ &= \langle a|a'\rangle\,\langle b|b'\rangle.\end{aligned} \tag{3.13}$$

The operation is performed “slot by slot”, by taking the inner products of the A-type and B-type vectors, and multiplying the results together. This is also consistent with the assumption that the four basis states in (3.5) form an orthonormal set.

The key features of the above example generalize to more complicated tensor products. Suppose the two subsystems A and B have orthonormal bases denoted as follows:

$$\Big\{|\alpha\rangle\Big\}\;\;\text{is a basis for}\;\;\mathscr{H}_A,\;\;\text{where}\;\;\alpha=1,2,\dots,\dim(\mathscr{H}_A) \tag{3.14}$$

$$\Big\{|\beta\rangle\Big\}\;\;\text{is a basis for}\;\;\mathscr{H}_B,\;\;\text{where}\;\;\beta=1,2,\dots,\dim(\mathscr{H}_B). \tag{3.15}$$

Note that the two bases may have different sizes (i.e., $\mathscr{H}_A$ and $\mathscr{H}_B$ may have different dimensions). Following the same reasoning as in the preceding example, we can set up a tensor product operation that obeys the factorization rules (3.1)–(3.2), and use (3.14)–(3.15) to construct a basis for the tensor product space:

$$\Big\{|\alpha\rangle|\beta\rangle\Big\}\;\;\text{is a basis for}\;\;\mathscr{H}_A\otimes\mathscr{H}_B,\;\;\text{where}\;\;\left\{\begin{array}{l}\alpha=1,2,\dots,\dim(\mathscr{H}_A),\\ \beta=1,2,\dots,\dim(\mathscr{H}_B).\end{array}\right. \tag{3.16}$$

The basis states are orthonormal:

$$\Big(\langle\alpha|\langle\beta|\Big)\Big(|\alpha'\rangle|\beta'\rangle\Big)=\langle\alpha|\alpha'\rangle\,\langle\beta|\beta'\rangle=\delta_{\alpha\alpha'}\delta_{\beta\beta'}. \tag{3.17}$$

As a corollary, the dimension of the tensor product space is

$$\dim\left[\mathscr{H}_A\otimes\mathscr{H}_B\right]=\dim(\mathscr{H}_A)\,\dim(\mathscr{H}_B). \tag{3.18}$$

3.1.2. Entanglement

The above discussion of tensor product spaces contains an important subtlety. Even though we used tensor products of the form

$$|a\rangle|b\rangle \tag{3.19}$$

to help define the tensor product space, vectors drawn from $\mathscr{H}_A \otimes \mathscr{H}_B$ do not necessarily have this form. This is because $\mathscr{H}_A \otimes \mathscr{H}_B$ contains not only tensor products, but also linear combinations of tensor products. The latter are *not* guaranteed to have the form (3.19).

In quantum mechanics, a tensor product like (3.19) is an obvious and natural way to describe a situation where subsystem A is in state $|a\rangle$, and B is in state $|b\rangle$. For instance, in our previous example of two spin-1/2 subsystems, if A and B are both in the spin-up state, the state of the combined system is

$$|\uparrow\rangle|\uparrow\rangle. \tag{3.20}$$

Similarly, suppose the states of A and B are

$$\begin{aligned} |a\rangle &= |\uparrow\rangle, \\ |b\rangle &= \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle + |\downarrow\rangle\Big). \end{aligned} \tag{3.21}$$

Then the state of the combined system is

$$|a\rangle\,|b\rangle = \frac{1}{\sqrt{2}}\,|\uparrow\rangle\,\Big(|\uparrow\rangle + |\downarrow\rangle\Big) \tag{3.22}$$

But now consider the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle\,|\downarrow\rangle\,-\,|\downarrow\rangle\,|\uparrow\rangle\Big). \tag{3.23}$$

Just like (3.20) and (3.22), this is a valid vector in $\mathscr{H}_A \otimes \mathscr{H}_B = \mathbb{C}^2 \otimes \mathbb{C}^2$. However, it turns out to be impossible to re-write Eq. (3.23) in the form $|a\rangle|b\rangle$! (We will prove this later, in Section 3.7.) In such a situation, A and B do not individually have stand-alone quantum states; only the combined system has a well-defined quantum state, $|\psi\rangle$. We then say A and B are **entangled**. Entanglement leads to many counterintuitive phenomena, which we will explore in the rest of this chapter.

3.1.3. Multiple subsystems

The tensor product concept can be extended to more than two subsystems. Given N subsystems with Hilbert spaces $\mathscr{H}_1, \mathscr{H}_2, \dots, \mathscr{H}_N$, the combined state space is

$$\mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_N, \tag{3.24}$$

which has dimension

$$\dim\left[\mathscr{H}_1 \otimes \cdots \otimes \mathscr{H}_N\right] = \dim\left[\mathscr{H}_1\right] \cdot \dim\left[\mathscr{H}_2\right] \cdots \dim\left[\mathscr{H}_N\right]. \tag{3.25}$$

Note that the dimension scales exponentially with N. For instance, if there are $N = 20$ subsystems each having a 2D Hilbert space, the combined Hilbert space has dimension $2^{20} = 1\,048\,576$. This implies that quantum systems containing only a modest number of particles can carry tremendous amounts of information in their quantum states. This is the primary motivation behind the active research field of quantum computing.

By the way, we assume for now that the subsystems in question are distinguishable. There are other complications arising if the subsystems "identical" particles, which will be the subject of the next chapter. (If you're unsure what this paragraph is talking about, never mind; just read on.)

3.2. PARTIAL MEASUREMENTS

Let us recall how measurements work in basic quantum theory. Each observable Q is described by some Hermitian operator $\hat{Q}$, which has an eigenbasis $\{|q\rangle\}$ such that

$$\hat{Q}|q\rangle = q|q\rangle. \tag{3.26}$$

For simplicity, let the eigenvalues $\{q\}$ be non-degenerate. Let the system initially be in a quantum state $|\psi\rangle$, which can be expanded in terms of the eigenbasis of $\hat{Q}$:

$$|\psi\rangle = \sum_q |q\rangle\psi_q, \;\; \text{where} \;\; \psi_q = \langle q|\psi\rangle. \tag{3.27}$$

The measurement postulate of quantum mechanics states that if we measure Q, then (i) the probability of obtaining each possible outcome q is

$$P(q) = |\psi_q|^2, \tag{3.28}$$

and (ii) upon obtaining this outcome, the system collapses into state $|q\rangle$.

Mathematically, these two rules can be summarized using the projection operator

$$\hat{\Pi}(q) = |q\rangle\langle q|. \tag{3.29}$$

Applying this operator to $|\psi\rangle$ gives the non-normalized state vector

$$|\psi'\rangle = \hat{\Pi}(q)|\psi\rangle = |q\rangle\langle q|\psi\rangle. \tag{3.30}$$

And from $|\psi'\rangle$, we can obtain:

- The probability of obtaining this outcome, which is $P(q) = \langle\psi'|\psi'\rangle = |\langle q|\psi\rangle|^2$.
- The post-measurement state, which is obtained by renormalizing $|\psi'\rangle$ to $|q\rangle$.

For combined systems (e.g., systems of multiple particles), there is a new complication: *what if a measurement is performed on just one subsystem*?

Suppose once again that we have two subsystems A and B, whose combined Hillbert space is $\mathscr{H}_A \otimes \mathscr{H}_B$. Let us perform a measurement on A, corresponding to a Hermitian operator acting upon $\mathscr{H}_A$ whose eigenstates are

$$\{\ |\alpha\rangle\ \}, \quad \text{where } \alpha = 1, 2, \ldots, \dim\left[\mathscr{H}_A\right].$$

To form a basis for $\mathscr{H}_A \otimes \mathscr{H}_B$, let us take tensor products of these A eigenstates with an arbitrary basis for B, denoted by $\{|\beta\rangle\}$. Any state $|\psi\rangle \in \mathscr{H}_A \otimes \mathscr{H}_B$ can be expressed as

$$|\psi\rangle = \sum_{\alpha\beta} \psi_{\alpha\beta}\, |\alpha\rangle|\beta\rangle \tag{3.31}$$

$$= \sum_{\alpha} |\alpha\rangle \underbrace{\left(\sum_{\beta} \psi_{\alpha\beta}\, |\beta\rangle\right)}_{\equiv\, |\varphi_\alpha\rangle}. \tag{3.32}$$

Note that $|\varphi_\alpha\rangle$ lies in $\mathscr{H}_B$; there is one such vector for each choice of α.

