A crash course in real-world quantum mechanics

Basic postulates for an isolated quantum system

- Pure states (minimum-uncertainty states) of a physical system are represented by vectors Ψ in a complex Hilbert space. Ψ may be thought of as the most efficient and complete mathematical representation of everything that you know about the state of the system.
- A system's dynamics are specified by a Hermitian operator **H**, and time-evolution is given by the Schrödinger Equation $i\hbar\dot{\Psi} = \mathbf{H}\Psi$.
- Mutually exclusive measurement outcomes correspond to orthogonal projection operators $\{\mathbf{P}_0, \mathbf{P}_{1,\ldots}\}$, and the probability of a particular outcome i is given by $|\mathbf{P}_i \Psi|^2$. For a complete measurement specification we must have $\sum_i \mathbf{P}_i = \mathbf{1}$. Note that if each of the $\mathbf{P}_i$ is rank one, the outcome probabilities are just the square magnitudes of the components of Ψ in some orthonormal basis.

Note that Ψ itself is NOT directly observable! But it does represent sufficient information to compute the sampling distribution for any possible measurement we might wish to perform...

Dirac notation for quantum states

States may be written as 'ket'

$$|\Psi_a\rangle \rightarrow \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix}, \qquad 2$$

or 'bra'

$$\langle\Psi_a| \rightarrow \begin{pmatrix} a_0^* & a_1^* & a_2^* \end{pmatrix}. \qquad 3$$

By convention, state vectors are assumed to be normalized: $\sum_i |a_i|^2 = 1$.

Bras and kets are related by Hermitian conjugation:

$$|\Psi_a\rangle = (\langle\Psi_a|)^\dagger, \qquad \langle\Psi_a| = (|\Psi_a\rangle)^\dagger. \qquad 4$$

The inner product of a bra and a ket is a complex number:

$$\langle \Psi_a \| \Psi_b \rangle = \begin{pmatrix} a_0^* & a_1^* & a_2^* \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ b_2 \end{pmatrix} = a_0^* b_0 + a_1^* b_1 + a_2^* b_2. \qquad 5$$

One typically drops one of the vertical bars and writes $\langle \Psi_a | \Psi_b \rangle$. Note that $\langle \Psi_a | \Psi_b \rangle = 0$ implies that the two vectors are orthogonal. Normalized states satisfy $\langle \Psi | \Psi \rangle = 1$.

The outer product of a ket and a bra is a linear operator (matrix):

$$|\Psi_a\rangle\langle\Psi_b| = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} \begin{pmatrix} b_0^* & b_1^* & b_2^* \end{pmatrix} = \begin{pmatrix} a_0 b_0^* & a_0 b_1^* & a_0 b_2^* \\ a_1 b_0^* & a_1 b_1^* & a_1 b_2^* \\ a_2 b_0^* & a_2 b_1^* & a_2 b_2^* \end{pmatrix}. \qquad 6$$

It is often convenient to work with basis kets or bras. For example,

$$|\Psi_a\rangle \rightarrow a_0|0\rangle + a_1|1\rangle + a_2|2\rangle$$

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \qquad \#$$

$$\langle \Psi_a | \rightarrow a_0^* \langle 0| + a_1^* \langle 1| + a_2^* \langle 2|, \qquad 7$$

where $\langle i|j\rangle = \delta(i,j)$. Hence,

$$(\, a_0|0\rangle + a_2|2\rangle \,)(\, b_0^*\langle 0| + b_1^*\langle 1| \,) = a_0 b_0^* |0\rangle\langle 0| + a_2 b_0^* |2\rangle\langle 0| + a_0 b_1^* |0\rangle\langle 1| + a_2 b_1^* |2\rangle\langle 1|$$

$$\rightarrow \begin{pmatrix} a_0 b_0^* & a_0 b_1^* & 0 \\ 0 & 0 & 0 \\ a_2 b_0^* & a_2 b_1^* & 0 \end{pmatrix}. \qquad 8$$

Of course, the same physical state $|\Psi_a\rangle$ can be expressed in (uncountably) many different bases. For example, if

$$|\Psi_a\rangle = a_0|0\rangle + a_1|1\rangle, \qquad 9$$

then in the basis $\left\{ |x\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), |y\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \right\}$,

$$|\Psi_a\rangle = \frac{1}{\sqrt{2}}(a_0 + a_1)|x\rangle + \frac{1}{\sqrt{2}}(a_0 - a_1)|y\rangle. \qquad 10$$

Hermitian conjugate of operators in Dirac notation: $(|a\rangle\langle b|)^\dagger = |b\rangle\langle a|$.

