Ph 12b Quantum Physics
19 January 2010
Quantum evolution

Note Title 1/19/2010

So far, our postulates of quantum physics (with a more logical ordering than Liboff's) are:

(1) States. A system is described by a Hilbert space $\mathcal{H}$, and a state of the system is a nonzero vector $|\psi\rangle \in \mathcal{H}$.

All that really matters, though, is the one-dimensional space spanned by $|\psi\rangle$; hence

$|\psi\rangle$ and $\lambda|\psi\rangle$ describe the same state, for $0 \neq \lambda \in \mathbb{C}$. We may by convention impose $\||\psi\rangle\|^2 = \langle\psi|\psi\rangle = 1$, and say that $|\psi\rangle$ and $\lambda|\psi\rangle$ describe the same state, where $|\lambda| = 1$

(2) Observables: An observable $\hat{A}$ is a Hermitian linear operator acting on $\mathcal{H}$.

Thus $\hat{A}$ has a spectral representation

$$\hat{A} = \sum_n a_n \hat{E}_n$$ where a_n is an eigenvalue of $\hat{A}$ and $\hat{E}_n$ is the orthogonal projector onto the space of eigenvectors with that eigenvalue. Thus $\hat{E}_n = |e_n\rangle\langle e_n|$ if the eigenvalue a_n is nondegenerate and

$$\hat{A}|e_n\rangle = a_n|e_n\rangle;$$

if a_n is a degenerate eigenvalue, and $\{|e_{n,i}\rangle\}$ span the eigenspace of eigenvalue a_n, then $\hat{E}_n = \sum_i |e_{n,i}\rangle\langle e_{n,i}|$.

Note that $\hat{E}_n = \hat{E}_n^\dagger$ and $\hat{E}_n \hat{E}_m = \delta_{nm} \hat{E}_n$

(3) Measurement: If observable $\hat{A}$ is measured, the outcome is an eigenvalue of $\hat{A}$. If the measurement is performed on the state $|\psi\rangle$, the outcome a_n occurs with probability

$$P(a_n) = \| \hat{E}_n |\psi\rangle \|^2 = \langle \psi | \hat{E}_n | \psi \rangle \quad (\text{"Born rule"})$$

If outcome a_n is obtained, the normalized state right after the measurement is

$$\frac{\hat{E}_n |\psi\rangle}{\| \hat{E}_n |\psi\rangle \|} = \frac{\hat{E}_n |\psi\rangle}{\sqrt{\langle \psi | \hat{E}_n | \psi \rangle}}$$

Note that if outcome a_n is obtained, and then the same measurement is immediately repeated, then in the second measurement outcome a_n occurs with probability one.

The probability distribution for measurement outcomes, in which a_n occurs with probability $P(a_n)$, yields an expectation value

$$\langle \hat{A} \rangle \equiv \langle a_n \rangle \equiv \sum_n a_n P(a_n) = \sum_n a_n \langle \psi | \hat{E}_n | \psi \rangle$$

$$= \langle \psi | \sum_n a_n \hat{E}_n | \psi \rangle = \langle \psi | \hat{A} | \psi \rangle$$

That is how far we had gotten last time. So far we have not said anything about dynamics: how do quantum states move in time? Dynamics is formulated by our next postulate.

(4) Dynamics. The time-evolving state vector obeys the first-order differential equation

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

which is called the (time-dependent) Schrödinger equation. Here $\hat{H}$ is a Hermitian operator (which might depend explicitly on the time t) called the Hamiltonian of the system.

We may think of the evolution as a sequence of infinitesimal time steps, where in each step the time advances from t to $t+dt$, and the state vector evolves as

$$|\psi(t+dt)\rangle = |\psi(t)\rangle - \tfrac{i}{\hbar}\hat{H}(t)\,dt\,|\psi(t)\rangle + O(dt^2)$$

$$= \hat{U}(t, t+dt)\,|\psi(t)\rangle$$

where $\hat{U}(t, t+dt) = \hat{I} - \tfrac{i}{\hbar}\hat{H}(t)\,dt + O(dt^2)$

is the "time-evolution operator" describing evolution in an infinitesimal interval $[t, t+dt]$.

