10 Interpreting Quantum Mechanics

In this final chapter, I want to explore the process of *measurement* in quantum mechanics. According to the Copenhagen interpretation, when we perform a measurement the state of the particle collapses onto an eigenstate of the corresponding operator, with the probabiliity of different results being given by the Born rule (2.69). This entails a departure from the unitary (and hence deterministic) time–evolution of our system as described by Schrödinger's equation. However, the Copenhagen interpretation does not tell us exactly what physical process should count as a 'measurement': does the observer need to be alive? to be human? to have taken PQM? Without such a prescription, how can we know when it is appropriate to evolve our state as $|\psi(t)\rangle = U(t)|\psi(0)\rangle$ and when instead it should collapse?

A further problem with measurement is that the states we measure usually correspond to what we consider to be 'classically sensible' quantities. This seems to imply that measurements invovle a *preferred* choice of basis for the system's Hilbert space. To give a famous example, we are all familiar with living cats and dead cats, but no-one has ever seen a cat that is simultaneously alive + dead. But why should quantum mechanics distinguish the basis

$$\{|\text{alive}\rangle, |\text{dead}\rangle\} \qquad \text{over} \qquad \left\{ \frac{|\text{alive}\rangle + |\text{dead}\rangle}{\sqrt{2}}, \frac{|\text{alive}\rangle - |\text{dead}\rangle}{\sqrt{2}} \right\} ?$$

In this chapter, we'll examine these issues from the perspective of *decoherence*. The formalism I present here is completely standard, and indeed decoherence is an important, well-established property of any quantum system. However, I should caution you that the jury is still out on whether this finally resolves the infamous problems with measurement in quantum mechanics.

10.1 The Density Operator

To get started, we must first realise that during a measurement, we cannot treat out quantum system as being isolated. Any form of measurement requires that we bring the system under study into contact with some form of measuring apparatus. Up to this point, we've assumed that we know the precise quantum state our system is in. While this may be possible for a small, isolated quantum system, we cannot possibly hope to know the exact quantum state of a macroscopic measuring device, which may easily contain $\sim 10^{23}$ atoms. Thus, to talk about measurements, we first need a way to describe systems *even when we're not sure which state they're in.* In fact, even in purely classical systems, there's always some uncertainty in our knowledge of the system: we never actually know the momentum of a single particle with infinite precision even in classical mechanics, because all our measurements are subject to some experimental error.

Let's now see how to incorporate such imprecision in our knowledge into quantum mechanics. Suppose we know only that our system is in one of the states $\{|\psi_\alpha\rangle\}$, and that the probability it is in state $|\psi_\alpha\rangle$ is p_α. It's important to be clear that we're *not* saying

that system is in state

$$\text{“ } |\Psi\rangle = \sum_\alpha \sqrt{p_\alpha}|\psi_\alpha\rangle \text{ ”} ,$$

because $|\Psi\rangle$ itself is a well–defined quantum state. Rather, we're admitting that we don't know the true state of the system, which could be any of the states $\{|\psi_\alpha\rangle\}$. Indeed, these states *do not need to form a complete set*, and *do not even need to be orthogonal*, although we will take them each to be correctly normalized $\langle\psi_\alpha|\psi_\alpha\rangle = 1$ for each α.

In this case, the average result we obtain when measuring the value of some observable Q is

$$\overline{Q} = \sum_\alpha p_\alpha \, \langle\psi_\alpha|Q|\psi_\alpha\rangle \, . \tag{10.1}$$

This expression combines the quantum expectation value of Q in the state $|\psi_\alpha\rangle$ (which may not be an eigenstate of Q), together with our lack of knowledge of the system's state, represented by the p_αs. For future use, it'll be convenient to describe this using a *density operator* $\rho : \mathcal{H} \to \mathcal{H}$, defined by

$$\rho = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| \tag{10.2}$$

where the p_α are the probabilities introduced above. Then we can write the average (10.1) as

$$\overline{Q} = \mathrm{tr}_{\mathcal{H}}(\rho\, Q) \, . \tag{10.3}$$

(To see this, suppose $\{|q_n\rangle\}$ is a complete set of eigenstates of Q, with eigenvalues $\{q_n\}$. Using $\{|q_n\rangle\}$ as a basis for $\mathcal{H}$ we have

$$\begin{aligned} \mathrm{tr}_{\mathcal{H}}(\rho\, Q) &= \sum_n \langle q_n|\rho\, Q|q_n\rangle = \sum_{n,\alpha} p_\alpha \langle q_n|\psi_\alpha\rangle \, \langle\psi_\alpha|Q|q_n\rangle \\ &= \sum_{n,\alpha} p_\alpha q_n |\langle q_n|\psi_\alpha\rangle|^2 = \sum_\alpha p_\alpha \langle\psi_\alpha|Q|\psi_\alpha\rangle \end{aligned} \tag{10.4}$$

as before.)

The density operator has the following three properties: First, it is an Hermitian operator

$$\rho^\dagger = \rho \, , \tag{10.5a}$$

reflecting the fact that the probabilities p_α must be real. Second,

$$\mathrm{tr}_{\mathcal{H}}(\rho) = 1 \tag{10.5b}$$

since the probabilities sum to one, and third

$$\langle\chi|\rho\,|\chi\rangle \geq 0 \qquad \text{for all } |\chi\rangle \in \mathcal{H} \tag{10.5c}$$

since probabilities are non-negative. We often write this property as $\rho \geq 0$ for short. In fact, these three properties can be taken to be the defining properties of a density operator, in the sense that *any* operator obeying these three properties is the density operator for

some system. To see this, suppose the eigenvectors of ρ are $|\phi_r\rangle$, with $\rho|\phi_r\rangle = \rho_r|\phi_r\rangle$. Then since $\rho = \rho^\dagger$ we have $\rho_r \in \mathbb{R}$. The remaining two properties tell us that $\sum_r \rho_r = 1$ and $\rho_r \geq 0$. Any set of real numbers $\{\rho_r\}$ obeying these conditions can be taken to be a probability distribution for some system. Note that since the $|\phi_r\rangle$ are eigenvectors of the Hermitian operator ρ, they're necessarily orthogonal, in contrast to the arbitrary set of states we used in (10.2).

If we have perfect knowledge of our system, meaning $\rho = |\psi\rangle\langle\psi|$ so that with probability 1 the system is in state $|\psi\rangle$, then we refer to it as *pure*. Correspondingly, if our knowledge of the state is incomplete, so that $\rho = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ with more than one $p_\alpha > 0$, we say that the system is in an *impure* or *mixed* state. This terminology is somewhat misleading, because it is really just our knowledge that is incomplete — the system itself is presumably in some perfectly well–defined quantum state, it's just that we don't know which one.

The density operator and the operators for the Hamiltonian and other observables encapsulate a complete, self–contained theory of quantum dynamics. If we have incomplete knowledge of the system's quantum state, then use of this formalism is mandatory. If we *do* happen to know that our system is initially in the precise quantum state $|\psi\rangle$, we can still use this apparatus by setting $\rho = |\psi\rangle\langle\psi|$, rather than using the TDSE, though in this case use of the density operator is optional.