Operators act on kets from the left and on bras from the right. Using orthonormal basis vectors, it's easy to compute the results. For example,

$$\begin{aligned} \mathbf{O} &= |0\rangle\langle 1| + |1\rangle\langle 0|, \\ \mathbf{O}|\Psi_a\rangle &= (\, |0\rangle\langle 1| + |1\rangle\langle 0| \,)(\, a_0|0\rangle + a_1|1\rangle + a_2|2\rangle \,) \\ &= a_1|0\rangle + a_0|1\rangle, \\ \langle \Psi_a|\mathbf{O} &= (\, a_0^*\langle 0| + a_1^*\langle 1| + a_2^*\langle 2| \,)(\, |0\rangle\langle 1| + |1\rangle\langle 0| \,) \\ &= a_0^*\langle 1| + a_1^*\langle 0|. \end{aligned} \qquad 11$$

The outer product of any vector with itself is a (rank one) projection operator:

$$|\Psi\rangle\langle\Psi| = \mathbf{P}_\Psi,$$
$$(\mathbf{P}_\Psi)^2 = |\Psi\rangle\langle\Psi|\Psi\rangle\langle\Psi| = \mathbf{P}_\Psi. \quad 12$$

The Schrödinger Equation

The dynamics of a quantum system is specified by a Hermitian operator **H**, called the Hamiltonian.

Time-evolution of quantum states is given by the Schrödinger Equation,

$$i\hbar\frac{d}{dt}|\Psi\rangle = \mathbf{H}|\Psi\rangle, \quad 13$$

where $\hbar = h/2\pi$ and $h \simeq 6.6261 \times 10^{-34}$ [J sec] is Planck's constant.

For finite-dimensional systems, (13) is a coupled system of linear ordinary differential equations. If the physical system is truly isolated (autonomous), then **H** must be constant and we may write the formal solution

$$|\Psi(t)\rangle = \exp\left[\frac{-i}{\hbar}\mathbf{H}t\right]|\Psi(0)\rangle. \quad 14$$

In some cases it is actually possible to compute the operator exponential, which is defined (as usual) via Taylor expansion:

$$\exp[i\alpha\mathbf{O}] = \mathbf{1} + i\alpha\mathbf{O} - \frac{\alpha^2}{2}\mathbf{O}^2 - i\frac{\alpha^3}{3!}\mathbf{O}^3 + \frac{\alpha^4}{4!}\mathbf{O}^4 + \cdots. \quad 15$$

Here α is an arbitrary (real) scalar.

Note that if **O** is a Hermitian operator,

$$(\exp[i\alpha\mathbf{O}])^\dagger = \mathbf{1} - i\alpha\mathbf{O} - \frac{\alpha^2}{2}\mathbf{O}^2 + i\frac{\alpha^3}{3!}\mathbf{O}^3 + \frac{\alpha^4}{4!}\mathbf{O}^4 + \cdots \quad 16$$

and

$$\exp[i\alpha\mathbf{O}](\exp[i\alpha\mathbf{O}])^\dagger = (\exp[i\alpha\mathbf{O}])^\dagger \exp[i\alpha\mathbf{O}] = \mathbf{1}. \quad 17$$

That is, $\exp[i\alpha\mathbf{O}]$ is a ***unitary*** operator.

In the case of the Schrödinger Equation, we write

$$\mathbf{T}(t_2, t_1) = \exp\left[\frac{-i}{\hbar}\mathbf{H}(t_2 - t_1)\right] \quad 18$$

and refer to $\mathbf{T}(t_2, t_1)$ as the system's unitary "propagator" or "time development operator" from time t_1 to t_2.

Note that

$$(\mathbf{T}(t_2, t_1))^{-1} = (\mathbf{T}(t_2, t_1))^\dagger \sim \mathbf{T}(t_1, t_2) \quad 19$$

can be thought of as an operator that evolves a state backwards in time.

Recall that unitary operators may be thought of as the complex generalization of rotation operators in a real vector space. Hence **quantum evolution for an isolated system corresponds to a "rigid rotation" of the state space**. As a consequence, time evolution preserves the norms of individual state vectors, and preserves the inner product (angle) between arbitrary pairs of state vectors.

Note that by taking the Hermitian conjugate of the entire Schrödinger Equation, we get a time evolution equation for bras:

$$-i\hbar\frac{d}{dt}\langle\Psi| = \langle\Psi|\mathbf{H},$$
$$\langle\Psi(t_2)| = \langle\Psi(t_1)|\mathbf{T}(t_1,t_2). \quad (20)$$

Accordingly,

$$\langle\Psi_a(t_2)|\Psi_b(t_2)\rangle = \langle\Psi_a(t_1)|\mathbf{T}(t_1,t_2)\mathbf{T}(t_2,t_1)|\Psi_b(t_1)\rangle = \langle\Psi_a(t_1)|\Psi_b(t_1)\rangle, \quad (21)$$

as noted above.

Quantum computation

Let the initial state of a quantum register be given by

$$|x\rangle \in \text{span}\{|0\rangle, |1\rangle, |2\rangle, |3\rangle, |4\rangle, \ldots\}.$$

We can think of this as something like the input to a function $F(x)$. Physical implementation of the function evaluation corresponds to unitary evolution:

$$|x\rangle \mapsto \mathbf{U}|x\rangle \equiv |F(x)\rangle.$$

Note that the last equivalence is an association we make in order to view the unitary evolution as a computation. Since quantum mechanical evolution is unitary, we clearly have

$$\mathbf{U}\frac{1}{\sqrt{2}}(|i\rangle + |j\rangle) = \frac{1}{\sqrt{2}}(\mathbf{U}|i\rangle + \mathbf{U}|j\rangle) = \frac{1}{\sqrt{2}}(|F(i)\rangle + |F(j)\rangle).$$

This type of "parallelism" appears to be a key ingredient in quantum computation. Note that since the final state vector is not directly observable, we cannot simply read-out one or more evaluations of our choosing. Rather, we must do something sneaky to extract ***global*** information about the behavior of F. As one might imagine, this involves making a final measurement in a basis other than the computational basis $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle, |4\rangle, \ldots\}$. This effectively creates interference between different computational paths.

