B   Basic concepts from quantum theory

B.1   Introduction

B.1.a   BASES

In quantum mechanics certain physical quantities are quantized, such as the energy of an electron in an atom. Therefore an atom might be in certain distinct energy states $|\text{ground}\rangle$, $|\text{first excited}\rangle$, $|\text{second excited}\rangle$, ... Other particles might have distinct states such as spin-up $|\uparrow\rangle$ and spin-down $|\downarrow\rangle$. In each case these alternative states correspond to orthonormal vectors:

$\langle\uparrow|\downarrow\rangle = 0,$
$\langle\text{ground} \mid \text{first excited}\rangle = 0,$
$\langle\text{ground} \mid \text{second excited}\rangle = 0,$
$\langle\text{first excited} \mid \text{second excited}\rangle = 0.$

In general we may express the same state with respect to different bases, such as vertical or horizontal polarization $|\rightarrow\rangle$, $|\uparrow\rangle$; or orthogonal diagonal polarizations $|\nearrow\rangle$, $|\searrow\rangle$.

B.1.b   SUPERPOSITIONS OF BASIS STATES

One of the unique characteristics of quantum mechanics is that a physical system can be in a superposition of basis states, for example,

$$|\psi\rangle = c_0|\text{ground}\rangle + c_1|\text{first excited}\rangle + c_2|\text{second excited}\rangle,$$

where the c_j are complex numbers, called *(probability) amplitudes*. With respect to a given basis, a state $|\psi\rangle$ is interchangeable with its vector of coefficients, $\mathbf{c} = (c_0, c_1, \ldots, c_n)^{\mathrm{T}}$. When the basis is understood, we can use $|\psi\rangle$ as a name for this vector. This ability of a quantum system to be in many states simultaneously is the foundation of *quantum parallelism*.

As we will see, when we measure the quantum state

$$c_0|E_0\rangle + c_1|E_1\rangle + \ldots + c_n|E_n\rangle$$

with respect to the $|E_0\rangle, \ldots, |E_n\rangle$ basis, we will get the result $|E_j\rangle$ with probability $|c_j|^2$ and the state will "collapse" into state $|E_j\rangle$. Since the probabilities must add to 1, $|c_0|^2 + |c_1|^2 + \cdots + |c_n|^2 = 1$, we know $\||\psi\rangle\| = 1$, that is, the vector is normalized.
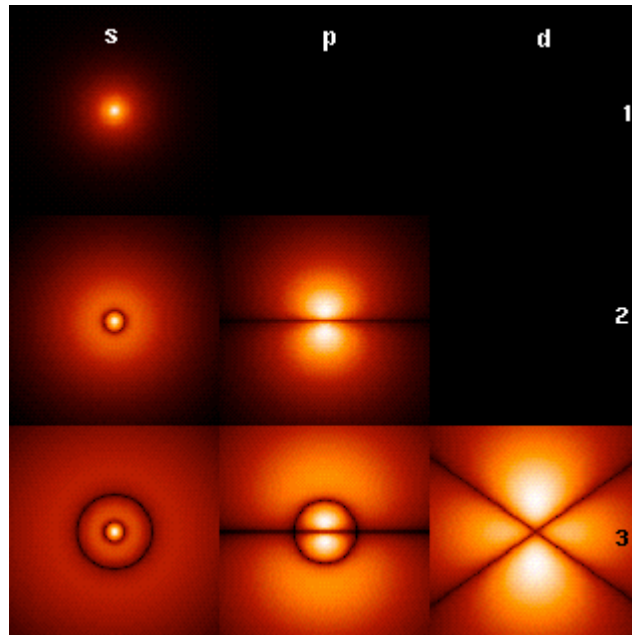
Figure III.1: Probability density of first six hydrogen orbitals. The main quantum number ($n = 1, 2, 3$) and the angular momentum quantum number ($\ell = 0, 1, 2 = $ s, p, d) are shown. (The magnetic quantum number $m = 0$ in these plots.) [fig. from wikipedia commons]

For the purposes of quantum computation, we usually pick two basis states and use them to represent the bits 1 and 0, for example, $|1\rangle = |\text{ground}\rangle$ and $|0\rangle = |\text{excited}\rangle$. We call this the *computational basis*. I've picked the opposite of the "obvious" assignment ($|0\rangle = |\text{ground}\rangle$) just to show that the assignment is arbitrary (just as for classical bits). Note that $|0\rangle \neq \mathbf{0}$, the zero element of the vector space, since $\||0\rangle\| = 1$ but $\|\mathbf{0}\| = 0$. (Thus $\mathbf{0}$ does not represent a physical state, since it is not normalized.)