10.1.1 The Bloch Sphere

As a simple example, consider a single spin-$\frac{1}{2}$ particle with $\{|\uparrow\rangle, |\downarrow\rangle\}$ forming a basis of $\mathcal{H} \cong \mathbb{C}^2$. If we know for sure that the system is in the state $|\uparrow\rangle$, then

$$\rho = |\uparrow\rangle\langle\uparrow| \,.$$

However, if we think there's only a $\frac{1}{2}$ chance that the system is actually in state $|\uparrow\rangle$, with a $\frac{1}{2}$ chance it might actually be in the state $|\downarrow\rangle$, then

$$\rho = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| = \frac{1}{2}\,1_{\mathcal{H}}$$

In this case, the average value of the spin along any axis is $\mathrm{tr}_{\mathcal{H}}(\rho\,\mathbf{S}) = 0$ and we'll see later that having ρ proportional to the identity matrix means we're maximally ignorant about the state of our system. As a further example, let $|\uparrow_x\rangle$ denote the eigenstate $S_x|\uparrow_x\rangle = \frac{\hbar}{2}|\uparrow_x\rangle$ of spin up along the x-axis. Then if we think there's probability $\frac{1}{2}$ our system is in state $|\uparrow\rangle$ and probability $\frac{1}{2}$ it's in the (non-orthogonal) state $|\uparrow_x\rangle$, then

$$\begin{aligned}
\rho &= \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\uparrow_x\rangle\langle\uparrow_x| \\
&= \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{4}(|\uparrow\rangle + |\downarrow\rangle)(\langle\uparrow| + \langle\downarrow|) \\
&= \frac{1}{4}\,1_{\mathcal{H}} + \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{4}|\uparrow\rangle\langle\downarrow| + \frac{1}{4}|\downarrow\rangle\langle\uparrow|
\end{aligned}$$

where we've used the result $|\uparrow_x\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ from section 5.3.4. With this density matrix, we find

$$\overline{S_x} = \frac{\hbar}{2} = \overline{S_z} \qquad \text{while} \qquad \overline{S_y} = 0\,,$$

reflecting the fact that we're more likely to have spin up than down along both the x and z-axes, but know nothing about the spin along the y-axis.

More generally, since any 2×2 Hermitian matrix can be written as a linear combination of the identity matrix and the the Pauli sigma matrices, we can write

$$\rho = \frac{1}{2}\,(1_{\mathcal{H}} + \mathbf{b}\cdot\boldsymbol{\sigma}) \tag{10.6}$$

for some vector $\mathbf{b}$, where we've used the fact that $\mathrm{tr}_{\mathcal{H}}(\boldsymbol{\sigma}) = 0$ and the condition $\mathrm{tr}_{\mathcal{H}}\rho = 1$ to fix the overall factor. Since $1 = \mathrm{tr}_{\mathcal{H}}\rho$ is the sum of it's eigenvalues, at least one must be positive. The other will also be non-negative (as required for their interpretation as probabilities) if

$$\det\,\rho = \frac{1}{4}(1 - \mathbf{b}\cdot\mathbf{b}) \geq 0\,. \tag{10.7}$$

Hence (10.6) is a well-defined density operator for our two–state system provided

$$|\mathbf{b}| \leq 1\,.$$

This condition is known as the *Bloch Ball*. Density matrices with $|\mathbf{b}| = 1$ on the *Bloch Sphere* correspond to pure states, where the system definitely has spin $+\hbar/2$ along the $\hat{\mathbf{b}}$-axis. On the other hand, states with $|\mathbf{b}| < 1$ must have both eigenvectors strictly positive, so there is no way to write such a density matrix as $|\uparrow_{\mathbf{n}}\rangle\langle\uparrow_{\mathbf{n}}|$ for any direction $\mathbf{n}$. For both mixed and pure states, the direction of $\mathbf{b}$ is said to define the *polarization* of the state: for any $\mathbf{b} \neq 0$, measurements of the spin will be preferentially aligned along $\mathbf{b}$.

10.2 Entropy

For pure states, where $\rho = |\psi\rangle\langle\psi|$ for some $|\psi\rangle$, it's easy to see that

$$\rho^n = \rho \qquad \text{(pure states)} \tag{10.8}$$

provided $|\psi\rangle$ is normalized. If an impure density operator has $p_\alpha = 0.99999999$ for some particular $|\psi_\alpha\rangle$, with the remaining probability spread in some way among other states, then although our knowledge of the system's state is imperfect, the effects of the impurity are likely to be negligible. On the other hand, if the density operator has $p_\alpha \leq 10^{-20}$ for every α so that a tremendous number of states are equally probable, then our knowledge of the true quantum state of a system is very poor indeed.

We'd like to have a way to quantify how much knowledge, or information, about a state we have once the probability distribution $\{p_i\}$ has been specified. To achieve this, define the *von Neumann entropy* $S(\rho)$ associated to a density operator by

$$S(\rho) = -\mathrm{tr}_{\mathcal{H}}(\rho\ln\rho)\,. \tag{10.9}$$

If $\{|\phi_r\rangle\}$ are the orthonormal eigenvectors of ρ then we can write

$$\ln\rho = \sum_r \ln(\rho_r)|\phi_r\rangle\langle\phi_r|\,.$$

Choosing any basis $\{|n\rangle\}$ for $\mathcal{H}$, we thus have

$$\begin{aligned} -\mathrm{tr}_{\mathcal{H}}(\rho \ln \rho) &= -\sum_n \left\langle n \left| \left(\sum_r \rho_r |\phi_r\rangle\langle\phi_r| \right) \left(\sum_{r'} \ln(\rho_{r'}) \, |\phi_{r'}\rangle\langle\phi_{r'}| \right) \right| n \right\rangle \\ &= -\sum_{n,r} \rho_r \ln(\rho_r) \;\; |\langle\phi_r|n\rangle|^2 = -\sum_r \rho_r \ln(\rho_r) \end{aligned} \tag{10.10}$$

in terms of the eigenvalues of the density operator.

Since $0 \leq \rho_r \leq 1$, it's easy to see from the form (10.10) that $S(\rho) \geq 0$ with $S(\rho) = 0$ iff ρ describes a pure state, where only one of the ρ_rs is non-zero (and hence equal to 1) as we have complete certainty about which state our system is in. We also claim that the maximum value of $S(\rho)$ is attained iff

$$\rho = \rho_{\max} = \frac{1}{\dim(\mathcal{H})} \, 1_{\mathcal{H}} \, . \tag{10.11}$$

When $\rho = \rho_{\max}$ all states are equally likely – meaning we have no idea about which state our system is actually in. To see that this indeed maximises the entropy, use the method of Lagrange multipliers to impose the constraint $\mathrm{tr}_{\mathcal{H}}(\rho) = 1$ and vary

$$S(\rho) - \lambda \left(\mathrm{tr}_{\mathcal{H}}(\rho) - 1 \right)$$

with respect to the probabilities and Lagrange multiplier λ. At an extremum,

$$\begin{aligned} 0 &= -\mathrm{tr}_{\mathcal{H}} \left[\delta\rho \, \ln \rho + \rho \rho^{-1} \delta\rho + \lambda \, \delta\rho \right] \\ 0 &= \delta\lambda \left(\mathrm{tr}_{\mathcal{H}}(\rho) - 1 \right) . \end{aligned} \tag{10.12}$$