Intrinsic uncertainty

Note that for ***any*** pure state $|\Psi\rangle$, we are guarenteed to be able to find uncountably many measurements $\{\mathbf{P}_0, \mathbf{P}_{1,\ldots}\}$ for which the result cannot be predicted with certainty. Hence quantum mechanics contains intrinsic uncertainty – no matter how much care you take in the "accurate" preparation of a quantum system, many of its qualities are unsharply defined.

Nonorthogonality and imperfect distinguishability

The following simple example is intended to highlight our first genuine example of a mysterious property of quantum mechanics that follows directly from the rules for representation and prediction.

Consider a nice simple two-dimensional Hilbert space with basis kets $|x\rangle$ and $|y\rangle$.

Given an arbitrary pair of states

$$\begin{aligned} |\Psi_c\rangle &= c_x|x\rangle + c_y|y\rangle, \\ |\Psi_d\rangle &= d_x|x\rangle + d_y|y\rangle, \end{aligned} \tag{28}$$

under what conditions is it possible to find a (standard) measurement that can distinguish them with zero probability of error?

Recall that a standard measurement is specified by a complete set of orthogonal projectors. Since for now we are working in just two dimensions, we actually only need to specify a single ket $|\phi\rangle$. Then unambiguously,

$$\begin{aligned} \mathbf{P}_1 &= |\phi\rangle\langle\phi|, \\ \mathbf{P}_2 &= \mathbf{1} - \mathbf{P}_1. \end{aligned} \tag{29}$$

In the current scenario, we are trying to pick $|\phi\rangle$ such that

$$\begin{aligned} \Pr(1|c) &= \langle\Psi_c|\mathbf{P}_1|\Psi_c\rangle = 1, \\ \Pr(1|d) &= \langle\Psi_d|\mathbf{P}_1|\Psi_d\rangle = 0, \\ \Pr(2|c) &= \langle\Psi_c|\mathbf{P}_2|\Psi_c\rangle = 0, \\ \Pr(2|d) &= \langle\Psi_d|\mathbf{P}_2|\Psi_d\rangle = 1. \end{aligned} \tag{30}$$

In order to satisfy the first condition, we clearly need to choose

$$|\phi\rangle = |\Psi_c\rangle. \tag{31}$$

As a consequence

$$\Pr(1|d) = \langle\Psi_d|\mathbf{P}_1|\Psi_d\rangle = |c_x^* d_x + c_y^* d_y|^2, \tag{32}$$

and we find that our two states Ψ_c and Ψ_d are not perfectly distinguishable ***unless*** they have zero overlap:

$$\Pr(1|d) = 0 \quad \textbf{iff} \quad \langle\Psi_c|\Psi_d\rangle = 0. \tag{33}$$

Hopefully it should be clear that among all possible pairs of vectors in a Hilbert space, only a ***vanishing*** fraction are orthogonal!

And yet, according to our quantum representation rule, every vector in the Hilbert space corresponds to a distinct physical state of the system – that is, to a distinct *preparation* procedure.

Even though quantum measurement theory allows for non-projective measurements (see third term of this course), it is nonetheless a theorem that

- No measurement can distinguish nonorthogonal states, with zero probability of error, in a single trial.

It is a profound mystery that quantum mechanics presents us with such a huge space of possible physical states without allowing us perfectly to distinguish between them. Why is it that we can "put more information into" the preparation of a quantum system than we can "get back out" in measurements of that very same system? In a sense it's embarassing that we don't yet have a good answer, but some of the most insightful scientists I know believe that this is the single most important question for contemporary research in quantum theory.

Ensembles of quantum states; the density operator

Let's say we're working in a nice, simple two-dimensional Hilbert space and that we've chosen orthonormal basis kets $|x\rangle$ and $|y\rangle$.

For the following discussion, we'll need to define two state vectors

$$\begin{aligned} |\Psi_A\rangle &= a_x|x\rangle + a_y|y\rangle, \\ |\Psi_B\rangle &= b_x|x\rangle + b_y|y\rangle. \end{aligned} \qquad 25$$

Suppose I ask you to perform a series of N measurements on this system (here N is just a large integer), corresponding to the projectors

$$\begin{aligned} \mathbf{P}_x &= |x\rangle\langle x|, \\ \mathbf{P}_y &= |y\rangle\langle y|. \end{aligned} \qquad 26$$

The trick is, in this series of measurements I will sometimes prepare the initial state $|\Psi_A\rangle$ (with probability p) and sometimes $|\Psi_B\rangle$ (with probability $1-p$). That is, I will be giving you a ***mixed*** ensemble of quantum states. How shall we predict the overall number of times n_x we expect to obtain the measurement outcome x?