Comparing Eq. (3.32) with Eq. (3.27), we see that $|\varphi_\alpha\rangle$ in (3.32) plays a role similar to ψ_q in (3.27), though the former is a vector and the latter is a scalar. Proceeding by analogy with Eq. (3.28), the probability for measurement outcome α should be

$$P(\alpha) = \langle\varphi_\alpha|\varphi_\alpha\rangle = \sum_{\beta} |\psi_{\alpha\beta}|^2. \tag{3.33}$$

To make this prediction more solid, recall how we previously showed that each measurement outcome is associated with a projection operator, Eq. (3.29). For a partial measurement, we can accordingly define the **partial projector**

$$\hat{\Pi}(\alpha) \;=\; |\alpha\rangle\langle\alpha| \otimes \hat{I}. \tag{3.34}$$

The A slot contains the projection operator associated with the measurement outcome α, similar to Eq. (3.29). The B slot contains the identity operator for $\mathscr{H}_B$, indicating that no measurement is being done on B. Applying this partial projector to Eq. (3.32) gives

$$|\psi'\rangle \;=\; \hat{\Pi}(\alpha)\, |\psi\rangle \;=\; |\alpha\rangle|\varphi_\alpha\rangle. \tag{3.35}$$

Then, following the same rules as before, the probability for the α outcome is

$$P(\alpha) = \langle\psi'|\psi'\rangle = \langle\alpha|\alpha\rangle\, \langle\varphi_\alpha|\varphi_\alpha\rangle = \sum_{\beta} |\psi_{\alpha\beta}|^2, \tag{3.36}$$

in agreement with Eq. (3.33). The post-measurement state is found by re-normalizing $|\psi'\rangle$:

$$\frac{1}{\sqrt{\langle\psi'|\psi'\rangle}}|\psi'\rangle = \frac{1}{\sqrt{\sum_{\beta'} |\psi_{\alpha\beta'}|^2}}\, \sum_{\beta} \psi_{\alpha\beta}|\alpha\rangle|\beta\rangle. \tag{3.37}$$

Example—A system of two spin-1/2 particles is in the “singlet state”

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle|\downarrow\rangle \,-\, |\downarrow\rangle|\uparrow\rangle\Big). \tag{3.38}$$

As usual, $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of the spin operator $\hat{S}_z$, corresponding to the eigenvalues $+\hbar/2$ and $-\hbar/2$ respectively.

If we measure S_z on A, what is the probability of each outcome, and the post-measurement state?

- **First outcome:** $+\hbar/2$.
  - The projected state is $|\psi'\rangle = \Big(|\!\uparrow\rangle\langle\uparrow\!| \otimes \hat{I}\Big)\,|\psi\rangle = \dfrac{1}{\sqrt{2}}\,|\!\uparrow\rangle|\!\downarrow\rangle$.
  - The outcome probability is $P(+) = \langle\psi'|\psi'\rangle = \dfrac{1}{2}$.
  - The post-collapse state is $|\!\uparrow\rangle|\!\downarrow\rangle$
- **Second outcome:** $-\hbar/2$.
  - The projected state is $|\psi'\rangle = \Big(|\!\downarrow\rangle\langle\downarrow\!| \otimes \hat{I}\Big)\,|\psi\rangle = -\dfrac{1}{\sqrt{2}}\,|\!\downarrow\rangle|\!\uparrow\rangle$.
  - The outcome probability is $P(-) = \langle\psi'|\psi'\rangle = \dfrac{1}{2}$.
  - The post-collapse state is $|\!\downarrow\rangle|\!\uparrow\rangle$.

The two possible outcomes are equally probable. Either way, the state collapses so that A and B have opposite spins. Note that A and B are not entangled after the collapse.

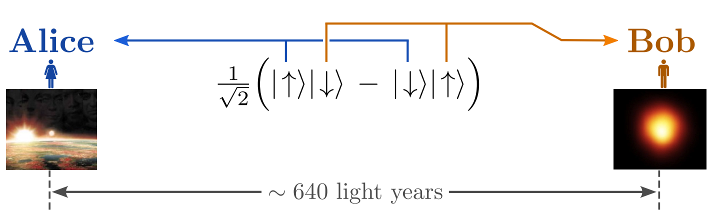
3.3. THE EINSTEIN-PODOLSKY-ROSEN "PARADOX"

In 1935, Einstein, Podolsky, and Rosen (EPR) formulated a thought experiment, now called the **EPR paradox**, highlighting the counter-intuitive features of quantum entanglement [3]. They intended for this to show that quantum theory cannot be a fundamental description of reality. Subsequently, it was shown that the EPR paradox is not an actual paradox—physical systems *really do* behave like the thought experiment! Nowadays, the EPR "paradox" is regarded not as an argument against quantum mechanics, but as an important tool for thinking about quantum entanglement.

Consider, once again, two spin-1/2 particles in the singlet state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|\!\uparrow\rangle|\!\downarrow\rangle \;-\; |\!\downarrow\rangle|\!\uparrow\rangle\Big), \tag{3.39}$$

where subsystems A and B correspond to the left and right slots of the tensor product respectively. We could prepare the state $|\psi\rangle$ in a laboratory on Earth, and subsequently transport A to Alice in the Alpha Centauri star system, and B to Bob in the Betelgeuse system:



In principle, this can be done carefully enough to avoid disturbing the two-particle state.

At a pre-scheduled time, Alice measures S_z on A. As we saw in the previous section, her measurement yields two equally probable outcomes. If the result is $+\hbar/2$, the combined state collapses to $|\uparrow\rangle|\downarrow\rangle$; if the result is $-\hbar/2$, the combined state collapses to $|\downarrow\rangle|\uparrow\rangle$. Immediately after Alice's scheduled measurement, Bob measures $\hat{S}_z$ on B. He obtains, with 100% probability, the result opposite to Alice's.

Notice that this thought experiment dispels some commonsensical but mistaken explanations for state collapse. For instance, it is sometimes claimed that in order to measure a particle's position, we must do something like shining light on it, which disturbs the particle's state. The EPR paradox shows that such stories do not capture the full weirdness of quantum measurement. We can collapse a particle's quantum state without interacting directly with it, by doing a measurement on another particle far away.

The postulates of quantum mechanics seem to indicate that the state collapses instantaneously. Alice and Bob are light years distant from each other, so during the time interval between their measurements, no classical signal could have passed between them, even at light speed. Yet Alice's measurement evidently affects Bob's measurement. Could this be a violation of the theory of relativity?

Not so fast: to achieve an actual violation of relativity, Alice and Bob must find a way to use the state collapse to perform superluminal communication. It is the combination of superluminal communication with relativity that generates cause-and-effect inconsistencies, such as the grandfather paradox. In the present setup, Alice and Bob individually see a statistical distribution of measurement outcomes equivalent to a coin flip (i.e., 50% chance of getting $+\hbar/2$, and 50% chance of getting $-\hbar/2$). Even if they repeat the experiment many times with many independently-prepared singlet states, each of them only receives a string of random bits, which carries no information.

Alice and Bob might try to get around this by varying their choice of measurement. For instance, instead of always measuring S_z, Alice might choose to measure S_x. This would cause the two-particle state to collapse to something like

$$\begin{aligned} &|\rightarrow\rangle \otimes |\leftarrow\rangle \qquad \text{(if Alice got } S_x = +\hbar/2) \\ &|\leftarrow\rangle \otimes |\rightarrow\rangle \qquad \text{(if Alice got } S_x = -\hbar/2), \end{aligned}$$

instead of $|\uparrow\rangle|\downarrow\rangle$ and $|\downarrow\rangle|\uparrow\rangle$. If Bob could thereby determine whether Alice had measured S_x or S_z, this would be a way to transmit one bit of information (e.g., S_x means 1 and S_z means 0) from Alice to Bob. This would work even if the determination is only statistical (e.g., if Bob can figure out that Alice picked S_x instead of S_z with 50.1% probability), since Alice and Bob can simply repeat the experiment many times to reduce the uncertainty.