In the first line, we've used the fact that $\mathrm{tr}(\rho \, \rho^{-1} \delta\rho) = \mathrm{tr}(\rho \, \delta\rho \, \rho^{-1})$ inside the trace, so the order of the variation in the logarithm doesn't matter. These equations must hold for arbitrary variations $\delta\rho$ and $\delta\lambda$, so the first tells us that

$$\rho = \mathrm{e}^{-\lambda - 1} 1_{\mathcal{H}} \, . \tag{10.13}$$

for some constant $\mathrm{e}^{-\lambda-1}$. Taking the trace, the second equation fixes the constant of proportionality so that

$$\rho = \rho_{\max} = \frac{1}{\dim(\mathcal{H})} \, 1_{\mathcal{H}} \, , \tag{10.14}$$

as claimed. The corresponding maximum entropy is

$$\begin{aligned} S(\rho_{\max}) &= -\mathrm{tr}_{\mathcal{H}} \left(\rho_{\max} \ln \rho_{\max} \right) \\ &= -\frac{\mathrm{tr}_{\mathcal{H}}(1_{\mathcal{H}})}{\dim(\mathcal{H})} \;\; \ln(\dim(\mathcal{H})^{-1}) \; = \ln \dim(\mathcal{H}) \, . \end{aligned} \tag{10.15}$$

Because it was defined as a trace, $S(\rho)$ doesn't depend on which basis we use to describe our Hilbert space.

10.2.1 The Gibbs Distribution

One of the main uses of the density operator and von Neumann entropy is in Quantum Statistical Mechanics. As an example, suppose we wish to extremize the entropy subject to both $\mathrm{tr}_{\mathcal{H}}(\rho) = 1$ and $\mathrm{tr}_{\mathcal{H}}(\rho H) = U$, saying that we know our system has a fixed average energy U. Then using two Lagrange multipliers λ and β, at an extremum we have

$$0 = \delta\left[S(\rho) - \lambda\left(\mathrm{tr}(\rho) \, - \, 1\right) - \beta\left(\mathrm{tr}(\rho H) - U\right)\right] \tag{10.16}$$

which gives the three conditions

$$\begin{aligned} 0 &= -\mathrm{tr}_{\mathcal{H}}\left[\delta\rho \, \left(\ln\rho + 1 + \beta H + \lambda\right)\right] \\ 0 &= \delta\lambda\left(\mathrm{tr}(\rho) - 1\right) \\ 0 &= \delta\beta\left(\mathrm{tr}_{\mathcal{H}}(\rho H) - U\right) \end{aligned} \tag{10.17}$$

Since these must hold for arbitrary variations, the first equation gives

$$\rho = \mathrm{e}^{-\beta H}\mathrm{e}^{-\lambda - 1}\,. \tag{10.18}$$

at a maximum of $S(\rho)$ with fixed energy. The second two conditions just enforce our constraints: to ensure $\mathrm{tr}_{\mathcal{H}}(\rho) = 1$ we must set $\mathrm{e}^{\lambda+1} = Z(\beta)$ where the constant

$$Z(\beta) = \mathrm{tr}_{\mathcal{H}}(\mathrm{e}^{-\beta H})\,. \tag{10.19}$$

is known as the *partition function* of our system. Thus, in a state of maximum entropy for fixed average energy, the density operator takes the form

$$\rho = \frac{1}{Z(\beta)}\mathrm{e}^{-\beta H} = \frac{1}{Z(\beta)}\sum_n \mathrm{e}^{-\beta E_n}|E_n\rangle\langle E_n|\,, \tag{10.20}$$

where in the final expression we have inserted a complete set of H eigenstates. This form of density operator is known as the *Gibbs distribution*, It plays a fundamental role in quantum statistical mechanics, as you'll see next term. β is usually denoted $1/\,k_{\mathrm{B}}T$ where T is called the *temperature* and k_{B} the Boltzmann constant. For fixed average energy U of the system, the temperature is determined by the constraint $\mathrm{tr}_{\mathcal{H}}(\rho H) = U$. In other words, the temperature T is determined by the average energy of the system. You'll work much more with the density operator and entropy if you take the Part II Statistical Mechanics course next term.

10.3 Reduced Density Operators

If our system comprises two (or more) identifiable subsystems A and B, then $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ so the full Hilbert space is the tensor product of the Hilbert spaces of the subsystems. Recall that a state $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ is called *entangled* if it cannot be written as a single product $|\phi\rangle \otimes |\chi\rangle$ of states $|\phi\rangle \in \mathcal{H}_A$ and $|\chi\rangle \in \mathcal{H}_B$.

We'll suppose A describes the system we're really interested in, whilst B is the 'environment'. That is, B describes the quantum state of everything in the Universe except

our immediate object of study A. Of course, we can't hope to know the precise quantum state of B.

We're going to be interested in the average value we obtain for measurements of a quantity Q that is an observable purely of A, represented on the full Hilbert space by $Q \otimes 1_B$, when the whole Universe is described by a density operator ρ_{AB}. We have

$$\overline{Q} = \mathrm{tr}_{\mathcal{H}_A \otimes \mathcal{H}_B}\big((Q \otimes 1_B)\,\rho_{AB}\,\big) = \mathrm{tr}_{\mathcal{H}_A}(Q\rho_A) \tag{10.21}$$

where we've used the fact that the traces can be performed independently. The second equality introduces the *reduced density operator* ρ_A of subsystem A, defined by

$$\rho_A = \mathrm{tr}_{\mathcal{H}_B}(\rho_{AB})\,, \tag{10.22}$$

taking the trace only over subsystem B.

The reduced density operator enables us to obtain expectation values of subsystem A's observables without bothering about the states of B. For example, suppose an atom is situated in a low-intensity radiation field. Every so often, a photon comes along. This photon may scatter off the atom, or be absorbed by the atom into an excited state which subsequently decays re-emitting the photon, or may even cause the atom to be temporarily ionized. If we wish to keep track of the whole system, then as more and more photons interact with the atom, we'd need to use a larger and larger Hilbert space encompassing further and further tensor products of the Hilbert spaces of individual photons. This is inconvenient, to say the least. However, if we're only really interested in the state of the atom, it's enough to keep track of the atom's reduced density operator, which refers solely to the Hilbert space of the atom.

10.4 Decoherence

We now show a very important result. Suppose the Universe itself is in a pure quantum state, so that $\rho_{AB} = |\Psi\rangle\langle\Psi|$ for some state $|\Psi\rangle$ written as

$$|\Psi\rangle = \sum_{a,\beta} c_{a,\beta}|a\rangle|\beta\rangle$$

in terms of orthonormal bases $\{|a\rangle\}$ for A and $\{|\beta\rangle\}$ for B. Then the reduced density matrix ρ_A is

$$\begin{aligned}\rho_A = \mathrm{tr}_{\mathcal{H}_B}\big(\rho_{AB}\big) &= \mathrm{tr}_{\mathcal{H}_B}\left(\sum_{a,a',\beta,\beta'} c_{a,\beta}\,\overline{c_{a',\beta'}}|a\rangle|\beta\rangle\ \langle a'|\langle\beta'|\right) \\ &= \sum_{a,a'} C_{a,a'}|a\rangle\langle a'|\,,\end{aligned} \tag{10.23}$$

where now

$$C_{aa'} = \sum_{\beta} c_{a,\beta}\,\overline{c_{a',\beta}}\,. \tag{10.24}$$

If the original state $|\Psi\rangle$ was *simple*, so that (say) the $c_{a,\beta}$ are non–zero only for a single value of β, for which $c_{a,\beta} = c_a$, then $C_{aa'} = c_a\overline{c_{a'}}$ with no sum. Then (10.23) is a pure

density operator for the state $|\phi\rangle = \sum_a c_a|a\rangle$. However, if $|\Psi\rangle$ is a more general, entangled state then the sum in (10.24) means that ρ_A is the density operator for a mixed state.