According to simple probability theory,

$$\begin{aligned} n_x &= N[\Pr(\Psi_A)\Pr(x|\Psi_A) + \Pr(\Psi_B)\Pr(x|\Psi_B)] \\ &= N[p\langle\Psi_A|\mathbf{P}_x|\Psi_A\rangle + (1-p)\langle\Psi_B|\mathbf{P}_x|\Psi_B\rangle] \\ &= N\big[p|a_x|^2 + (1-p)|b_x|^2\big]. \end{aligned} \qquad 27$$

Note that since $0 \le p \le 1$, the quantity n_x/N is bounded from below by the smaller of $|a_x|^2$ and $|b_x|^2$. In particular, if both of these quantities are nonzero than n_x must also be greater than zero.

A very different expression for n_x would be obtained if, instead of a mixed ensemble, I were to present you with a 'coherent superposition' of the states $|\Psi_A\rangle$ and $|\Psi_B\rangle$, corresponding to the 'pure' state $|\Psi(p_A,p_B)\rangle$

$$\begin{aligned} |\Psi(p_A,p_B)\rangle &= p_A|\Psi_A\rangle + p_B|\Psi_B\rangle \\ &= (p_A a_x + p_B b_x)|x\rangle + (p_A a_y + p_B b_y)|y\rangle. \end{aligned} \qquad 28$$

(Note that we should be careful in choosing p_A and p_B such that $|\Psi(p_A,p_B)\rangle$ is normalized.) In this case, we would predict

$$n_x = N\langle \Psi(p_A,p_B)\,|\mathbf{P}_x|\,\Psi(p_A,p_B)\,\rangle$$
$$= N|p_A a_x + p_B b_x|^2. \qquad 29$$

Note that in certain cases, *e.g.* $p_A a_x = -p_B b_x \neq 0$, it is possible to choose p_A, p_B such that $n_x = 0 < |a_x|^2, |b_x|^2$ through the phenomenon of *destructive interference*. This is the truly important distinction between coherent superpositions (of the type that produce a single pure state) and incoherent admixtures (of the type that produce a mixed ensemble of quantum states).

A simplifying notation can be introduced for performing computations with mixed quantum ensembles. If the states composing the ensemble are labelled $|\Psi_i\rangle$ and have probabilities p_i, then the ***density operator*** for this ensemble is defined as

$$\boldsymbol{\rho} = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|. \qquad 30$$

Note that $\boldsymbol{\rho}$ is indeed an operator on the Hilbert space, and has the form of a linear combination of projection operators. However, the ensemble representation used to define a density operator is not necessarily also a spectral decomposition, as the various $|\Psi_i\rangle$ that constitute an ensemble do not need to be mutually orthogonal.

The density operator is automatically Hermitian, and furthermore has the property that

$$\mathrm{Tr}\,\boldsymbol{\rho} = 1. \qquad 31$$

Here Tr denotes the 'trace' operation

$$\mathrm{Tr}\,\boldsymbol{\rho} = \sum_k \langle k|\boldsymbol{\rho}|k\rangle, \qquad 32$$

where $\{|k\rangle\}$ is ***any*** orthonormal basis for the Hilbert space – the numerical result is independent of choice of basis.

In particular, since $\boldsymbol{\rho}$ is Hermitian we can chose to take the trace in its own eigenbasis, which makes it clear that

$$\mathrm{Tr}\,\boldsymbol{\rho} = \sum_i \lambda_i^{\rho}, \qquad 33$$

where λ_i^{ρ} are the eigenvalues of $\boldsymbol{\rho}$. Note that if $\boldsymbol{\rho}$ happens to be available in matrix form, we can further make use of the fact that the sum of the eigenvalues of a matrix is equal to the sum of its diagonal elements.

Density operators can represent either pure states,

$$\boldsymbol{\rho} = |\Psi\rangle\langle\Psi|, \qquad 34$$

or mixed states

$$\boldsymbol{\rho} = \sum_i p_i |\Psi_i\rangle\langle\Psi_i| \qquad 35$$

where there is more than one $p_i > 0$.

Note that in the former (pure state) case $\boldsymbol{\rho}$ is a true projection operator, so

$$\textbf{pure}: \quad \boldsymbol{\rho}^2 = \boldsymbol{\rho}. \qquad 36$$

In particular, $\mathrm{Tr}\,\boldsymbol{\rho}^2 = 1$ for a pure state.

For a mixed state, however, we can use the spectral decomposition to show that $\mathrm{Tr}\,\boldsymbol{\rho}^2 < 1$. We start by writing

$$\boldsymbol{\rho}^2 = \left(\sum_i \lambda_i^\rho \mathbf{P}_i^\rho \right)^2$$
$$= \sum_i (\lambda_i^\rho)^2 \mathbf{P}_i^\rho, \qquad 37$$

and note that since $\mathrm{Tr}\,\boldsymbol{\rho} = \sum_i \lambda_i^\rho = 1$, each of the λ_i^ρ must be strictly less than one for a mixed state. Hence the eigenvalues of $\boldsymbol{\rho}^2$, which are equal to the $(\lambda_i^\rho)^2$, must add up to *less than* one.