Upon closer inspection, it turns out that such schemes do *not* allow Alice and Bob to communicate. The key point is that quantum states themselves cannot be measured; only observables are measured. By calculating the various measurement probabilities, we can prove the following (see Exercise 1):

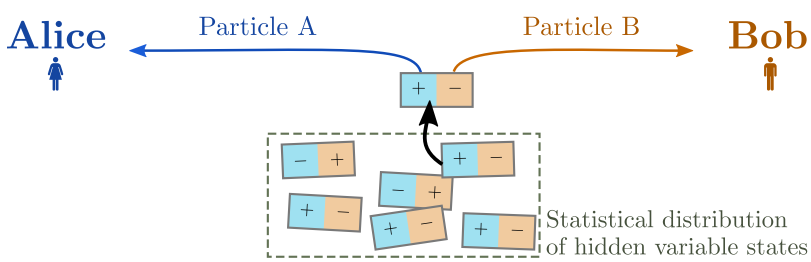
- If Alice measures along axis n, and Bob then measures along axis n', the overall probability for Bob to get either result (i.e., $+\hbar/2$ or $-\hbar/2$) is 0.5, regardless of the choices of n and n'.

- If $n = n'$, Bob always gets the opposite of Alice's result.

Since Bob always has equal probability to get either outcome, he is unable to extract any information from the state collapse induced by Alice. This implies that the EPR thought experiment does not contradict relativity. Nonetheless, EPR argued that the situation is unsatisfactory. A central element of quantum theory—i.e., the quantum state—is changing faster than the speed of light. Even if that change cannot be directly measured or used to transmit information, this seems to violate the *spirit* of relativity.

EPR suggested an alternative: maybe quantum mechanics is an approximation of some deeper theory, whose details are currently unknown. Such a **hidden-variable theory** could give the appearance of quantum state collapse, but without any faster-than-light changes actually happening.

Suppose, contrary to quantum theory, that each particle has a definite value of S_z, i.e., $S_z = +\hbar/2$ or $-\hbar/2$. For simplicity, let us denote these options as $+$ or $-$. Let us hypothesize that the two-particle quantum state $|\psi\rangle$ is actually a statistical distribution of two kinds of "**hidden-variable states**": $\boxed{+|-}$ (i.e., $S_z = +\hbar/2$ for A and $S_z = -\hbar/2$ for B), or $\boxed{-|+}$ (vice versa). When the state $|\psi\rangle$ is prepared, one of these hidden-variable states is randomly drawn from the distribution, but its contents are initially hidden.



When Alice measures S_z, the hidden variable is revealed. If she got $+$, that means the hidden-variable state must have been $\boxed{+|-}$, whereas if she got $-z$, the hidden-variable state was $\boxed{-|+}$. When Bob subsequently measures S_z, his result will be the opposite of Alice's. These outcomes were predetermined when the hidden-variable state was drawn, so there is no physical effect traveling between Alice and Bob akin to the instantaneous state collapse of quantum theory.

Clearly, there are many theoretical details missing. The hidden-variable theory would need to replicate all the successful predictions made by quantum theory. Trying to come up with a suitable theory of this sort seems like a tall order, but with enough hard work, might it be doable?

Well, no.

3.4. BELL'S THEOREM

In 1964, Bell published a bombshell paper showing that the predictions of quantum theory are inherently inconsistent with hidden-variable theories [4]. The amazing thing about this proof, which is called **Bell's theorem**, is that it requires no knowledge about the details of the hidden-variable theory, merely the fact that it is deterministic and local. Here, we present a simplified version of Bell's theorem due to Mermin [5].

Yet again, we consider pairs of spin-1/2 particles, with particle A sent to Alice and particle

B to Bob, with the two-particle state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\Big). \tag{3.40}$$

In each round of the thought experiment, Alice and Bob are each allowed to measure their particle's spin along one of three possible spin axes, whose observables are denoted by S_1, S_2, S_3 (we'll specify the directions of these spin axes later). Each experimentalist chooses S_1, S_2, or S_3, *randomly and with equal probabilities.*

Many rounds of the experiment are conducted. Afterwards, we bring together Alice's and Bob's experimental records, and examine their axis choices and results. For example:

	Alice		**Bob**	
	Axis	Result	Axis	Result
Round 1	S_1	−	S_2	+
Round 2	S_3	+	S_2	+
Round 3	S_2	+	S_1	−
Round 4	S_3	−	S_3	+
Round 5	S_3	−	S_1	−
⋮	⋮	⋮	⋮	⋮

If the results are consistent with quantum theory, whenever Alice and Bob chose the same axis (by random chance), they must have obtained opposite results. For example, in the above records, they both chose axis S_3 during Round 4; Alice got $-$, and Bob got $+$.

Can a hidden-variable theory reproduce such behavior? In a hidden-variable theory, each particle has a definite value for each spin observable. For example, A might have $S_1 = +\hbar/2$, $S_2 = +\hbar/2$, $S_3 = -\hbar/2$, which we can denote more concisely as '$++-$'. For every spin axis, the two particles' hidden variables must have opposite values. Hence, there are 8 possible hidden-variable states, which we can denote like this:

$$\boxed{+++|---}\quad \boxed{++-|--+}\quad \boxed{+-+|-+-}\quad \boxed{+--|-++}$$
$$\boxed{-++|+--}\quad \boxed{-+-|+-+}\quad \boxed{--+|++-}\quad \boxed{---|+++}$$

For instance, $\boxed{++-|--+}$ indicates that A has $S_1 = S_2 = +\hbar/2$ and $S_3 = -\hbar/2$, while B has $S_1 = S_2 = -\hbar/2$ and $S_3 = +\hbar/2$. The hidden-variable theory postulates that the two-particle state (3.40) is actually some kind of statistical distribution involving 8 hidden-variable states:

$$\Big\{P\big(\boxed{+++|---}\big),\; P\big(\boxed{++-|--+}\big), \dots, P\big(\boxed{---|+++}\big)\Big\}.$$

Let us focus on the rounds in which Alice and Bob *chose different spin axes.* Within this subset, what is the probability *for their measurement results to have opposite signs*? To answer this question, we first consider these 6 hidden-variable states:

$$\boxed{++-|--+}\quad \boxed{+-+|-+-}\quad \boxed{+--|-++}$$
$$\boxed{-++|+--}\quad \boxed{-+-|+-+}\quad \boxed{--+|++-}$$

These are the cases for which each particle's spin variables are not all $+$ or all $-$. Take the first case, $\boxed{++-|--+}$. Under our assumption that Alice and Bob chose different measurement axes, there are two choices that give opposite signs for the measurement results: (S_1, S_2) or (S_2, S_1). Conversely, there are four choices that give the same sign: (S_1, S_3), (S_2, S_3), (S_3, S_1) and (S_3, S_2). Since the axis choices are totally random, the probability of obtaining opposite signs for this hidden-variable state is 1/3. Going through the rest of the 6 hidden-variable states listed above, we find that the probability to get opposite signs is likewise 1/3. In the notation of conditional probabilities,

$$P\big(\text{opp.}|\boxed{++-|--+}\big) = P\big(\text{opp.}|\boxed{+-+|-+-}\big) = \cdots = \frac{1}{3}, \tag{3.41}$$

where "opp." stands for opposite signs being obtained in the two measurement results.

Now look at the remaining 2 hidden-variable states:

$$\boxed{+++|---} \qquad \boxed{---|+++}$$

For these, the conditional probabilities are

$$P\big(\text{opp.}|\boxed{+++|---}\big) = P\big(\text{opp.}|\boxed{---|+++}\big) = 1. \tag{3.42}$$

By the law of conditional probabilities, the probability for the "opposite signs" outcome is

$$\begin{aligned} P\big(\text{opp.}\big) = \;\; & P\big(\text{opp.}|\boxed{++-|--+}\big)P\big(\boxed{++-|--+}\big) \\ & + P\big(\text{opp.}|\boxed{+-+|-+-}\big)P\big(\boxed{+-+|-+-}\big) \\ & + \;\; \cdots \\ & + P\big(\text{opp.}|\boxed{---|+++}\big)P\big(\boxed{---|+++}\big), \end{aligned} \tag{3.43}$$

where the sum runs over all 8 possibilities (hidden-variable states). We can use Eqs. (3.41) and (3.42) to insert the conditional probabilities, resulting in

$$\begin{aligned} P\big(\text{opp.}\big) = \frac{1}{3}\Big[& \underbrace{P\big(\boxed{++-|--+}\big) + P\big(\boxed{+-+|-+-}\big) + \cdots + P\big(\boxed{--+|++-}\big)}_{\text{6 hidden-variable states obeying Eq. (3.41)}}\Big] \\ & + \underbrace{P\big(\boxed{+++|---}\big) + P\big(\boxed{---|+++}\big)}_{\text{2 hidden-variable states obeying (3.42)}}. \end{aligned} \tag{3.44}$$

It follows that

$$P\big(\text{opp.}\big) \ge \frac{1}{3}\Big[\underbrace{P\big(\boxed{++-|--+}\big) + \cdots + P\big(\boxed{---|+++}\big)}_{\text{all 8 hidden-variable states}}\Big]. \tag{3.45}$$

The probabilities in the square brackets must sum to one. Therefore,

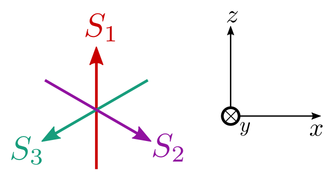
$$P\big(\text{opp.}\big) \ge \frac{1}{3}. \tag{3.46}$$

This result, called **Bell's inequality**, can be summarized as follows:

In a hidden-variable theory, for the rounds where Alice and Bob choose different spin axes, their measurement results have opposite signs with probability $\geq 1/3$.