For example, suppose our Universe consists of just two spin-$\frac{1}{2}$ particles, prepared in the pure but entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\big)$$

where $|\uparrow\downarrow\rangle = |\uparrow\rangle|\downarrow\rangle$ *etc.*. The associated density operator is

$$\begin{aligned}\rho_{AB} &= |\psi\rangle\langle\psi| \\ &= \frac{1}{2}\big(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow| - |\uparrow\downarrow\rangle\langle\downarrow\uparrow| - |\downarrow\uparrow\rangle\langle\uparrow\downarrow|\big)\,.\end{aligned} \tag{10.25}$$

Tracing over the second spin gives the reduced density operator

$$\rho_A = \mathrm{tr}_{\mathcal{H}_B}\big(\rho_{AB}\big) = \frac{1}{2}\big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\big) = \frac{1}{2}\,1_A \tag{10.26}$$

which is mixed, and indeed the state of maximum entropy.

Although we won't prove this here, the von Neumann entropy (10.9) obeys

$$S(\rho_{AB}) \le S(\rho_A) + S(\rho_B) \tag{10.27}$$

where ρ_A and ρ_B are the reduced density matrices for the two subsystems. The equality is saturated if and only if the two subsystems are uncorrelated (unentangled) so that $\rho_{AB} = \rho_A \otimes \rho_B$. This property is known as *subadditivity* and it tells us that the entropy of a whole is no greater than the sum of entropies of its parts. It follows from subadditivity that if $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ then

$$S(\rho_{ABC}) \le S(\rho_A) + S(\rho_{BC}) \le S(\rho_A) + S(\rho_B) + S(\rho_C) \tag{10.28}$$

but in fact something stronger is true: we have

$$S(\rho_{ABC}) + S(\rho_B) \le S(\rho_{AB}) + S(\rho_{BC}) \tag{10.29}$$

which is known as *strong subadditivity* and was proved in 1973 by Elliott Lieb and Mary Beth Ruskai. To interpret it, we consider AB and BC are each subsystems of ABC, with $AB \cap BC = B$. Strong subadditivity states that the entropy of the whole is no greater than the entropies of the overlapping subsystems AB and BC, even when the entropy of the overlap B is removed.

10.5 Time Evolution of Density Operators and Reduced Density Operators

In the Schrödinger picture, states evolve in time according to

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \tag{10.30}$$

where $U(t) = \mathrm{e}^{-\mathrm{i}Ht/\hbar}$ in the case that the Hamiltonian itself is time–independent. This implies that the density operator evolves (like any other operator) as

$$\rho(t) = U(t)\rho(0)\,U^{-1}(t)\,, \tag{10.31}$$

Figure 19: *Strong subadditivity of the von Neumann entropy.*

or

$$\mathrm{i}\hbar\frac{d\rho}{dt} = U(t)(H\rho(0) - \rho(0)H)U^{-1}(t) = [H, \rho(t)] \tag{10.32}$$

infinitesimally. This is the quantum analogue of Liouville's equation $d\rho/dt = \{H, \rho\}$ in Classical Dynamics, which governs the time evolution of a probability density ρ on phase space. In particular, if the density operator can be written purely in terms of the Hamiltonian then it is time–independent. The Gibbs ensemble we obtained above is a good example.

To obtain the time evolution of an arbitrary expectation value (of a quantity that has no explicit time dependence in the Schrödinger picture) we use (10.32) to find

$$\mathrm{i}\hbar\frac{d}{dt}\mathrm{tr}_{\mathcal{H}}(\rho\, Q) = \mathrm{tr}_{\mathcal{H}}\left([H, \rho]Q\right) = \mathrm{tr}_{\mathcal{H}}(\rho\,[Q, H]) \tag{10.33}$$

where the last equality uses the cyclicity of the trace. We know from before that the rate of change of the expectation value of Q in any pure quantum state is given by the expectation value of $[Q, H]/\mathrm{i}\hbar$. Equation (10.33) states that – even when our knowledge of the quantum state is imprecise – the expected rate of change of Q is the appropriately weighted average of the rates of change of Q for each of the possible states of the system.

Let's now consider how the reduced density operator evolves. Suppose that at $t = 0$ both A and B start in pure quantum states $|\phi\rangle$ and $|\chi\rangle$, respectively. Initially then,

$$\rho_{AB}(0) = |\Psi_0\rangle\langle\Psi_0| \tag{10.34}$$

where

$$|\Psi_0\rangle = |\phi\rangle|\chi\rangle\,, \tag{10.35}$$

so that the two systems are unentangled. The whole system will evolve unitarily in time via the operator $U_{AB}(t)$ built from the Hamiltonian of the full system. This means that the reduced density operator for system A evolves as

$$\rho_A(t) = \mathrm{tr}_{\mathcal{H}_B}\big(U_{AB}(t)|\Psi_0\rangle\langle\Psi_0|U_{AB}^{-1}(t)\big) = \sum_{\beta}\langle\beta|U_{AB}(t)|\Psi_0\rangle\,\langle\Psi_0|U_{AB}^{-1}(t)|\beta\rangle \tag{10.36}$$

where we're using the orthonormal basis $\{|\beta\rangle\}$ of $\mathcal{H}_B$ to perform the trace.

We're motivated to define operators $M_\beta(t) : \mathcal{H}_A \to \mathcal{H}_A$ by

$$M_\beta(t) = \langle\beta|U_{AB}(t)|\chi\rangle = \mathrm{tr}_{\mathcal{H}_B}\big(U_{AB}(t)|\chi\rangle\langle\beta|\big)\,, \tag{10.37}$$

where we not that this is an operator acting on $\mathcal{H}_A$ since we've used the time evolution operator $U_{AB}(t)$ for $\mathcal{H}_A \otimes \mathcal{H}_B$. Since $U_{AB}(t)$ is unitary, the $M_\beta(t)$s obey a completeness relation

$$\sum_\beta M_\beta^\dagger(t) M_\beta(t) = \sum_\beta \langle\chi|\langle\beta|U_{AB}(t)|\chi\rangle = 1_A \tag{10.38}$$

provided $|\chi\rangle$ was properly normalized. Putting all this together,

$$\rho_A(t) = \sum_\beta M_\beta(t)\rho_A(0)M_\beta^\dagger(t) \tag{10.39}$$

is the evolution of the reduced density matrix.