Joint state space for two subsystems

Suppose we have two *independent* quantum systems. It seems clear that we can separately consider the representation of their physical states in two independent Hilbert spaces. Labelling the systems A and B, we can simply chose state vectors

$$|\Psi_A\rangle \in H_A, \qquad 3$$

and

$$|\Psi_B\rangle \in H_B. \qquad 4$$

What if we need to bring these systems together and let them interact?

The joint state space for two such systems corresponds to the ***tensor product*** of H_A and H_B, denoted $H_{AB} = H_A \otimes H_B$.

Let N_A be the dimension of H_A, and N_B the dimension of H_B. If $\{|1_A\rangle, |2_A\rangle, |3_A\rangle, \dots\}$ is a complete orthonormal basis for H_A and $\{|1_B\rangle, |2_B\rangle, |3_B\rangle, \dots\}$ is a complete orthonormal basis for H_B, then $H_A \otimes H_B$ is the Hilbert space of dimension $N_{AB} = N_A N_B$ spanned by the vectors of the form $|i_A\rangle \otimes |j_B\rangle$. (Note that by extension, this means we can build a quantum register whose state lives in a Hilbert space of dimension $2^L - 1$ from L constituent qubits.)

Hence arbitrary states in H_{AB} have the form

$$|\Psi_{AB}\rangle = \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} c_{ij} |i_A\rangle \otimes |j_B\rangle. \qquad 5$$

As long as we fix an ordering for the new basis states $|i_A\rangle \otimes |j_B\rangle$, the set of $N_A N_B$ complex coefficients can be used as a vector representation for kets in H_{AB}.

The tensor product operation between vectors has the following properties:

1. Linearity: $(\alpha |\Psi_A\rangle) \otimes |\Psi_B\rangle = \alpha (|\Psi_A\rangle \otimes |\Psi_B\rangle)$, where α is a complex number
2. Distributivity: $|\Psi_A\rangle \otimes (|\Psi_B^1\rangle + |\Psi_B^2\rangle) = |\Psi_A\rangle \otimes |\Psi_B^1\rangle + |\Psi_A\rangle \otimes |\Psi_B^2\rangle$.
3. 'Commutativity': formally, $|\Psi_A\rangle \otimes |\Psi_B\rangle$ is the same as $|\Psi_B\rangle \otimes |\Psi_A\rangle$. In practice however, it is wise to use consistent ordering.

4. Adjoint: $(|\Psi_A\rangle \otimes |\Psi_B\rangle)^\dagger = \langle\Psi_A| \otimes \langle\Psi_B|$.

5. Scalar product: $(\langle\Psi_A^1| \otimes \langle\Psi_B^1|)(|\Psi_A^2\rangle \otimes |\Psi_B^2\rangle) = \langle\Psi_A^1|\Psi_A^2\rangle\langle\Psi_B^1|\Psi_B^2\rangle$.

It is important to note that basis kets $|i_A\rangle \otimes |j_B\rangle \in H_{AB}$ thus inherit orthogonality from their 'factors' in H_A and H_B.

Entanglement

The most profound consequence of this mathematical rule for representation of joint states is that there exist $|\Psi_{AB}\rangle \in H_{AB}$ that cannot be expressed the tensor product of a state $|\Psi_A\rangle \in H_A$ with a state $|\Psi_B\rangle \in H_B$. Such 'nonfactorizable' states are said to be ***entangled***.

For example, let's consider two two-dimensional systems. Say we have chosen orthonormal bases $\{|0_A\rangle, |1_A\rangle\}$ for H_A and $\{|0_B\rangle, |1_B\rangle\}$ for H_B. Then H_{AB} is spanned by the four states

$$|0_A\rangle \otimes |0_B\rangle, \quad |0_A\rangle \otimes |1_B\rangle, \quad |1_A\rangle \otimes |0_B\rangle, \quad |1_A\rangle \otimes |1_B\rangle. \tag{6}$$

Factorizable (nonentangled) states in H_{AB} are all of the form

$$\begin{aligned} |\Psi_{AB}^{fac}\rangle &= (c_0^A|0_A\rangle + c_1^A|1_A\rangle) \otimes (c_0^B|0_B\rangle + c_1^B|1_B\rangle) \\ &= c_0^A c_0^B |0_A\rangle \otimes |0_B\rangle + c_0^A c_1^B |0_A\rangle \otimes |1_B\rangle \\ &\quad + c_1^A c_0^B |1_A\rangle \otimes |0_B\rangle + c_1^A c_1^B |1_A\rangle \otimes |1_B\rangle. \end{aligned} \tag{7}$$

That is, a certain relationship exists between the coefficients of the four basis states in H_{AB}.