If we can find a situation where quantum theory predicts a violation of Bell's inequality, that would prove quantum theory is inconsistent with a broad class of hidden-variable theories. It would not matter how complicated the inner workings of the hidden-variable theory are, so long as it meets the modest assumptions presented above (e.g., there are local deterministic hidden variables for each measurement, the hidden-variable states are associated with probabilities summing to one, etc.).

Thus, we seek a set of spin operators $\{S_1, S_2, S_3\}$ such that quantum theory violates Bell's inequality. One way to accomplish this is to align S_1 with the z axis, and place S_2 and S_3 in the x-z plane at 120° ($2\pi/3$ radians) from S_1, as shown below:



Referring to this diagram, we can express the three spin operators as

$$\begin{aligned} \hat{S}_1 &= \frac{\hbar}{2}\,\hat{\sigma}_3 && = \hat{S}_z \\ \hat{S}_2 &= \frac{\hbar}{2}\,[\cos(2\pi/3)\hat{\sigma}_3 + \sin(2\pi/3)\hat{\sigma}_1] && = \hat{U}^\dagger \hat{S}_z \hat{U} \\ \hat{S}_3 &= \frac{\hbar}{2}\,[\cos(2\pi/3)\hat{\sigma}_3 - \sin(2\pi/3)\hat{\sigma}_1] && = \hat{U} \hat{S}_z \hat{U}^\dagger, \end{aligned} \tag{3.47}$$

where $\hat{U}$ is the following unitary rotation operator:

$$\hat{U} = e^{(i\pi/3)\hat{\sigma}_2} = \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix}. \tag{3.48}$$

Suppose Alice chooses S_1, while Bob chooses S_2. Note that the eigenstates of $\hat{S}_2$ are

$$|\pm s_2\rangle = \hat{U}^\dagger |\updownarrow\rangle, \tag{3.49}$$

since

$$\hat{S}_2 \left(\hat{U}^\dagger |\updownarrow\rangle\right) = \hat{U}^\dagger \hat{S}_z \hat{U} \left(\hat{U}^\dagger |\updownarrow\rangle\right) = \pm\frac{\hbar}{2}\,\hat{U}^\dagger |\updownarrow\rangle. \tag{3.50}$$

The probability that Alice and Bob obtain opposite results, for this choice of axes, can be written in the form

$$P(\text{opp.}) = P(A_+)P(B_-|A_+) + P(A_+)P(B_-|A_+). \tag{3.51}$$

For example, $P(A_+)$ denotes the probability of Alice obtaining +, whereupon Bob performs his measurement on the $|\downarrow\rangle$ state; and we want the probability of Bob obtaining −, corresponding to the eigenstate $|-s_2\rangle$. Therefore,

$$\begin{aligned} P(\text{opp.}) &= \frac{1}{2}\left|\langle -s_2|\downarrow\rangle\right|^2 + \frac{1}{2}\left|\langle +s_2|\uparrow\rangle\right|^2 && (3.52)\\ &= \frac{1}{2}\left(\left|\langle\downarrow|\hat{U}|\downarrow\rangle\right|^2 + \left|\langle\uparrow|\hat{U}|\uparrow\rangle\right|^2\right) && (3.53)\\ &= \frac{1}{4}. && (3.54)\end{aligned}$$

In obtaining Eq. (3.53), we have used Eq. (3.49), and in obtaining Eq. (3.54), we have used Eq. (3.48).

In a similar fashion, we can work through all the other possible choices of spin axes (subject to the over-arching constraint that Alice and Bob pick different axes). All the cases yield the same result as Eq. (3.54). In other words, the probability for Alice and Bob obtain opposite results is $1/4$, so Bell's inequality is violated!

Last of all, we must consult Nature. Is it possible to experimentally observe a violation of Bell's inequality? In the decades following Bell's paper, many experiments were performed to answer this question. These experiments are all substantially more complicated than the above toy model, and are subject to various real-world imperfections. But in the end, the experimental consensus is a clear *yes*: Nature agrees with quantum mechanics, not the hidden-variable theories! The experimental evidence is reviewed in a paper by Aspect [6].

3.5. QUANTUM CRYPTOGRAPHY

One of the most remarkable consequences of Bell's thought experiment is that it provides a way to perform cryptography that is more secure, in certain respects, than conventional cryptography. The possibility of **quantum cryptography** is poised to be one of the most important technological applications of quantum entanglement. Here, we describe one of the earliest quantum cryptography schemes, devised by Ekert in 1991 [7].

Ekert's scheme allows two participants, Alice and Bob, to share with each other a string of random binary digits (0 or 1), called a "key". The objective is to make this sharing secure, in the sense that no one else can eavesdrop and learn the key. After Alice and Bob have established the key, they can use it alongside various non-quantum methods to encrypt messages between each other (e.g., by using the key as a one-time pad).

The scheme closely follows the Bell thought experiment from Section 3.4. Alice and Bob take part in multiple rounds of measurements; during each round, a pair of spin-1/2 particles is prepared in the singlet state (3.40), with particle A going to Alice and B going to Bob. Each participant randomly chooses an axis (S_1, S_2, or S_3), performs the corresponding spin measurement, and secretly records down the result.

Alice and Bob then tell each other what axes they chose during the measurement rounds. These announcements are assumed to take place over a communication channel that isn't necessarily secure, in the sense that it might be eavesdropped upon; however, it is assumed that the communications cannot be jammed or altered by any third party. From this information, Alice and Bob identify the rounds in which they picked the same axis (about 1/3 of the rounds), during which they must have obtained exactly opposite measurement results. These measurement results are thus a string of random binary digits known to both Alice and Bob, and no one else.

How might a third party, Eve, attempt to eavesdrop? Suppose Eve was able to intercept some or all of the B particles intended for Bob. She can try to extract some information from them (which, according to quantum theory, means doing measurements on them), and then sending some replacement particles to Bob (hoping he does not notice). However, such measurements would break the entanglement between the particles received by Alice and Bob. The situation turns into a kind of hidden-variable theory, where the hidden variables represent the information extracted by Eve.

To check for Eve's tampering, Alice and Bob can publicly announce their measurement results for the rounds in which their axes were different. (Remember, these rounds are not needed for the secret key.) Each of them can then check for a violation of Bell's inequality, which would guarantee no eavesdropping has taken place. For details, refer to Ref. [7].

Alternatively, Eve might duplicate or "clone" the quantum state of B before it goes to Bob. Then she can wait for Bob to announce his choice of measurement axis for that round, perform that measurement on her cloned particle, and reproduce Bob's result. Though plausible at first glance, this turns out to be incompatible with the laws of quantum mechanics.

The so-called **no-cloning theorem** can be proven as follows. Eve desires to clone an arbitrary state of a spin-half particle B onto another spin-half particle C. The two-particle Hilbert space is $\mathscr{H} \otimes \mathscr{H}$. With particle C initially prepared in some state $|0\rangle$, Eve must devise a unitary operation $\hat{U}$, representing the cloning process, such that

$$\hat{U}|\psi\rangle|0\rangle = e^{i\phi}|\psi\rangle|\psi\rangle \tag{3.55}$$

for all $|\psi\rangle \in \mathscr{H}$. The phase factor ϕ can depend on $|\psi\rangle$.