In the exceptional case that the full Hamiltonian does not couple A and B, so that $H = H_A \otimes I + I \otimes H_B$ and $U_{AB}(t) = U_A(t) \otimes U_B(t)$, we have

$$M_\beta(t) = \langle\beta|U_B(t)|m\rangle\; U_A(t)\,.$$

The completeness relation then shows that

$$\rho_A(t) = U_A(t)\rho_A(0)U_A^{-1}(t)\,. \tag{10.40}$$

Thus, if A starts in a pure state *and it does not interact with the environment* then it will remain in a pure state. However, in every realistic case, subsystems are coupled to each other — however weak, there is some term H_{AB} in the Hamiltonian that is not diagonal with respect to the splitting $\mathcal{H}_A \otimes \mathcal{H}_B$. In the presence of an interaction term H_{AB}, the time evolution operator is not generically a product of the time evolution operators of the two subsystems, and states of A and B will typically become entangled, leading to $\rho_A(t)$ describing a mixed state at some later time t.

In general, interactions between an experimental system and the wider environment mean that the state of the whole Universe rapidly becomes entangled. Since we don't keep track of all the details of the environment, sooner or later we're obliged to describe our experimental system by its reduced density operator, which will be impure. The tendency for subsystems to evolve from pure quantum states to impure states through interactions with the environment is known as *quantum decoherence*. Trying to isolate a system from the environment so as to prevent it from becoming impure is one of the main challenges to be overcome in building a practical quantum computer.

10.5.1 Decoherence and Measurement

We're at last ready to explore what all this has to do with measurements in quantum mechanics.

Let's suppose our system A consists of a single qubit, either $|\uparrow\rangle$ or $|\downarrow\rangle$. To keep things simple we'll imagine the environment (or measuring apparatus) has only three possible

states, $|0\rangle$, $|1\rangle$ and $|2\rangle$. An ideal measurement will change the state of the measuring apparatus without affecting the system A under study. Let's suppose the measurement process is described via evolution by a unitary operator U, representing the usual evolution of the system and apparatus by a coupled Hamiltonian. We suppose our apparatus is designed in such a way that U is defined by[80]

$$\begin{aligned} U|\uparrow\rangle \otimes |0\rangle &= |\uparrow\rangle\big(\sqrt{1-p}\,|0\rangle + \sqrt{p}\,|1\rangle\big) \\ U|\downarrow\rangle \otimes |0\rangle &= |\downarrow\rangle\big(\sqrt{1-p}\,|0\rangle + \sqrt{p}\,|2\rangle\big)\,. \end{aligned} \tag{10.41}$$

In other words, the apparatus starts in the 'quiescent' state $|0\rangle$. When we bring it into contact with our system A, the apparatus changes its state with probability p, becoming $|1\rangle$ if A is in $|\uparrow\rangle$, or $|2\rangle$ if A is $|\downarrow\rangle$. The apparatus is not perfectly efficient, so stays in the quiescent state with probability $1-p$.

Now let's suppose the system A is initially described by some density matrix

$$\rho_A = \begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix}$$

For this evolution, we have

$$\begin{aligned} M_0 &= \langle 0|U|0\rangle = \sqrt{1-p}\;1_A \\ M_1 &= \langle 1|U|0\rangle = \sqrt{p}\;|\uparrow\rangle\langle\uparrow| \\ M_2 &= \langle 2|U|0\rangle = \sqrt{p}\;|\downarrow\rangle\langle\downarrow| \end{aligned} \tag{10.42}$$

and these indeed obey $\sum_\beta M_\beta^\dagger M_\beta = 1_A$. Contact with our measuring apparatus thus causes ρ_A to evolve as

$$\rho_A = \begin{pmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix} \mapsto \begin{pmatrix} \rho_{\uparrow\uparrow} & (1-p)\rho_{\uparrow\downarrow} \\ (1-p)\rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{pmatrix}\,, \tag{10.43}$$

suppressing the off–diagonal components. These off-diagonal components encode possible superpositions between $|\uparrow\rangle$ and $|\downarrow\rangle$, so as our system becomes entangled with the measuring apparatus, we're less likely to find it in such a superposition.

Let's go further and look at successive evolution. The probability the apparatus changed away from the quiescent state during one measurement period was p, so if we suppose this measurement took a short time δt, then we can a rate $\Gamma = p/\delta t$. After a total time $t = N\delta t$, the off–diagonal terms will thus be suppressed by

$$(1-p)^n = \left(1 - \Gamma\frac{t}{N}\right)^N \approx \mathrm{e}^{-\Gamma t} \tag{10.44}$$

for large N. In particular, if we initially prepare A to be in the superposition

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle \qquad \text{where } |a|^2 + |b|^2 = 1$$

[80] By assigning appropriate values to U acting on $|1\rangle$ and $|2\rangle$, this U can indeed be completed to a unitary operator (exercise!).

then eventually, A's density matrix will become

$$\lim_{t\to\infty} \rho_A(t) = \lim_{t\to\infty} \begin{pmatrix} |a|^2 & a\overline{b}\,\mathrm{e}^{-\Gamma t} \\ \overline{a}b\,\mathrm{e}^{-\Gamma t} & |b|^2 \end{pmatrix} = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix} .$$

This is sometimes called *phase damping*, because the late–time density matrix only has real entries.

Now we come to the punchline. What exactly was it that made our measurement cause A to evolve into either $|\uparrow\rangle$ or $|\downarrow\rangle$, but not a superposition? Clearly, this must have had something to do with our choice of U in (10.41). To get an idea, let's imagine the two–state system A actually corresponds to a dust particle which can sit either at x_0 or x_1. The measuring apparatus may be a photon which, with probability p, can scatter into a different direction, depending on where the dust is located. The fact that U is defined *wrt* to the preferred basis $|\uparrow\rangle = |x_0\rangle$ and $|\downarrow\rangle = |x_1\rangle$ then corresponds to the fact that the interactions are *local*: The interactions we can described between the dust and photons will be built out of operators such as $\mathbf{X}_{\rm dust}$, so decoherence will take place in the basis $\{|x_0\rangle, |x_1\rangle\}$ where the dust particle has a definite location, rather than the $\big(|x_0\rangle \pm |x_1\rangle\big)/\sqrt{2}$ basis.

Locality of interactions is one of the key features of all physical laws, and has deep–rooted origins in quantum field theory. Combined with decoherence, many physicists believe[81] that this explains why we see cats either in the state $|\text{alive}\rangle$ or the state $|\text{dead}\rangle$, but never $\big(|\text{alive}\rangle + |\text{dead}\rangle\big)/\sqrt{2}$.

10.6 Quantum Mechanics or Hidden Variables?

Einstein was never happy with the probabilistic nature of quantum mechanics. He, Podolsky and Rosen devised a thought experiment that they hoped would show quantum mechanics was incomplete as a theory of Nature.

In the EPR thought experiment, an electron and a positron[82] are produced in a state with net spin 0, perhaps by the decay of some nucleus from a spin-0 excited state to a lower spin-0 state. The electron and positron travel in opposite directions, each carrying the same amount of momentum. At some distance from the decaying nucleus Alice detects the electron and measures the component of its spin in a direction $\mathbf{a}$ of her choice. Since electrons have spin-$\frac{1}{2}$, Alice inevitably discovers either $+\hbar/2$ or $-\hbar/2$. Meanwhile Bob, who is sitting at a similar distance on the opposite side of the nucleus, detects the positron and measures its spin in some direction $\mathbf{b}$ of *his* choice.