A simple example of an entangled state, whose coefficients do not exhibit the above relationship, is

$$\begin{aligned} |\Psi_{AB}\rangle &= \frac{1}{\sqrt{2}}(|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle) \\ &\neq |\Psi_A\rangle \otimes |\Psi_B\rangle. \end{aligned} \tag{8}$$

When the joint state of two subsystems is entangled, ***there is no way to assign a pure quantum state to either subsystem alone***. As we shall see below, it is possible to ascribe *mixed* quantum states to each of the subsystems considered alone, but first we'll need to have a look at operators on H_{AB}.

Tensor products of operators

If **A** is an operator on H_A and **B** is an operator on H_B, then

$$\mathbf{A} \otimes \mathbf{B} \tag{9}$$

is a valid operator on H_{AB}. Its action on an arbitrary state

$$|\Psi_{AB}\rangle = \sum_{i,j} c_{ij} |i_A\rangle \otimes |j_B\rangle \tag{10}$$

is defined by

$$(\mathbf{A} \otimes \mathbf{B})|\Psi_{AB}\rangle = \sum_{i,j} c_{ij}(\mathbf{A}|i_A\rangle) \otimes (\mathbf{B}|j_B\rangle). \quad 11$$

Note that the usual relationship holds between projectors on the joint state space and outer-products of joint state vectors:

$$\begin{aligned}(|\Psi_A\rangle \otimes |\Psi_B\rangle)(\langle\Psi_A| \otimes \langle\Psi_B|) &= |\Psi_A\rangle\langle\Psi_A| \otimes |\Psi_B\rangle\langle\Psi_B| \\ &= \mathbf{P}_A \otimes \mathbf{P}_B. \quad 13\end{aligned}$$

Hence any complete set of joint projectors (summing to the identity operator on H_{AB}) specifies a complete measurement.

As was the case with state vectors, linear combinations of tensor-product operators are also valid opeators on H_{AB}:

$$\mathbf{O}_{AB} = \sum_m c_m \mathbf{A}_m \otimes \mathbf{B}_m. \quad 14$$

Hence, not all operators on a joint state space are factorizable.

Given subsystem density operators $\boldsymbol{\rho}_A$ and $\boldsymbol{\rho}_B$, we can form a tensor-product density operator that describes a mixed ensemble of states in H_{AB}:

$$\boldsymbol{\rho}_{AB} = \boldsymbol{\rho}_A \otimes \boldsymbol{\rho}_B. \quad 15$$

In general, one can form convex combinations of such $\boldsymbol{\rho}_{AB}$ to construct new joint density operators, which may or may not be factorizable.

One can also construct joint density operators directly from ensembles of pure states in H_{AB}. For instance, the density operator corresponding to the entangled state described above is

$$\begin{aligned}|\Psi_{AB}\rangle &= \frac{1}{\sqrt{2}}[|0_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle] \\ \boldsymbol{\rho}_{AB} &= |\Psi_{AB}\rangle\langle\Psi_{AB}| \\ &= \frac{1}{2}\begin{bmatrix} |0_A\rangle\langle 0_A| \otimes |0_B\rangle\langle 0_B| + |0_A\rangle\langle 1_A| \otimes |0_B\rangle\langle 1_B| \\ +|1_A\rangle\langle 0_A| \otimes |1_B\rangle\langle 0_B| + |1_A\rangle\langle 1_A| \otimes |1_B\rangle\langle 1_B| \end{bmatrix}, \quad 16\end{aligned}$$

and in general

$$\boldsymbol{\rho}_{AB} = \sum_i p_i |\Psi^i_{AB}\rangle\langle\Psi^i_{AB}|. \quad 17$$

Note that operators on a tensor-product space can be expressed as complex matrices o_{kl}:

$$\mathbf{O}_{AB} = \sum_{kl} o_{kl}|k_{AB}\rangle\langle l_{AB}|, \quad 18$$

where the summations both run over a complete set of N_{AB} basis vectors.

Given matrix representations for subsystem operators **A** and **B**, it is customary to choose an ordering for the basis states of the joint space such that

$$\mathbf{A}\otimes\mathbf{B}\leftrightarrow\begin{pmatrix} a_{11}B & a_{12}B & a_{13}B & \\ a_{21}B & a_{22}B & a_{23}B & \cdots \\ a_{31}B & a_{32}B & a_{33}B & \\ \vdots & & & \ddots \end{pmatrix}. \qquad 19$$

For example if $\{|1_A\rangle, |2_A\rangle, \dots\}$ is the orthnormal basis for H_A used in defining the matrix representation of A, and similarly for H_B, then

$$\begin{aligned} |1_{AB}\rangle &\leftrightarrow |1_A\rangle\otimes|1_B\rangle, \\ |2_{AB}\rangle &\leftrightarrow |1_A\rangle\otimes|2_B\rangle, \\ |3_{AB}\rangle &\leftrightarrow |1_A\rangle\otimes|3_B\rangle, \\ &\vdots \\ |(N_B+1)_{AB}\rangle &\leftrightarrow |2_A\rangle\otimes|1_B\rangle, \\ &\vdots \end{aligned} \qquad 20$$

As a result, the common class of operators $\mathbf{1}^A\otimes\mathbf{B}$ will have block-diagonal representations.