Now replace $|\psi\rangle$ in the above equation with two arbitrary states denoted by $|\psi_1\rangle$ and $|\psi_2\rangle$, and take their inner product. According to Eq. (3.55),

$$\begin{aligned}\Big(\langle\psi_1|\langle 0|\hat{U}^\dagger\Big)\Big(\hat{U}|\psi_2\rangle|0\rangle\Big) &= \Big(\langle\psi_1|\langle\psi_1|e^{-i\phi_1}\Big)\Big(e^{i\phi_2}|\psi_2\rangle|\psi_2\rangle\Big) &(3.56)\\ &= e^{-i(\phi_1-\phi_2)}\Big(\langle\psi_1|\psi_2\rangle\Big)^2. &(3.57)\end{aligned}$$

Here, ϕ_1 and ϕ_2 are the phase factors from Eq. (3.55) for the two chosen states. On the other hand, since $\hat{U}$ is unitary,

$$\begin{aligned}\langle\psi_1|\langle 0|\hat{U}^\dagger\hat{U}|\psi_2\rangle|0\rangle &= \Big(\langle\psi_1|\langle 0|\Big)\Big(|\psi_2\rangle|0\rangle\Big) &(3.58)\\ &= \langle\psi_1|\psi_2\rangle. &(3.59)\end{aligned}$$

Comparing the magnitudes of (3.57) and (3.59),

$$\big|\langle\psi_1|\psi_2\rangle\big|^2 = \big|\langle\psi_1|\psi_2\rangle\big| \;\;\Rightarrow\;\; \big|\langle\psi_1|\psi_2\rangle\big| = 0 \text{ or } 1. \tag{3.60}$$

But aside from the trivial case of a one-dimensional Hilbert space, this cannot be true for arbitrary $|\psi_1\rangle$ and $|\psi_2\rangle$. For instance, for a two-dimensional space spanned by an orthonormal basis $\{|0\rangle, |1\rangle\}$, we can pick

$$|\psi_1\rangle = |0\rangle,\; |\psi_2\rangle = \frac{1}{\sqrt{2}}\big(|0\rangle + |1\rangle\big) \;\;\Rightarrow\;\; \big|\langle\psi_1|\psi_2\rangle\big| = \frac{1}{\sqrt{2}}. \tag{3.61}$$

3.6. DENSITY OPERATORS

We now introduce **density operators**, which help streamline calculations involving systems of multiple particles (or, more generally, multiple subsystems).

As a warm-up, consider a quantum system in a state $|\psi\rangle \in \mathscr{H}$. We can define the Hermitian operator

$$\hat{\rho} = |\psi\rangle\,\langle\psi|. \tag{3.62}$$

This is just the projector for $|\psi\rangle$, but in this context we call it a "density operator". It is also commonly called a **density matrix**.

In Section 3.2, we had gone through the rules for calculating the probabilities for measurements done on $|\psi\rangle$. Using $\hat{\rho}$, these rules can be re-stated as follows:

1. If we measure an observable $\hat{Q}$, whose eigenvalues are $\{q\}$ and eigenstates are $\{|q\rangle\}$, the probability of obtaining q is

$$P(q) = \big|\langle q|\psi\rangle\big|^2 = \langle q|\,\hat{\rho}\,|q\rangle. \tag{3.63}$$

2. The expectation value of the observable is

$$\langle Q\rangle = \sum_q q P(q) = \sum_q \langle q|\hat{Q}\,\hat{\rho}|q\rangle = \mathrm{Tr}\big[\,\hat{Q}\,\hat{\rho}\,\big]. \tag{3.64}$$

   Here, $\mathrm{Tr}[\cdots]$ denotes the trace, which is the sum of the diagonal elements of the matrix representation of the operator. Its value is basis independent.

Let us move on to partial measurements. Consider, once again, two subsystems A and B, with Hilbert spaces $\mathscr{H}_A$ and $\mathscr{H}_B$. Suppose we are specifically interested in partial measurements performed on A. As detailed in Section 3.2 the probabilities of these partial measurement outcomes can be calculated from the state of the combined system,

$$|\psi\rangle \in \mathscr{H}_A \otimes \mathscr{H}_B.$$

However, $|\psi\rangle$ also contains information about B, which we are not interested in. Is there a more economical way to encode just the properties of the A subsystem?

To do this, we define the density operator for A, sometimes called the **reduced density operator**, as follows:

$$\hat{\rho}_A = \mathrm{Tr}_B\left[\,\hat{\rho}\,\right]. \tag{3.65}$$

Here, $\hat{\rho}$ is the density matrix for the combined system, as defined in Eq. (3.62). $\mathrm{Tr}_B[\cdots]$ denotes a **partial trace**, which means tracing out the B part of the Hilbert space. To be precise, given a basis $\{|\beta\rangle\}$ for $\mathscr{H}_B$, the partial trace is

$$\hat{\rho}_A = \sum_\beta \Big(\hat{I}_A \otimes \langle\beta|\Big)\;|\psi\rangle\langle\psi|\;\Big(\hat{I}_A \otimes |\beta\rangle\Big). \tag{3.66}$$

In the A part of the Hilbert space, we do nothing (i.e., apply identity operators), while in the B part we perform a trace. Whereas the standard trace turns an operator to a scalar, this partial trace turns an operator acting on $\mathscr{H}_A \otimes \mathscr{H}_B$ into an operator acting on just $\mathscr{H}_A$.

Like the standard trace, the partial trace turns out to be basis independent—i.e., even if we use a different basis in Eq. (3.66), we end up with the same operator.

Now, suppose we measure an observable $\hat{Q}_A$ on subsystem A, which has eigenstates $\{|\alpha\rangle\}$ and eigenvalues $\{\alpha\}$. According to the rules for partial measurements (Section 3.2), the probability of obtaining α is

$$\begin{aligned} P(\alpha) &= \langle\psi| \Big(|\alpha\rangle\langle\alpha| \otimes \hat{I}_B\Big)|\psi\rangle &(3.67)\\ &= \langle\psi| \left[|\alpha\rangle\langle\alpha| \otimes \left(\sum_\beta |\beta\rangle\langle\beta|\right)\right] |\psi\rangle &(3.68)\\ &= \sum_\beta \Big(\langle\alpha|\langle\beta|\Big) |\psi\rangle\langle\psi| \Big(|\alpha\rangle|\beta\rangle\Big) &(3.69)\\ &= \langle\alpha|\hat{\rho}_A|\alpha\rangle. &(3.70)\end{aligned}$$

This result is clearly analogous to Eq. (3.63). Hence, we can use $\hat{\rho}_A$ to directly calculate the probabilities for any measurement on A. As a corollary,

$$\langle Q_A\rangle = \sum_\alpha \alpha\langle\alpha|\hat{\rho}_A|\alpha\rangle = \mathrm{Tr}\Big[\hat{Q}_A\,\hat{\rho}_A\Big], \tag{3.71}$$

which is analogous to Eq. (3.64).

To better understand these results, let us expand the state of the combined system as

$$|\psi\rangle = \sum_{\alpha\beta} \psi_{\alpha\beta}|\alpha\rangle|\beta\rangle, \tag{3.72}$$

where $\sum_{\alpha\beta}|\psi_{\alpha\beta}|^2 = 1$. Then

$$\hat{\rho} = \sum_{\alpha\alpha'\beta\beta'} \psi_{\alpha\beta}\psi^*_{\alpha'\beta'}\;|\alpha\rangle|\beta\rangle\,\langle\alpha'|\langle\beta'|, \tag{3.73}$$

and the reduced density operator is

$$\begin{aligned}\hat{\rho}_A &= \sum_{\alpha\alpha'\beta} \psi_{\alpha\beta}\psi^*_{\alpha'\beta}|\alpha\rangle\langle\alpha'|\\ &= \sum_\beta \left(\sum_\alpha \psi_{\alpha\beta}|\alpha\rangle\right)\left(\sum_{\alpha'}\psi^*_{\alpha'\beta}\langle\alpha'|\right) \qquad (3.74)\\ &= \sum_\beta |\varphi_\beta\rangle\langle\varphi_\beta|, \quad \text{where} \quad |\varphi_\beta\rangle = \sum_\alpha \psi_{\alpha\beta}|\alpha\rangle.\end{aligned}$$

But $|\varphi_\beta\rangle$ is not necessarily normalized to unity:

$$\langle\varphi_\beta|\varphi_\beta\rangle = \sum_\alpha |\psi_{\alpha\beta}|^2 \le 1. \tag{3.75}$$

Let us therefore define the re-normalized states

$$|\Psi_\beta\rangle = \frac{1}{\sqrt{P_\beta}}|\varphi_\beta\rangle, \quad \text{where}\;\; P_\beta = \sum_\alpha |\psi_{\alpha\beta}|^2. \tag{3.76}$$

Note that each P_β is a non-negative real number in the range $[0,1]$. Eq. (3.74) now becomes

$$\hat{\rho}_A = \sum_\beta P_\beta \,|\Psi_\beta\rangle\langle\Psi_\beta|, \quad \text{where} \quad \left\{ \begin{array}{l} \text{each } P_\beta \text{ is a real number in } [0,1], \text{ and} \\ \text{each } |\Psi_\beta\rangle \in \mathscr{H}_A, \;\; \text{with } \;\langle\Psi_\beta|\Psi_\beta\rangle = 1. \end{array}\right. \tag{3.77}$$

This has the form of a sum of density operators for a set of quantum states $\{|\Psi_\beta\rangle\}$, weighted by a set of classical probabilities $\{P_\beta\}$. This called an **ensemble** of states. Note that the states in the ensemble need not be orthogonal to each other.