We're free to choose the $\mathbf{z}$-axis to be aligned with Alice's direction $\mathbf{a}$. Since the electron–positron system has combined spin zero, it must be in the state

$$|\text{EPR}\rangle = \frac{1}{\sqrt{2}}\,\big(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\big) \tag{10.45}$$

[81] The matter is still not fully resolved. The leading proponents of the 'measurement=decoherence' paradigm are H.D. Zeh and W. Zurek, see for example Zurek, W., *Quantum Darwinism*, Nature Physics **5**(3), 181 (2009) for a review. Prominent opponents include R. Kastner, see *e.g.* Kastner, R., Stud. Hist. Phil. Science **B48** 56 (2014).

[82] Here we'll describe a slightly sharper version of EPR's original thought experiment, due to Bohm. The positron is the antiparticle of the electron, predicted in the relativistic theory by Dirac's equation. It has the same mass and spin as an electron, but opposite sign electric charge.

that entangles the separate spins of the electron and positron. We'll call this the EPR state. According to the Copenhagen interpretation, when Alice measures $+\hbar/2$ for the electron spin, the system collapses into the state

$$|\psi'\rangle = |\uparrow\rangle|\downarrow\rangle\,. \tag{10.46}$$

Thus, whilst before Alice's measurement the amplitude for the *positron* to have spin $+\hbar/2$ along $\mathbf{a}$ was $1/2$, after she has measured the electron spin, there is no chance that the positron also has spin up along the same axis.

The state of the positron corresponding to definitely having spin $+\hbar/2$ along the $\mathbf{b}$-axis is

$$|\uparrow_{\mathbf{b}}\rangle = \cos\left(\frac{\theta}{2}\right) \mathrm{e}^{-\mathrm{i}\phi/2}|\uparrow\rangle + \sin\left(\frac{\theta}{2}\right) \mathrm{e}^{\mathrm{i}\phi/2}|\downarrow\rangle \tag{10.47}$$

as we found in the second problem sheet, where $\theta = \cos^{-1}(\mathbf{a}\cdot\mathbf{b})$ and ϕ is the azimuthal angle around $\hat{\mathbf{z}} = \hat{\mathbf{a}}$. Given that after Alice's measurement the positron is certainly in state $|\downarrow\rangle$, it follows from (10.47) that the probability Bob measures spin up along $\mathbf{b}$ is

$$|\langle\uparrow_{\mathbf{b}}|\downarrow\rangle|^2 = \sin^2\left(\frac{\theta}{2}\right)\,. \tag{10.48}$$

In particular, there is only a small probability he would find spin-up along a direction closely aligned with Alice's choice $\mathbf{a}$.

We've supposed that Alice measures first, but if the electron and positron are far apart when the measurements are made, a light signal sent to Bob by Alice when she makes her measurement would not have arrived at Bob by the time he makes his measurement, and *vice versa*. In these circumstances, relativity tells us that the order in which the measurements appear to be made depend on the velocity of the observer who is judging the matter. Consequently, for consistency the predictions of quantum mechanics must be independent of who is supposed to make the first measurement and thus collapse the state. This condition is satisfied by the above discussion, since the final probability depends only on $\mathbf{a}\cdot\mathbf{b}$ and is thus symmetric between Alice and Bob.

What bothered EPR is that after Alice's measurement there is a direction ($\mathbf{a}$) along which Bob can never find $+\hbar/2$ for the positron's spin, and this direction depends on what exactly Alice chooses to measure. This fact seems to imply that the positron somehow 'knows' what Alice measured for the electron, and the collapse of the entangled wavefunction

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right) \qquad \longrightarrow \qquad |\uparrow\rangle|\downarrow\rangle$$

apparently confirms this suspicion. Since relativity forbids news of Alice's work on the electron from influencing the positron at the time of Bob's measurement, EPR argued that the required information must have travelled out in the form of a *hidden variable* which was correlated at the time of the nuclear decay with a matching hidden variable in the electron. These hidden variables would then explain the probabilistic nature of quantum mechanics — QM would contain no uncertainties once replaced by a 'better' theory taking into account these hidden variables.

10.6.1 Bell's Inequality

Remarkably, Bell was able to show that the predictions of *any* theory of hidden variables are in conflict with the predictions of quantum mechanics.

Suppose we assume that the result of measuring the electron's spin in the **a**-direction is completely determined by the values taken by hidden variables in addition to **a**. We suppose there are n such hidden variables, so that the result of measuring the electron's spin is a function

$$s_{\rm e} : \mathbb{R}^3 \times \mathbb{R}^n \to \left\{ -\frac{\hbar}{2}, +\frac{\hbar}{2} \right\} \tag{10.49}$$

that returns either $+\hbar/2$ or $-\hbar/2$, depending only on the direction $\mathbf{a} \in \mathbb{R}^3$ along which we measure the spin and the values $\mathbf{v} \in \mathbb{R}^n$ of the hidden variables carried by the electron. In other words, if Alice knew the value of the hidden variable $\mathbf{v} \in \mathbb{R}^n$, we could predict *with certainty* the result of measuring the component of the electron's spin along any direction **a**. Alice is only uncertain of the outcome because she does *not* know the values of the hidden variables. Similarly, the result of measuring the positron's spin along **b** is some function $s_{\rm p}(\mathbf{b}, \mathbf{v})$. We have

$$s_{\rm e}(\mathbf{a}, \mathbf{v}) + s_{\rm p}(\mathbf{a}, \mathbf{v}) = 0 \tag{10.50}$$

by conservation of angular momentum.

Let's suppose that $\mathbf{v}$ has a probability distribution $p(\mathbf{v})$, such that the probability dP that $\mathbf{v}$ lies in the infinitesimal volume $d^n\mathbf{v}$ is

$$dP = p(\mathbf{v})\, d^n\mathbf{v}\,. \tag{10.51}$$

Then the expectation value of interest is

$$\begin{aligned} \langle s_{\rm e}(\mathbf{a}, \mathbf{v})\, s_{\rm p}(\mathbf{b}, \mathbf{v}) \rangle &= \int p(\mathbf{v})\, s_{\rm e}(\mathbf{a}, \mathbf{v})\, s_{\rm p}(\mathbf{b}, \mathbf{v})\, d^n\mathbf{v} \\ &= -\int p(\mathbf{v})\, s_{\rm e}(\mathbf{a}, \mathbf{v})\, s_{\rm e}(\mathbf{b}, \mathbf{v})\, d^n\mathbf{v}\,. \end{aligned} \tag{10.52}$$