Partial trace and reduced density operators

We can now define the partial trace operation. Let $\boldsymbol{\rho}_{AB}$ be a density operator on H_{AB}:

$$\boldsymbol{\rho}_{AB}=\sum_{ijkl}\rho_{ijkl}|i_A\rangle\otimes|j_B\rangle\langle k_A|\otimes\langle l_B|, \qquad 36$$

where the summations are take over orthonormal bases for H_A and H_B. We define the partial trace of $\boldsymbol{\rho}_{AB}$ over the B subsystem to be

$$\begin{aligned} \tilde{\boldsymbol{\rho}}_A &\equiv \mathrm{Tr}_B[\boldsymbol{\rho}_{AB}] \\ &= \sum_{m=1}^{N_B}\sum_{i,k=1}^{N_A}\rho_{imkm}|i_A\rangle\langle k_A| \\ &= \sum_{i,k=1}^{N_A}\left(\sum_{m=1}^{N_B}\rho_{imkm}\right)|i_A\rangle\langle k_A| \end{aligned} \qquad 38$$

Here $\tilde{\boldsymbol{\rho}}_A$ is called the 'reduced density operator' for subsystem A. It provides the best possible representation of subsystem A within H_A, when the joint state of A and B is entangled/nonfactorizable. A notationally convenient (but mathematically imprecise) way of computing the partial trace is as follows:

$$\begin{aligned}\mathrm{Tr}_B[\boldsymbol{\rho}_{AB}] &= \sum_{m=1}^{N_B} \langle m_B | \boldsymbol{\rho}_{AB} | m_B \rangle \\ &= \sum_{m=1}^{N_B} \langle m_B | \left(\sum_{ijkl} \rho_{ijkl} | i_A \rangle \otimes | j_B \rangle \langle k_A | \otimes \langle l_B | \right) | m_B \rangle \\ &= \sum_{m=1}^{N_B} \sum_{i,k=1}^{N_A} \rho_{imkm} | i_A \rangle \langle k_A |. \end{aligned} \tag{39}$$

Note that if we start with a pure entangled state and take the partial trace over one subsystem, the reduced density operator for the remaining subsystem will represent a mixed state! Hence we see that entanglement between a system of interest and "reservoir" degrees of freedom removes coherence and gives rise to excess uncertainties...

Finally, let us see that a pair of systems that starts out in a factorizable initial state can evolve into an entangled state via Hamiltonian evolution. Let's work again with our same two two-dimensional quantum systems. Let the initial state be

$$\begin{aligned} |\Psi_{AB}(0)\rangle &= \tfrac{1}{2}(|0_A\rangle + |1_A\rangle) \otimes (|0_B\rangle + |1_B\rangle) \\ &= \tfrac{1}{2}(|0_A\rangle \otimes |0_B\rangle + |0_A\rangle \otimes |1_B\rangle + |1_A\rangle \otimes |0_B\rangle + |1_A\rangle \otimes |1_B\rangle), \end{aligned} \tag{21}$$

and suppose the Hamiltonian is

$$\mathbf{H} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{22}$$

where the ordering of basis states in H_{AB} is

$$|0_A\rangle \otimes |0_B\rangle, \quad |0_A\rangle \otimes |1_B\rangle, \quad |1_A\rangle \otimes |0_B\rangle, \quad |1_A\rangle \otimes |1_B\rangle. \tag{23}$$

The unitary evolution operator is

$$\mathbf{T}(t,0) = \exp\left(\frac{-i}{\hbar}\mathbf{H}t\right). \tag{24}$$

After a time $t = \frac{1}{2}\pi\hbar$,

$$\begin{aligned} \mathbf{T}(t,0) &= \begin{pmatrix} e^{-i\pi/2} & 0 & 0 & 0 \\ 0 & e^{-i\pi/2} & 0 & 0 \\ 0 & 0 & e^{-i\pi/2} & 0 \\ 0 & 0 & 0 & e^{+i\pi/2} \end{pmatrix} \\ &= \begin{pmatrix} -i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}, \end{aligned} \tag{25}$$

and

$$|\Psi_{AB}(t)\rangle = \mathbf{T}(t,0)|\Psi_{AB}(0)\rangle$$
$$= \frac{-i}{2}(|0_A\rangle \otimes |0_B\rangle + |0_A\rangle \otimes |1_B\rangle + |1_A\rangle \otimes |0_B\rangle - |1_A\rangle \otimes |1_B\rangle), \quad 26$$

which is an entangled state.