B.2 Postulates of QM

In this section you will learn the four fundamental postulates of quantum mechanics.[1]

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[1]Quotes are from Nielsen & Chuang (2010) unless otherwise specified.

B.2.a POSTULATE 1: STATE SPACE

Postulate 1: Associated with any isolated physical system is a *state space*, which is a Hilbert space. The state of the system "is completely defined by its *state vector*, which is a unit vector in the system's state space" (Nielsen & Chuang, 2010). The state vector has to be normalized so that the total probability is 1; it is equivalent to the probability axiom that states that the maximum probability (probability of the whole sample space) = 1.

In previous examples, the state vectors have been finite dimensional, but Hilbert spaces can be infinite dimensional as well. For example, a quantum system might have an unlimited number of energy levels, $|0\rangle, |1\rangle, |2\rangle, \ldots$. If the state of the system is a superposition, $|\psi\rangle = \sum_{k=0}^{\infty} c_k |k\rangle$, then the squared amplitudes must sum to 1, $\sum_{k=0}^{\infty} |c_k|^2 = 1$.

A quantum state $|\psi\rangle$ is often a *wavefunction*, which defines the *probability amplitude* distribution (actually, the probability density function) of some continuous quantity. For example, $|\psi\rangle$ may define the complex amplitude $\psi(\mathbf{r})$ associated with each location $\mathbf{r}$ in space, and $|\Psi\rangle$ may define the complex amplitude of $\Psi(\mathbf{p})$ associated with each momentum $\mathbf{p}$ (see Fig. III.1). Infinite dimensional Hilbert spaces also include spaces of wavefunctions such as these. The inner product of wavefunctions is defined:

$$\langle \phi \mid \psi \rangle = \int_{\mathbb{R}^3} \overline{\phi(\mathbf{r})} \psi(\mathbf{r}) \mathrm{d}\mathbf{r}.$$

(For this example we are assuming the domain is 3D space.) Wavefunctions are also normalized, $1 = \||\psi\rangle\|^2 = \int_{\mathbb{R}^3} |\psi(\mathbf{r})|^2 \mathrm{d}\mathbf{r}$. For our purposes, finite dimensional spaces are usually adequate.

In quantum mechanics, global phase has no physical meaning; all that matters is relative phase. In other words, if you consider all the angles around the circle, there is no distinguished 0° (see Fig. III.2). Likewise, in a continuous wave (such as a sine wave), there is no distinguished starting point (see Fig. III.3).

To say all quantum states are normalized is equivalent to saying that their absolute length has no physical meaning. That is, only their *form* (shape) matters, not their absolute size. This is a characteristic of *information*.

Another way of looking at quantum states is as *rays* in a *projective Hilbert space*. A *ray* is an equivalence class of nonzero vectors under the relation, $\phi \cong \psi$ iff $\exists z \neq 0 \in \mathbb{C} : \phi = z\psi$, where $\phi, \psi \neq \mathbf{0}$. That is, global magnitude and phase (r and ϕ in $z = re^{i\phi}$) are irrelevant (i.e., have no physical meaning).
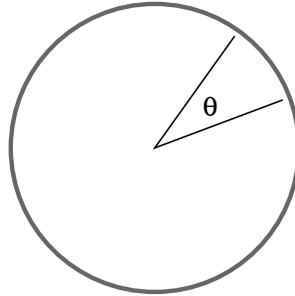
Figure III.2: Relative phase vs. global phase. What matters in quantum mechanics is the relative phase between state vectors (e.g., θ in the figure). Global phase "has no physical meaning"; i.e., we can choose to put the 0° point anywhere we like.
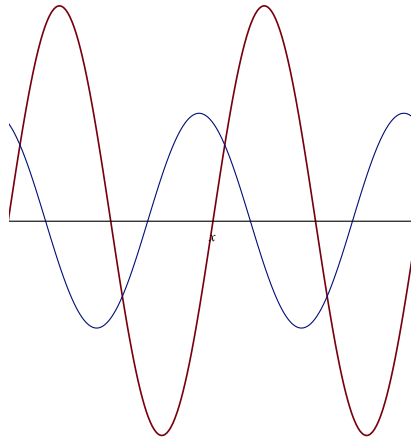