Now suppose Bob sometimes measures the spin of the positron parallel to $\mathbf{b}'$ rather than **b**. The fact that $s_{\rm p}(\mathbf{b}, \mathbf{v})^2 = \frac{\hbar^2}{4}$ allows us to write

$$\begin{aligned} \langle s_{\rm e}(\mathbf{a}, \mathbf{v})\, s_{\rm p}(\mathbf{b}, \mathbf{v}) \rangle - \langle s_{\rm e}(\mathbf{a}, \mathbf{v})\, s_{\rm p}(\mathbf{b}', \mathbf{v}) \rangle &= -\int p(\mathbf{v})\, s_{\rm e}(\mathbf{a}, \mathbf{v})\, [s_{\rm p}(\mathbf{b}, \mathbf{v}) - s_{\rm p}(\mathbf{b}', \mathbf{v})]\, d^n\mathbf{v} \\ &= -\int p(\mathbf{v})\, s_{\rm e}(\mathbf{a}, \mathbf{v})\, s_{\rm e}(\mathbf{b}, \mathbf{v})\, \left[1 - \frac{4}{\hbar^2}\, s_{\rm e}(\mathbf{b}, \mathbf{v})\, s_{\rm e}(\mathbf{b}', \mathbf{v}) \right] d^n\mathbf{v}\,. \end{aligned} \tag{10.53}$$

The expression $[1 - 4s_{\rm e}(\mathbf{b}, \mathbf{v}) s_{\rm e}(\mathbf{b}', \mathbf{v})]$ is non–negative, while the product $s_{\rm e}(\mathbf{a}, \mathbf{v})\, s_{\rm e}(\mathbf{b}, \mathbf{v})$ fluctuates between $\pm\hbar^2/4$. Hence we obtain the bound

$$\begin{aligned} \left| \langle s_{\rm e}(\mathbf{a}, \mathbf{v})\, s_{\rm p}(\mathbf{b}, \mathbf{v}) \rangle - \langle s_{\rm e}(\mathbf{a}, \mathbf{v})\, s_{\rm p}(\mathbf{b}', \mathbf{v}) \rangle \right| &\le \frac{\hbar^2}{4} \int p(\mathbf{v}) \left[1 - \frac{4}{\hbar^2}\, s_{\rm e}(\mathbf{b}, \mathbf{v})\, s_{\rm e}(\mathbf{b}', \mathbf{v}) \right] d^n\mathbf{v} \\ &= \frac{\hbar^2}{4} - \langle s_{\rm e}(\mathbf{b}, \mathbf{v})\, s_{\rm p}(\mathbf{b}', \mathbf{v}) \rangle \end{aligned} \tag{10.54}$$

This is *Bell's inequality*. It must hold for any three unit vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{b}'$ if the probabilistic nature of QM really comes from some underlying hidden variables.

We now show that quantum mechanics itself *violates* Bell's inequality. To do this, we must treat the spins as operators and compute their expectation values in some state, and we'll choose the EPR state (10.45). Because $|\mathrm{EPR}\rangle$ has total spin zero, it obeys

$$(\mathbf{S}_\mathrm{e} \otimes 1_\mathrm{p} + 1_\mathrm{e} \otimes \mathbf{S}_\mathrm{p})|\mathrm{EPR}\rangle = 0$$

so that we always find the spin of the electron and positron to be anti-aligned whenever we measure them along any one given axis, no matter in which direction this is. In particular, this allows us to write

$$\begin{aligned}\big(\mathbf{a}\cdot\mathbf{S}_\mathrm{e}\otimes 1_\mathrm{p}\big)\big(1_\mathrm{e}\otimes\mathbf{b}\cdot\mathbf{S}_\mathrm{p}\big) &= -\big(\mathbf{a}\cdot\mathbf{S}_\mathrm{e}\otimes 1_\mathrm{p}\big)\big(\mathbf{b}\cdot\mathbf{S}_\mathrm{e}\otimes 1_\mathrm{p}\big)\\ &= -(\mathbf{a}\cdot\mathbf{S}_\mathrm{e}\,\mathbf{b}\cdot\mathbf{S}_\mathrm{e})\otimes 1_\mathrm{p}\end{aligned} \tag{10.55}$$

when acting on $|\mathrm{EPR}\rangle$. For any (single) spin-$\frac{1}{2}$ particle, the spin operator obeys

$$\mathbf{a}\cdot\mathbf{S}\;\mathbf{b}\cdot\mathbf{S} = \frac{\hbar^2}{4}\mathbf{a}\cdot\mathbf{b} + \frac{\mathrm{i}\hbar}{2}(\mathbf{a}\times\mathbf{b})\cdot\mathbf{S}\,.$$

Therefore

$$\langle\mathbf{a}\cdot\mathbf{S}_\mathrm{e}\;\mathbf{b}\cdot\mathbf{S}_\mathrm{p}\rangle_\mathrm{EPR} = -\frac{\hbar^2}{4}\mathbf{a}\cdot\mathbf{b} - \frac{\mathrm{i}\hbar}{2}(\mathbf{a}\times\mathbf{b})\cdot\langle\mathbf{S}_\mathrm{e}\rangle_\mathrm{EPR}\,. \tag{10.56}$$

Finally, we note that the expectation value of the electron's spin

$$\langle\mathrm{EPR}|\mathbf{S}_\mathrm{e}\otimes 1_\mathrm{p}|\mathrm{EPR}\rangle = 0$$

along any axis. This is clear for the z-axis, but since $|\mathrm{EPR}\rangle$ has no preferred direction it must be true of the other directions also. Thus we find that the EPR state obeys

$$\langle\mathbf{a}\cdot\mathbf{S}_\mathrm{e}\otimes\mathbf{b}\cdot\mathbf{S}_\mathrm{p}\rangle_\mathrm{EPR} = -\frac{\hbar^2}{4}\mathbf{a}\cdot\mathbf{b} \tag{10.57}$$

for any two directions $\mathbf{a}$ and $\mathbf{b}$. Using this correlation in either side of Bell's inequality we find

$$\mathrm{LHS} = \frac{\hbar^2}{4}|\mathbf{a}\cdot(\mathbf{b}-\mathbf{b}')| \qquad \text{whereas} \qquad \mathrm{RHS} = \frac{\hbar^2}{4}(1-\mathbf{b}\cdot\mathbf{b}')$$

In particular, suppose $\mathbf{a}$ and $\mathbf{b}$ are unit vectors, with $\mathbf{a}\cdot\mathbf{b}=0$ and $\mathbf{b}' = \mathbf{b}\cos\alpha + \mathbf{a}\sin\alpha$. Then we find

$$\mathrm{LHS} = \frac{\hbar^2}{4}|\sin\alpha| \qquad \text{whereas} \qquad \mathrm{RHS} = \frac{\hbar^2}{4}(1-\cos\alpha)$$

and it's easy to see that Bell's inequality is violated for all $\alpha \neq 0, \pi/2$. The predictions of quantum mechanics are thus inconsistent with the existence of hidden variables.

10.6.2 The CHSH Inequality

There's a slightly simpler context in which we can see the essentials of the conflict between quantum probability and hidden variables theories, discovered by Clauser, Horne, Shimony & Holt.

Suppose Alice and Bob are each sent a two-state system as in the EPR experiment. Alice chooses to measure one of two possible observables, either A_1 and A_2. Similarly, Bob can choose to measure either B_1 or B_2. To keep things simple, let's assume that there are only two possible outcomes, $+1$ and -1, for the result when measuring any of the four quantities A_i or B_i. We'll require that

$$[A_i, B_j] = 0 \qquad \text{for } i = 1, 2$$

so that the measurement Alice makes does not interfere with the one made by Bob. However, we do not require that either $[A_1, A_2] = 0$ or $[B_1, B_2] = 0$.