Although we have derived Eq. (3.77) from $|\psi\rangle$, the state of the combined system, we cannot work backwards from $\hat{\rho}_A$ to figure out $|\psi\rangle$ (specifically, the coefficients $\psi_{\alpha\beta}$). In other words, $\hat{\rho}_A$ provides all the necessary information regarding measurements on A, discarding extraneous information about subsystem B and how it is entangled with A. This means that we don't have to keep thinking of $\hat{\rho}_A$ as a reduced density operator derived from some larger state; we can simply present it as "the density operator for A".

From this point of view, a density operator of the form $|\psi\rangle\langle\psi|$, which we started with back in Eq. (3.62), is the special case of an ensemble of one quantum state $|\psi\rangle$ with probability $P = 1$. We call such an ensemble a **pure state**. If an ensemble is not a pure state, we call it a **mixed state**, and this implies that the system is entangled with something else.

Using Eq. (3.77), we can show that the density matrix $\hat{\rho}_A$ (be it for a pure state or a mixed state) has the following properties:

1. $\hat{\rho}_A$ is Hermitian.

2. $\langle\varphi|\hat{\rho}_A|\varphi\rangle \geq 0$ for any $|\varphi\rangle \in \mathscr{H}_A$ (i.e., the operator is positive semidefinite).

3. For any observable $\hat{Q}_A$ acting on $\mathscr{H}_A$,

$$\langle Q_A\rangle = \mathrm{Tr}_A\left[\hat{Q}_A\,\hat{\rho}_A\right]. \tag{3.78}$$

   This also gives the probability for any measurement outcome: if $|\alpha\rangle$ is the eigenstate associated with the outcome, the outcome probability is $\langle\alpha|\hat{\rho}_A|\alpha\rangle$, consistent with Eq. (3.70). To see this, take $\hat{Q}_A = |\alpha\rangle\langle\alpha|$.

4. The eigenvalues of $\hat{\rho}_A$, denoted by $\{p_1, p_2, \dots, p_{d_A}\}$, form a set of probabilities. In other words, they satisfy

$$p_n \in \mathbb{R} \;\; \text{and} \;\; 0 \leq p_n \leq 1 \;\; \text{for} \;\; n = 1, \dots, d_A, \quad \text{with} \; \sum_{n=1}^{d_A} p_n = 1. \tag{3.79}$$

   From this, it directly follows that

$$\mathrm{Tr}_A[\hat{\rho}_A] = 1. \tag{3.80}$$

   Property 4 follows from Property 3. First, take $\hat{Q}_A = |j\rangle\langle j|$, where $|j\rangle$ is any eigenvector of $\hat{\rho}_A$ with eigenvalue p_j, and use Property 3 to prove that $0 \leq p_j \leq 1$. Then take $\hat{Q} = \hat{I}_A$ and use Property 3 to prove that the eigenvalues sum to 1.

In some circumstances, we can assume that a system is in a given mixed state, without deriving its density matrix via a partial trace. For example, if a system has energy eigenbasis $\{|\psi_n\rangle\}$ and energies $\{E_n\}$, and is in thermal equilibrium with an external heat bath of temperature T, its density operator can be assumed to be

$$\hat{\rho}_A = \sum_n \frac{\exp(-E_n/k_B T)}{Z}\, |E_n\rangle\langle E_n|, \tag{3.81}$$

where $Z = \sum_n \exp(-E_n/k_B T)$. This is justified by the postulates of statistical mechanics, rather than any actual derivation based on tracing out the heat bath's quantum degrees of freedom, which would be hopelessly complicated. So long as the weights in the sum are classical probabilities (i.e., non-negative real numbers adding up to 1), the density matrix $\hat{\rho}_A$ will satisfy the general properties 1–4 described above.

3.7. ENTANGLEMENT ENTROPY

Previously, we said that a multi-particle system is entangled if the individual particles lack definite quantum states. It would be nice to make this statement more precise, and in fact physicists have come up with several different quantitive measures of entanglement. In this section, we will describe the most common measure, **entanglement entropy**, which is closely related to the entropy concept from thermodynamics, statistical mechanics, and information theory.

We have seen from the previous section that if a subsystem A is (possibly) entangled with some other subsystem B, the information required to calculate all partial measurement outcomes on A is given by a reduced density operator $\hat{\rho}_A$. We can use this to define a quantity called the **entanglement entropy**:

$$S_A = -k_b \,\mathrm{Tr}_A\Big\{\hat{\rho}_A \,\ln\big[\hat{\rho}_A\big]\Big\}. \tag{3.82}$$

In this formula, $\ln[\cdots]$ denotes the logarithm of an operator, which is the inverse of the exponential: $\ln(\hat{P}) = \hat{Q} \Rightarrow \exp(\hat{Q}) = \hat{P}$. The prefactor k_b is Boltzmann's constant, and ensures that S_A has the same units as thermodynamic entropy.

In classical statistical mechanics, entropy is a quantitative measure of uncertainty (i.e, lack of information) about a system's underlying microscopic state, or "microstate". Suppose a system has W possible microstates occurring with probabilities $\{p_1, p_2, \dots, p_W\}$. Then the classical entropy is defined as

$$S_{\mathrm{cl.}} = -k_b \sum_{i=1}^{W} p_i \ln(p_i). \tag{3.83}$$

It can be shown (see Appendix C) that for *any* probability distribution,

$$0 \le S_{\mathrm{cl.}} \le k_b \ln W. \tag{3.84}$$

The lower bound, $S_{\mathrm{cl.}} = 0$, occurs if and only if $p_i = \delta_{ik}$ for a specific k, which can be interpreted as a situation of "complete certainty" about the microstate. The upper bound, $S_{\mathrm{cl.}} = k_b \ln W$, occurs if and only if all microstates are equally probable (i.e., $p_i = 1/W$), which corresponds to "complete uncertainty" about the system's microstate.

The entanglement entropy (3.82) similarly aims to quantify the uncertainty arising from a quantum system's lack of a definite quantum state, due to it being possibly entangled with another system. In formulating this concept, we need to be careful about how classical notions of probability apply to quantum systems. We have seen that when performing a measurement on A whose possible outcomes are $\{q\}$, the probability of each outcome is $P(q) = \langle q|\hat{\rho}_A|q\rangle$. However, it is problematic to directly substitute these probabilities $\{P(q)\}$ into the classical entropy formula (3.83), since they are basis-dependent. Eq. (3.82) bypasses this problem by using the trace, which is basis-independent.

In one specific basis, the eigenbasis for $\hat{\rho}_A$, the entanglement entropy does match the classical entropy formula. Let $\{|n\rangle\}$ be the eigenstates of $\hat{\rho}_A$; as shown in Eq. (3.79), the corresponding eigenvalues $\{p_n\}$ form a set of probabilities. Then

$$\begin{aligned} S_A &= -k_b \sum_n \langle n|\hat{\rho}_A \ln(\hat{\rho}_A)|n\rangle \\ &= -k_b \sum_n p_n \ln(p_n). \end{aligned} \tag{3.85}$$

From this, we can see that the entanglement entropy obeys the following bounds, similar to the classical entropy formula:

$$0 \le S_A \le k_b \ln(d_A), \quad \text{where } d_A = \dim\left[\mathscr{H}_A\right]. \tag{3.86}$$

The lower bound, $S_A = 0$, holds if and only if one of the p_n's in Eq. (3.85) is 1, and all the others are zero, meaning A is in a pure state. Conversely, $S_A \neq 0$ when $\hat{\rho}_A$ describes a mixed state—i.e., A is entangled with some other quantum system.