Figure III.3: Relative phase vs. global phase of sine waves. There is no privileged point from which to start measuring absolute phase, but there is a definite relative phase between the two waves.

This is another way of expressing the fact that the *form* is significant, but not the *size*. However, it is more convenient to use normalized vectors in ordinary Hilbert spaces and to ignore global phase.

B.2.b Postulate 2: evolution

Postulate 2: "The evolution of a closed quantum system is described by a unitary transformation" (Nielsen & Chuang, 2010). Therefore a closed quantum system evolves by "complex rotation" of a Hilbert space. More precisely, the state $|\psi\rangle$ of the system at time t is related to the state $|\psi'\rangle$ of the system at time t' by a unitary operator U which depends only on the times t and t',

$$|\psi'\rangle = U(t, t')|\psi\rangle = U|\psi\rangle.$$

This postulate describes the evolution of systems that don't interact with the rest of the world. That is, the quantum system is a dynamical system of relatively low dimension, whereas the environment, including any measurement apparatus, is a thermodynamical system (recall Ch. II, Sec. B).

Dynamics (supplementary) The laws of quantum mechanics, like the laws of classical mechanics, are expressed in differential equations. However, in quantum computation we usually deal with quantum gates operating in discrete time, so it is worth mentioning their relation.

   The continuous-time evolution of a closed quantum mechanical system is given by the Schrödinger equation:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle,$$

or more compactly, $i\hbar|\dot\psi\rangle = H|\psi\rangle$. H is the Hamiltonian of the system (a fixed Hermitian operator), and $\hbar$ is the reduced Planck constant (often absorbed into H).

   Since H is Hermitian, it has a spectral decomposition, $H = \sum_E E|E\rangle\langle E|$, where the normalized $|E\rangle$ are *energy eigenstates* (or *stationary states*) with corresponding energies E. The lowest energy is the *ground state energy*.

   In quantum computing, we are generally interested in the discrete-time dynamics of quantum systems. Stone's theorem shows that the solution to the Schrödinger equation is:

$$|\psi(t + s)\rangle = e^{-iHt/\hbar}|\psi(s)\rangle.$$

Therefore define $U(t) \overset{\text{def}}{=} \exp(-iHt/\hbar)$; then $|\psi(t+s)\rangle = U(t)|\psi(s)\rangle$. It turns out that U is unitary (Exer. III.3). Hence the evolution of a closed quantum mechanical system from a state $|\psi\rangle$ at time t to a state $|\psi'\rangle$ at time t' can be described by a unitary operator, $|\psi'\rangle = U|\psi\rangle$. Conversely, for any unitary operator U there is a Hermitian K such that $U = \exp(iK)$ (Exer. III.4).

B.2.c   POSTULATE 3: QUANTUM MEASUREMENT

What happens if the system is no longer closed, that is, if it interacts with the larger environment? In particular, what happens if a quantum system interacts with a much larger measurement apparatus, the purpose of which is to translate a microscopic state into a macroscopic, observable effect? For example, suppose we have a quantum system that can be in two distinct states, for example, an atom that can be in a ground state $|0\rangle$ and an excited state $|1\rangle$. Since they are distinct states, they correspond to orthogonal vectors, $\langle 0 \mid 1 \rangle = 0$. Suppose further that we have a measurement apparatus that turns on one light if it measures state $|0\rangle$ and a different light if it measures state $|1\rangle$.