Now consider the observable

$$C = (A_1 + A_2)B_1 + (A_1 - A_2)B_2\,. \tag{10.58}$$

In a hidden variable theory, the outcomes of measuring the A_i or B_j would be entirely determined by the value $\mathbf{v}$ of some hidden variables carried by the state, so we'd have functions

$$a_i : \mathbb{R}^n \to \{+1, -1\} \qquad \text{and} \qquad b_j : \mathbb{R}^n \to \{+1, -1\}\,. \tag{10.59}$$

The average value of C in a hidden variable theory is

$$\langle C\rangle = \int \big(\big[a_1(\mathbf{v}) + a_2(\mathbf{v})\big]b_1(\mathbf{v}) + \big[a_1(\mathbf{v}) - a_2(\mathbf{v})\big]b_2(\mathbf{v})\big)\; p(\mathbf{v})\, d^n\mathbf{v}\,, \tag{10.60}$$

where again $p(\mathbf{v})$ is the probability density for the hidden variables. Since each $a_i(\mathbf{v})$ can take only the values ± 1, either $\mathbf{v}$ is such that the outcomes of A_1 and A_2 are different, in which case

$$a_1(\mathbf{v}) + a_2(\mathbf{v}) = 0 \qquad \text{while} \qquad a_1(\mathbf{v}) - a_2(\mathbf{v}) = \pm 2\,,$$

or else the value of $\mathbf{v}$ ensures that the outcomes of A_1 and A_2 are the same, so that

$$a_1(\mathbf{v}) - a_2(\mathbf{v}) = 0 \qquad \text{while} \qquad a_1(\mathbf{v}) + a_2(\mathbf{v}) = \pm 2\,.$$

Thus, whatever the value of $\mathbf{v}$, only one of the two terms in the integral (10.60) can be non-zero. Multiplying the non-zero term by $b_i(\mathbf{v}$ at most changes its sign, so we always have

$$\big[a_1(\mathbf{v}) + a_2(\mathbf{v})\big]b_1(\mathbf{v}) + \big[a_1(\mathbf{v}) - a_2(\mathbf{v})\big]b_2(\mathbf{v} = \pm 2$$

fluctuating as $\mathbf{v}$ moves around. Consequently, we can bound the average by

$$-2 \le \langle C\rangle \le 2\,. \tag{10.61}$$

This is known as the *CHSH inequality* and it's obeyed in any hidden variables theory.

Now let's look at the same observable in quantum theory. Since the eigenvalues of A_i and B_j are just ± 1, we have $A_i^2 = 1$ and $B_j^2 = 1$. Consequently one finds

$$\begin{aligned} C^2 &= (A_1 + A_2)^2 B_1 + (A_1 - A_2)^2 B_2^2 + (A_1 + A_2)(A_1 - A_2) B_1 B_2 + (A_1 - A_2)(A_1 + A_2) B_2 B_1 \\ &= 4 - A_1 A_2 B_1 B_2 + A_2 A_1 B_1 B_2 - A_1 A_2 B_2 B_1 + A_2 A_1 B_2 B_1 \\ &= 4 - [A_1, A_2]\,[B_1, B_2]\,, \end{aligned} \tag{10.62}$$

where the first equality uses our assumption $[A_i, B_j = 0$. We have that

$$|\langle [A_1, A_2] \rangle| \leq |\langle A_1 A_2 \rangle| + |\langle A_2 A_1 \rangle| \leq 2\,, \tag{10.63}$$

with the final bound again coming since the eigenvalues of A_i are just ± 1. Thus we have $\langle C^2 \rangle \leq 8$ in quantum theory. Finally, since $\langle C^2 \rangle \leq \langle C \rangle^2$ for any Hermitian operator, we obtain the *Cirel'son bound*

$$-2\sqrt{2} \leq \langle C \rangle \leq 2\sqrt{2} \tag{10.64}$$

in quantum theory. This shows that quantum theory permits a *wider* range of values for $\langle C \rangle$ than allowed by the CHSH bound (10.61) for hidden variable theories.

Again, it's straightforward to show that the EPR state saturate the Cirel'son inequality. Recall from (10.57) that

$$\langle \hat{\mathbf{a}} \cdot \boldsymbol{\sigma}_{\mathrm{e}} \otimes \hat{\mathbf{b}} \cdot \boldsymbol{\sigma}_{\mathrm{p}} \rangle_{\mathrm{EPR}} = -\hat{\mathbf{a}} \cdot \hat{\mathbf{b}} = -\cos\theta \tag{10.65}$$

for any two unit vectors. (We're using the Pauli matrices rather than spins $\mathbf{S} = \hbar\boldsymbol{\sigma}/2$ to ensure the eigenvalues are ± 1 as in the CHSH & Cirel'son bounds.) To apply this to the Cirel'son case, let A_i be the Pauli matrices for the electron and B_j those for the proton and choose A_2, B_1, A_1, B_2 to all lie in (say) the (x, z)-plane at angles 0, $\pi/4$, $\pi/2$ and $3\pi/4$ to the z-axis, respectively. Then

$$\langle A_1 B_1 \rangle = \langle A_1 B_2 \rangle = \langle A_2 B_1 \rangle = -\frac{1}{\sqrt{2}}$$

for the EPR state, while

$$\langle A_2 B_2 \rangle = +\frac{1}{\sqrt{2}}\,.$$

Consequently, we have

$$\langle C \rangle_{\mathrm{EPR}} = -2\sqrt{2} \tag{10.66}$$

saturating the Cirel'son bound.

Impressively, this inequality has actually been tested experimentally by Aspect *et al.*, following the suggestion of Clauser *et al.*[83] In the experiment, two photons are emitted from successive decays of excited states of calcium. The first comes from the decay of a

[83] See Freedman, S. & Clauser, J., *Experimental Test of Local Hidden Variable Theories*, Phys. Rev. Lett. **28**, 938 (1972) an Aspect, A. & Roger, G. *Experimental Realization of the Einstein–Podolski–Rosen–Bohm Gedankenexperiment: A New Violation of Bell's Inequalities*, Phys. Rev. Lett. **49**, 91 (1982). An earlier version of the experiment was performed by Kocher, C. and Commins, E. Phys. Rev. Lett. **18**, 575 (1979).

parity-even state with $j = 0$ to a short-lived parity-odd state with $j = 1$, while the second photon comes from the decay of this short-lived state to a further x parity-even state of $j = 0$ (of lower energy than the initial state). The photons are directed into a combination of polarizers and photomultipliers which read out ± 1 according to whether the photons are found to be linearly polarized along some directions **a** and **b**. The experiment found

$$|\langle C\rangle_{\rm expt}| = 2.697 \pm 0.0515 \tag{10.67}$$

This is slightly less than the idealised result $|\langle C\rangle_{\rm EPR}| = 2\sqrt{2} \approx 2.828$, with most of the disagreement coming because the polarizers used in the experiment were not perfectly efficient. When the efficiency of the polarizers is taken into account, Aspect's result is in good agreement with what was is predicted by quantum mechanics, and in clear violation of the CHSH bound for hidden variable theories.

In the final problem set, you'll explore an even more striking conflict between the predictions of Quantum Mechanics and classical hidden variables by considering entanglement between three qubits rather than two.