A system is said to be **maximally entangled** if it saturates the upper bound of (3.86). This occurs if and only if the eigenvalues of the density operator are all equal to $1/d_A$.

Example—Consider the singlet state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\Big). \tag{3.87}$$

The corresponding density operator is

$$\hat{\rho}(\psi) = \frac{1}{2}\Big(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\Big)\Big(\langle\uparrow|\langle\downarrow| - \langle\downarrow|\langle\uparrow|\Big). \tag{3.88}$$

Tracing over system B (the second slot) yields the reduced density operator

$$\hat{\rho}_A(\psi) = \frac{1}{2}\Big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\Big). \tag{3.89}$$

This can be expressed as a matrix in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis:

$$\hat{\rho}_A(\psi) = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \tag{3.90}$$

Now we can use $\hat{\rho}_A$ to compute the entanglement entropy:

$$S_A = -k_b \mathrm{Tr}\left\{\hat{\rho}_A \ln(\rho_A)\right\} = -k_b \mathrm{Tr}\begin{pmatrix} \frac{1}{2}\ln\left(\frac{1}{2}\right) & 0 \\ 0 & \frac{1}{2}\ln\left(\frac{1}{2}\right) \end{pmatrix} = k_b \ln(2). \tag{3.91}$$

Hence, A and B are maximally entangled.

3.8. THE MANY WORLDS INTERPRETATION

We conclude this chapter with a set of interesting but controversial ideas related to the entanglement phenomenon: the **Many Worlds Interpretation** of quantum mechanics [8].

So far, when describing the phenomenon of state collapse, we have relied on the measurement postulate (see Section 3.2), which is part of the **Copenhagen Interpretation** of quantum mechanics. This is how quantum mechanics is typically taught, and also how physicists usually think about measurement when doing practical calculations.

However, the measurement postulate has two bad features:

1. It stands apart from the other postulates of quantum mechanics as the only place where randomness (or "indeterminism") creeps into quantum theory. The other postulates do not refer to probabilities. In particular, the Schrödinger equation
$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle \tag{3.92}$$
is completely deterministic. If you know $\hat{H}(t)$ and the initial state $|\psi(t_0)\rangle$ at time t_0, you can in principle calculate $|\psi(t)\rangle$ for all t. This time evolution describes a smooth, deterministic rotation of the state vector. A measurement process is completely different: during state collapse, the state vector jumps instantaneously to a random value. It seems strange for quantum theory to contain two completely different ways for a state to change.

2. The measurement postulate is silent on what constitutes a measurement. Does measurement require a conscious observer? Surely not: as Einstein once exasperatedly asked, are we to believe that the Moon exists only when we look at it? But if a given device interacts with a particle, what determines whether it acts via the Schrödinger equation, or performs a measurement?

The Many Worlds Interpretation of quantum mechanics seeks to resolve these problems by positing that the measurement postulate is *not* a fundamental postulate of quantum mechanics. It says that the key features of quantum measurement—e.g., the randomness of outcomes, and the quantum state collapsing after a measurement—are emergent properties of large and complex quantum systems obeying the Schrödinger equation. They can be derived, rather than posited, by adopting quantum descriptions for both the system being measured *and* the system doing the measurement.

We can use a toy model to illustrate this idea [9]. Suppose we have (i) a spin-1/2 particle, whose Hilbert space is $\mathscr{H}_S$, and (ii) an apparatus that measures S_z on that particle, whose Hilbert space is $\mathscr{H}_A$. The apparatus has a vast number of degrees of freedom, for it comprises a macroscopic device that performs the S_z measurement (and, optionally, an experimentalist who looks at the result, etc.). Its Hilbert space thus has a mind-bogglingly high dimension:

$$d_A = \dim[\mathscr{H}_A] \gg 1. \tag{3.93}$$

The Hilbert space for the combined system of spin and apparatus is

$$\mathscr{H}_S \otimes \mathscr{H}_A. \tag{3.94}$$

Let us suppose the combined system is prepared in an initial state

$$|\psi(0)\rangle = \Big(a_1|\uparrow\rangle + a_2|\downarrow\rangle\Big) \otimes |\Psi\rangle, \tag{3.95}$$

where a_1 and a_2 are the spin-up and spin-down quantum amplitudes, and $|\Psi\rangle \in \mathscr{H}_A$ is some initial state for the apparatus, which is initially not entangled with the spin.

We aim to show that the apparatus behaves as though is "measuring" the spin, simply by evolving the combined system using a Hamiltonian of the form

$$\hat{H} = \hat{S}_z \otimes \hat{V}. \tag{3.96}$$

This will only involve unitary time evolution via the Schrödinger equation, *without* invoking the measurement postulate. Also, it turns out that we will not need to make any special choices for $|\Psi\rangle$ in Eq. (3.95), or $\hat{V}$ in Eq. (3.96), so we leave these unspecified for now.

The assumed Hamiltonian (3.96) is time-independent, so the state after some time t is

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}\,|\psi(0)\rangle. \tag{3.97}$$

To find this, observe how the Hamiltonian (3.96) acts on each term of the initial state defined in Eq. (3.95):

$$\hat{H}|\uparrow\rangle|\Psi\rangle = +\frac{\hbar}{2}\,|\uparrow\rangle \otimes \Big(\hat{V}|\Psi\rangle\Big), \tag{3.98}$$

$$\hat{H}|\downarrow\rangle|\Psi\rangle = -\frac{\hbar}{2}\,|\downarrow\rangle \otimes \Big(\hat{V}|\Psi\rangle\Big). \tag{3.99}$$

Hence,

$$e^{-i\hat{H}t/\hbar}\,|\updownarrow\rangle|\Psi\rangle = |\updownarrow\rangle \otimes \Big(e^{\mp i\hat{V}t/2}|\Psi\rangle\Big). \tag{3.100}$$

Applying this to Eq. (3.97) yields

$$|\psi(t)\rangle = a_1|\uparrow\rangle|\Psi_\uparrow(t)\rangle + a_2|\downarrow\rangle|\Psi_\downarrow(t)\rangle, \tag{3.101}$$

where

$$|\Psi_\updownarrow(t)\rangle = e^{\mp i\hat{V}t/2}|\Psi\rangle \;\;\in \mathscr{H}_A. \tag{3.102}$$

Based on Eq. (3.101), we can interpret $|\Psi_\uparrow(t)\rangle$ and $|\Psi_\downarrow(t)\rangle$ as apparatus states corresponding to each possible measurement result. For example, $|\Psi_\uparrow(t)\rangle$ may represent a state in which the device has printed a message saying "$S_z = +\hbar/2$" on its screen; also, if the apparatus subsystem contains an experimentalist, that person has read the message and observed that the result is spin-up. For this interpretation to work, $|\Psi_\uparrow(t)\rangle$ and $|\Psi_\downarrow(t)\rangle$ ought to be almost exactly orthogonal, since they refer to utterly different states of $\mathscr{H}_A$. This turns out to be readily satisfied; we will show (and later verify numerically) that if $d_A \gg 1$,

$$\langle\Psi_\uparrow(t)|\Psi_\downarrow(t)\rangle \to 0 \tag{3.103}$$

after the passage of a short time t.

In the Many Worlds Interpretation, the two terms in Eq. (3.101) represent two disinct "worlds". Within each world, it appears that the spin has collapsed to a particular eigenstate, and the apparatus has measured the corresponding value of S_z. But from the point of view of the combined state $|\psi(t)\rangle$, which contains both worlds, the spin and apparatus are entangled. The two worlds' relative importance is quantified by the weights $|a_1|^2$ and $|a_2|^2$, which are precisely the two measurement probabilities specified by the initial state (3.95).