Now consider an atom in a quantum state $|\psi\rangle = \frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle$, a superposition of the states $|0\rangle$ and $|1\rangle$. When we measure $|\psi\rangle$ in the computational basis, we will measure $|0\rangle$ with probability $\left|\frac{1}{2}\right|^2 = \frac{1}{4}$, and we will measure $|1\rangle$ with probability $\left|\frac{\sqrt{3}}{2}\right|^2 = \frac{3}{4}$. After measurement, the system is in the state we measured ($|0\rangle$ or $|1\rangle$, respectively); this is the "collapse" of the wavefunction. We depict the possibilities as follows:

$$|\psi\rangle \xrightarrow{1/4} |0\rangle,$$
$$|\psi\rangle \xrightarrow{3/4} |1\rangle.$$

Now consider a more complicated example, a quantum system that can be in three distinct states, say an atom that can be in a ground state $|0\rangle$ or two excited states, $|1\rangle$ and $|2\rangle$. Note that $\langle 0 \mid 1 \rangle = \langle 1 \mid 2 \rangle = \langle 0 \mid 2 \rangle = 0$. Suppose the quantum system is in state $|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|1\rangle + \frac{1}{2}|2\rangle$. Further, suppose we have a measurement apparatus that turns on a light if it measures state $|0\rangle$ and does not turn it on otherwise. When we measure $|\psi\rangle$, with probability $\left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$ we will measure $|0\rangle$ and after measurement it will collapse to state $|0\rangle$. With probability $\left|\frac{1}{2}\right|^2 + \left|\frac{1}{2}\right|^2 = \frac{1}{2}$ it will not measure state $|0\rangle$ and the

light won't go on. In this case, it will collapse to state $\frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle$, which we get by renormalizing the state measured:

$$\frac{\frac{1}{2}|1\rangle + \frac{1}{2}|2\rangle}{\sqrt{\left|\frac{1}{2}\right|^2 + \left|\frac{1}{2}\right|^2}} = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle.$$

We can depict the possible outcomes as follows:

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|1\rangle + \frac{1}{2}|2\rangle \quad \begin{cases} \xrightarrow{1/2} & |0\rangle \\ \xrightarrow{1/2} & \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle \end{cases}.$$

In other words, we zero out the coefficients of the states we didn't measure and renormalize (because quantum states are always normalized). Now we develop these ideas more formally.

A measurement can be characterized by a set of projectors P_m, for each possible measurement outcome m. In the first example above, the measurement operators are $P_1 = |0\rangle\langle 0|$ and $P_2 = |1\rangle\langle 1|$. In the second example, the operators are $P_1 = |0\rangle\langle 0|$ and $P_2 = |1\rangle\langle 1| + |2\rangle\langle 2|$. In the latter case, P_1 projects the quantum state into the subspace spanned by $\{|0\rangle\}$, and P_2 projects the quantum state into the subspace spanned by $\{|1\rangle, |2\rangle\}$. These are *orthogonal subspaces* of the original space (spanned by $\{|0\rangle, |1\rangle, |2\rangle\}$).

Since a measurement must measure some definite state, a projective measurement is a set of projectors $P_1, \ldots, P_N$ satisfying: (1) They project into orthogonal subspaces, so for $m \neq n$ we have $P_m P_n = \mathbf{0}$, the identically zero operator. (2) They are complete, that is, $I = \sum_{m=1}^{N} P_m$, so measurement always produces a result. Projectors are also idempotent, $P_m P_m = P_m$, since if a vector is already projected into the m subspace, projecting it again has no effect. Finally, projectors are Hermitian (self-adjoint), as we can see:

$$P_m^\dagger = \left(\sum_j |\eta_j\rangle\langle\eta_j|\right)^\dagger = \sum_j (|\eta_j\rangle\langle\eta_j|)^\dagger = \sum_j |\eta_j\rangle\langle\eta_j| = P_m.$$

Now we can state Postulate 3.

Postulate 3: Quantum measurements are described by a complete set of orthogonal *projectors*, P_m, for each possible measurement outcome m.