How do we know that this is an entangled state? Probably by inspection, but let's also check the trace of $\tilde{\boldsymbol{\rho}}_A^2$. First off, the joint density operator is

$$\begin{aligned}\boldsymbol{\rho}_{AB} &= |\Psi_{AB}(t)\rangle\langle\Psi_{AB}(t)| \\ &= \frac{1}{4}(|0_A0_B\rangle\langle 0_A0_B| + |0_A0_B\rangle\langle 0_A1_B| + |0_A0_B\rangle\langle 1_A0_B| - |0_A0_B\rangle\langle 1_A1_B| \\ &\quad + |0_A1_B\rangle\langle 0_A0_B| + |0_A1_B\rangle\langle 0_A1_B| + |0_A1_B\rangle\langle 1_A0_B| - |0_A1_B\rangle\langle 1_A1_B| \\ &\quad + |1_A0_B\rangle\langle 0_A0_B| + |1_A0_B\rangle\langle 0_A1_B| + |1_A0_B\rangle\langle 1_A0_B| - |1_A0_B\rangle\langle 1_A1_B| \\ &\quad - |1_A1_B\rangle\langle 0_A0_B| - |1_A1_B\rangle\langle 0_A1_B| - |1_A1_B\rangle\langle 1_A0_B| + |1_A1_B\rangle\langle 1_A1_B|). \end{aligned} \quad 27$$

Next we take the partial trace over B:

$$\begin{aligned}\tilde{\boldsymbol{\rho}}_A &= \mathrm{Tr}_B\,[\boldsymbol{\rho}_{AB}] \\ &= \langle 0_B|\boldsymbol{\rho}_{AB}|0_B\rangle + \langle 1_B|\boldsymbol{\rho}_{AB}|1_B\rangle \\ &= \frac{1}{4}(|0_A\rangle\langle 0_A| + |0_A\rangle\langle 1_A| + |1_A\rangle\langle 0_A| + |1_A\rangle\langle 1_A| \\ &\quad + |0_A\rangle\langle 0_A| - |0_A\rangle\langle 1_A| - |1_A\rangle\langle 1_A| + |1_A\rangle\langle 1_A|) \\ &= \frac{1}{2}(|0_A\rangle\langle 0_A| + |1_A\rangle\langle 1_A|) \\ &= \frac{1}{2}\mathbf{1}^A. \end{aligned} \quad 28$$

Hence $\tilde{\boldsymbol{\rho}}_A^2 = \frac{1}{4}\mathbf{1}^A$, and $\mathrm{Tr}\,[\tilde{\boldsymbol{\rho}}_A^2] = \frac{1}{2}$, which is clearly less than one. Since density operators that correspond to pure states are projectors, we conclude that no pure state can be assigned to subsystem A when the joint state of the AB system is $|\Psi_{AB}(t)\rangle$.

Note that evolutions producing entanglement between a pair of qubits represent quantum logic gates. Luckily, arbitrary unitary transformations on a Hilbert space of dimension $2^L - 1$ can be decomposed into "circuits" made up of sequences of one- and two-qubit gates. As it turns out, a gate set composed of single-qubit gates plus the above "controlled sign" gate (a special case of a "quantum phase gate") is universal for quantum computing.

On the other hand, entangling evolution between a system and reservoir will compromise the purity of the system's quantum state. Essentially any Hamiltonian that couples system and reservoir degrees-of-freedom will create entanglement, hence the ubiquity of environmental decoherence in real physical systems.

Open systems

The evolution of a real (open) system is generally described by a Master Equation. In simple cases, this takes the form of a differential equation for the system density operator:

$$\frac{d}{dt}\boldsymbol{\rho}(t) = \frac{-i}{\hbar}\{\mathbf{H}\boldsymbol{\rho}(t) - \boldsymbol{\rho}(t)\mathbf{H}\} + \sum_j \left\{2\mathbf{L}_j\boldsymbol{\rho}(t)\mathbf{L}_j^\dagger - \mathbf{L}_j^\dagger\mathbf{L}_j\boldsymbol{\rho}(t) - \boldsymbol{\rho}(t)\mathbf{L}_j^\dagger\mathbf{L}_j\right\}.$$

The first term represents the coherent part of a system's evolution, while the terms in the sum represent the decohering effects of residual couplings to the environment. They can be thought of as arising from continual entangling with and tracing over reservoir degrees of freedom. They're not unitary! Next time, we'll look at an example of a realistic Master Equation (for atoms trapped in an optical cavity) and discuss the significance of each of the terms that appear there...

Overview of recommended reading for Thursday and Friday

Cavity QED

1. Turchette 1995 – Original experimental demonstration of an optical quantum gate

2. Cirac 1997 – Proposed scheme for quantum communication with atoms and photons

3. Ye 1999 – Recent progress on trapping atoms in cavities

4. Pellizzari 1995 – An early proposed scheme for quantum computing with atoms in cavities

Trapped ions

1. Kielpinski 2002 – Proposal for scalable ion-trap computing, based on demonstrated techniques

2. Monroe 1995 – Original experimental demonstration of an ion-trap quantum gate

3. King 1998 – Crucial technical demonstration of cooling multiple ions

4. Wineland review – A glimpse at the true technical complexity of experiments like this!

5. Kielpinski 2001 – Demonstration of a decoherence-free subspace technique with ions

6. Cirac 1995 – Theoretical proposal that led to Monroe 1995

Ensemble NMR

1. Vandersypen 2001 – Crowning glory of NMR thus far: Shor's algorithm to factor 15

2. Havel 2002 – Review by another leading group in NMR quantum computing

3. Menicucci 2002 – Arguments for a conservative interpretation of NMR experiments

4. Braunstein 1999 – Earlier version of the above

5. Chuang 1998b – An early demonstration of quantum algorithms via NMR