To back this up, let us perform an explicit numerical calculation. Since we have little hope of formulating a realistic model for a measurement apparatus, let us choose the apparatus state $|\Psi\rangle$ in Eq. (3.95), and the operator $\hat{V}$ in Eq. (3.96), in a generic way. For $|\Psi\rangle$, we pick a random complex vector in an arbitrary basis, with each component having its real and imaginary parts drawn from the normal distribution $N(0,1)$:

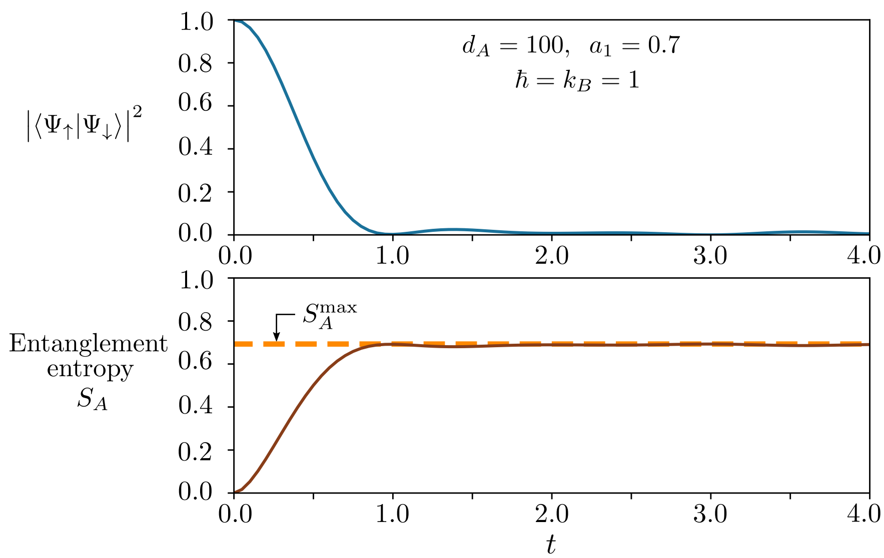
$$|\Psi\rangle = \frac{1}{\sqrt{\mathcal{N}}}\begin{pmatrix}\Psi_1\\ \vdots \\ \Psi_{d_A}\end{pmatrix}, \;\; \text{where } \; \mathrm{Re}(\Psi_j), \mathrm{Im}(\Psi_j) \sim N(0,1). \tag{3.104}$$

Here, the constant $\mathcal{N}$ is chosen so that $|\Psi\rangle$ is normalized to unity. Similarly, we let $\hat{V}$ be a random Hermitian $d_A \times d_A$ matrix:

$$\hat{V} = \frac{1}{2\sqrt{d_A}}\left(\hat{A} + \hat{A}^\dagger\right), \;\; \text{where } \; \mathrm{Re}(A_{ij}), \mathrm{Im}(A_{ij}) \sim N(0,1). \tag{3.105}$$

(The prefactor of $1/2\sqrt{d_A}$ is unimportant for our present discussion; it simply ensures that the eigenvalues of $\hat{V}$ lie in the range $[-2,2]$ rather than scaling with d_A, according to the theory of random matrices [10].) In this example, we will choose $d_A = 100$.

Now we simply have to pick the inital state (say, $a_1 = 0.7$ and $a_2 = \sqrt{1-a_1^2}$), and solve the Schrödinger equation numerically (for details, refer to Appendix D). Then we can generate plots like this:



The upper plot shows $|\langle\Psi_\uparrow|\Psi_\downarrow\rangle|^2$ versus t. This is equal to 1 at $t = 0$, but then drops rapidly to around zero, and stays there, in agreement with Eq. (3.103).

The lower plot shows the entanglement entropy of the spin and apparatus (see Section 3.7). At $t = 0$, this is zero, consistent with the two subsystems being initially unentangled [Eq. (3.95)]. Subsequently, S_A increases up to

$$S_A^{\max} = -k_b\Big(|a_1|^2 \ln |a_1|^2 + |a_2|^2 \ln |a_2|^2\Big) \approx 0.693\, k_b. \tag{3.106}$$

This corresponds to the classical entropy for a probability distribution $\{|a_1|^2, |a_2|^2\}$, and is indicated by a horizontal dashed line in the above figure. Note that S_A reaches $S_A^{\max}$ roughly when $|\langle\Psi_+|\Psi_-\rangle|^2$ reaches zero. This tells us that the establishment of entanglement between the spin and the apparatus (from the combined state's point of view) is associated with the process of measurement, and the formation of a "world".

Such a view of measurement can be generalized from the above toy model to the set of all measurement processes occurring everywhere. According to the Many Worlds Interpretation, the universe itself can be described by an extremely high-dimensional state vector. As this universal state evolves according to the Schrödinger equation, it repeatedly "branches" to produce more and more worlds, just like in Eq. (3.101). The world we inhabit, with its well-defined measurement results and collapsed quantum states, is just one of a vast multitude.

It is up to you to decide whether this conception of reality seems reasonable. It is essentially a matter of preference, because the Copenhagen Interpretation and the Many Worlds Interpretation have identical physical consequences—which is why they are referred to as different "interpretations" of quantum mechanics, rather than different theories.

EXERCISES

1. Consider the singlet state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle|\downarrow\rangle \;-\; |\downarrow\rangle|\uparrow\rangle\Big), \tag{3.107}$$

where the left- and right-hand slots refer to subsystems A and B respectively, and $\{|\uparrow\rangle, |\downarrow\rangle\}$ denote the eigenstates of the spin operator $\hat{S}_z$ with eigenvalue $\pm\hbar/2$.

(a) Suppose we perform a measurement on A using a rotated spin observable

$$\hat{S}_n = \hat{U}^\dagger \hat{S}_z \hat{U}, \tag{3.108}$$

where $\hat{U}$ is a unitary rotation matrix. The eigenstates of $\hat{S}_n$ are $|\pm n\rangle = \hat{U}^\dagger|\updownarrow\rangle$, with eigenvalues $\pm\hbar/2$. For each measurement outcome $\pm\hbar/2$, prove that the collapsed two-particle state is (up to arbitrary phase and normalization factors)

$$|\psi'\rangle \propto |\pm n\rangle\;|\mp n\rangle. \tag{3.109}$$

Hint: you don't need the explicit form of $\hat{U}$, only the fact that it is unitary.

(b) Denote the probabilities of the two outcomes in part (a) by $P(A_+)$ and $P(A_-)$. Derive expressions for these two probabilities.

(c) For each of the two outcomes from measuring S_n on A, find the measurement probabilities for a subsequent S_z measurement on B, denoted by $P(B_+|A_\pm)$ and $P(B_-|A_\pm)$. Hence, show that

$$P(B_+) = P(B_+|A_+)P(A_+) + P(B_+|A_-)P(A_-) = \frac{1}{2} \tag{3.110}$$

$$P(B_-) = P(B_-|A_+)P(A_+) + P(B_-|A_-)P(A_-) = \frac{1}{2}, \tag{3.111}$$

regardless of n. Optional: generalize this to any B measurement axis.

2. Consider two spin-1/2 subsystems, with the density operator

$$\hat{\rho} = \frac{1}{2}|\uparrow\rangle\langle\uparrow| \,+\, \frac{1}{2}|\rightarrow\rangle\langle\rightarrow|, \tag{3.112}$$

   where

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right). \tag{3.113}$$

   Find the entanglement entropy.

3. Consider two distinguishable particles, A and B. The 2D Hilbert space of A is spanned by $\{|m\rangle, |n\rangle\}$, and the 3D Hilbert space of B is spanned by $\{|p\rangle, |q\rangle, |r\rangle\}$. The two-particle state is

$$|\psi\rangle = \frac{1}{3}\,|m\rangle|p\rangle + \frac{1}{\sqrt{6}}\,|m\rangle|q\rangle + \frac{1}{\sqrt{18}}\,|m\rangle|r\rangle + \frac{\sqrt{2}}{3}\,|n\rangle|p\rangle + \frac{1}{\sqrt{3}}\,|n\rangle|q\rangle + \frac{1}{3}\,|n\rangle|r\rangle. \tag{3.114}$$

   Find the entanglement entropy.

FURTHER READING

[1] Bransden & Joachain, §14.1—14.4, §17.1–17.5

[2] Sakurai, §3.9

[3] A. Einstein, B. Podolsky, and N. Rosen, *Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?*, Physical Review **47**, 777 (1935). [link]

[4] J. S. Bell, *On the Einstein-Podolsky-Rosen paradox*, Physics **1**, 195 (1964). [link]

[5] N. D. Mermin, *Bringing home the atomic world: Quantum mysteries for anybody*, American Journal of Physics **49**, 940 (1981). [link]

[6] A. Aspect, *Bell's inequality test: more ideal than ever*, Nature (News and Views) **398**, 189 (1999). [link]

[7] A. K. Ekert, *Quantum Cryptography Based on Bell's Theorem*, Physical Review Letters **67**, 661 (1991). [link]

[8] H. Everett, III, *The Theory of the Universal Wave Function* (PhD thesis), Princeton University (1956) [link]

[9] A. Albrecht, *Following a "collapsing" wave function*, Physical Review D 48, 3768 (1993). [link]

[10] A. Edelman and N. R. Rao, *Random matrix theory*, Acta Numerica **14**, 233 (2005). [link]