Measurement projects the state into a subspace with a probability given by the squared magnitude of the projection. Therefore, the probability of measurement m of state $|\psi\rangle$ is given by:

$$p(m) = \||P_m|\psi\rangle\|^2 = \langle\psi \mid P_m^\dagger P_m \mid \psi\rangle = \langle\psi \mid P_m P_m \mid \psi\rangle = \langle\psi \mid P_m \mid \psi\rangle.$$
(III.1)

This is *Born's Rule*, which gives the probability of a measurement outcome. The measurement probabilities must sum to 1, which we can check:

$$\sum_m p(m) = \sum_m \langle\psi \mid P_m \mid \psi\rangle = \langle\psi|\left(\sum_m P_m\right)|\psi\rangle = \langle\psi \mid I \mid \psi\rangle = \langle\psi \mid \psi\rangle = 1.$$

This follows from the completeness if the projectors, $\sum_m P_m = I$.

For an example, suppose $P_m = |m\rangle\langle m|$, and write the quantum state in the measurement basis: $|\psi\rangle = \sum_m c_m|m\rangle$. Then the probability $p(m)$ of measuring m is:

$$
\begin{aligned}
p(m) &= \langle\psi \mid P_m \mid \psi\rangle \\
&= \langle\psi|(|m\rangle\langle m|)|\psi\rangle \\
&= \langle\psi \mid m\rangle\langle m \mid \psi\rangle \\
&= \overline{\langle m \mid \psi\rangle}\langle m \mid \psi\rangle \\
&= |\langle m \mid \psi\rangle|^2 \\
&= |c_m|^2.
\end{aligned}
$$

More generally, the same holds if P_m projects into a subspace, $P_m = \sum_k |k\rangle\langle k|$; the probability is $p(m) = \sum_k |c_k|^2$. Alternatively, we can "zero out" the c_j for the orthogonal subspace, that is, for the $|j\rangle\langle j|$ omitted by P_m. To maintain a total probability of 1, the normalized state vector after measurement is

$$\frac{P_m|\psi\rangle}{\sqrt{p(m)}} = \frac{P_m|\psi\rangle}{\||P_m|\psi\rangle\|}.$$

B.2.d POSTULATE 4: COMPOSITE SYSTEMS

Postulate 4: "The state space of a composite physical system is the tensor product of the state spaces of the component physical systems" (Nielsen & Chuang, 2010). If there are n subsystems, and subsystem j is prepared in

state $|\psi_j\rangle$, then the composite system is in state

$$|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle = \bigotimes_{j=1}^{n} |\psi_j\rangle.$$

B.3 Wave-particle duality (supplementary)

Some of the capabilities of quantum computation depend on the fact that microscopic objects behave as both particles and waves. To see why, imagine performing the double-slit experiment with three different kinds of objects.

Imagine a stream of classical particles impinging on the two slits and consider the probability of their arriving on a screen. Define $P_j(x)$ to be the probability of a particle arriving at x with just slit j open, and $P_{12}(x)$ to be the probability of a particle arriving at x with both open. We observe $P_{12} = P_1 + P_2$, as expected.

Now consider classical waves, such as water waves, passing through the two slits. The energy I of a water wave depends on the square of its height H, which may be positive or negative. Hence,

$$I_{12} = H_{12}^2 = (H_1 + H_2)^2 = H_1^2 + 2H_1H_2 + H_2^2 = I_1 + 2H_1H_2 + I_2.$$

The $2H_1H_2$ term may be positive or negative, which leads to constructive and destructive interference.

Finally, consider quantum particles. The probability of observing a particle is given by the rule for waves. In particular, the probability P is given by the square of a complex amplitude A:

$$\begin{aligned} P_{12} &= |A_1 + A_2|^2 = \overline{A_1}A_1 + \overline{A_1}A_2 + \overline{A_2}A_1 + \overline{A_2}A_2, \\ &= P_1 + \overline{A_1}A_2 + A_1\overline{A_2} + P_2. \end{aligned}$$

Again, the interference terms $\overline{A_1}A_2 + A_1\overline{A_2}$ can be positive or negative leading to constructive and destructive interference. How does a particle going through one slit "know" whether or not the other slit is open?