Because $\hat{H}$ is Hermitian, the time evolution operator is unitary. We say a linear operator $\hat{U}$ is unitary if

$$\hat{U}^\dagger \hat{U} = \hat{U}\hat{U}^\dagger = \hat{I}$$

For the infinitesimal time evolution operator

$$\hat{U}(t, t+dt)^{+}\hat{U}(t, t+dt)$$

$$= \left[\hat{I} + \tfrac{i}{\hbar}\hat{H}^{+}dt + O(dt^2)\right]\left[\hat{I} - \tfrac{i}{\hbar}\hat{H}dt + O(dt^2)\right]$$

$$= \hat{I} - \tfrac{i}{\hbar}(\hat{H} - \hat{H}^{+})dt + O(dt^2) = \hat{I} + O(dt^2)$$

The significance of unitarity is that a unitary transformation preserves inner products. If

$$|\psi'\rangle = \hat{U}|\psi\rangle$$
$$|\varphi'\rangle = \hat{U}|\varphi\rangle$$

then $\langle\varphi'|\psi'\rangle = \langle\varphi|\hat{U}^{+}\hat{U}|\psi\rangle$

$$= \langle\varphi|\hat{I}|\psi\rangle = \langle\varphi|\psi\rangle$$

So in particular, a unitary transformation preserves the norm of a vector! $\|\psi'\|^2 = \langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle = \|\psi\|^2$

A unitary transformation maps an orthonormal basis $\{|e_a\rangle\}$ to a new orthonormal basis $\{|e_a'\rangle = \hat{U}|e_a\rangle\}$ and in fact we may express $\hat{U}$ acting on an N-dimensional space as

$$\hat{U} = \sum_{a=1}^{N} |e_a'\rangle\langle e_a|$$

The product of two unitary transformations is also unitary — if $\hat{U}_1$ and $\hat{U}_2$ map ON bases to ON bases, then so does their product $\hat{U}_2\hat{U}_1$ (i.e. $\hat{U}_1$ followed by $\hat{U}_2$):

$$\hat{U}_1 = \sum_a |e_a'\rangle\langle e_a|, \quad \hat{U}_2 = \sum_a |e_a''\rangle\langle e_a'|$$

$$\Rightarrow \quad \hat{U}_2 \hat{U}_1 = \sum_a |a''_a\rangle\langle a_a|$$

Since time evolution for a finite time interval may be obtained from a sequence of many infinitesimal time steps, the evolution operator $\hat{U}(t, t+T)$ for the finite time interval $[t, t+T]$

is also unitary. This means that our normalization convention $\|\psi\|^2 = 1$ is compatible with time evolution:

If $\langle\psi(t)|\psi(t)\rangle = 1$, then

$$\langle\psi(t+T')|\psi(t+T)\rangle = \langle\psi(t)|\hat{U}(t,t+T)^\dagger \hat{U}(t,t+T)|\psi(t)\rangle$$

$$= \langle\psi(t)|\hat{I}|\psi(t)\rangle = 1$$

Physically, unitarity of time evolution is important because it means that "probability is conserved" — i.e., that at any time the probabilities assigned to measurement outcomes sum to 1:

$$\sum_n P(a_n) = \sum_n \langle\psi|\hat{E}_n|\psi\rangle = \langle\psi|\hat{I}|\psi\rangle = \langle\psi|\psi\rangle = 1$$

Let's consider time evolution in the case where the Hamiltonian $\hat{H}$ is time independent. Since $\hat{H}$ is Hermitian, $\hat{H}$ has an ON basis of eigenstates $\{|\psi_n\rangle\}$:

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle, \qquad \langle\psi_n|\psi_m\rangle = \delta_{nm}$$

This eigenvalue condition is called the "time-independent Schrodinger equation"!

The eigenvalues $\{E_n\}$ are the possible outcomes when we measure the energy of the system. In the case of an atom, for example, there is a discrete set of allowed energies, explaining the atomic spectrum (The frequencies $\omega_{nm} = (E_m - E_n)/\hbar$ of light emitted by the atom). That is why the set of eigenvalues is called the "spectrum" of a Hermitian operator.

It is easy to solve the Schrödinger equation if the initial state is an eigenstate of $\hat{H}$:

$$|\psi(0)\rangle = |\psi_n\rangle.$$

Then $\frac{d}{dt}|\psi(t)\rangle = -\frac{i}{\hbar}\hat{H}|\psi(t)\rangle$ is solved by

$$|\psi(t)\rangle = e^{-iE_nt/\hbar}|\psi_n\rangle$$

The state remains an eigenstate at all times — in fact only its phase changes, and since the overall phase of a state vector has no significance, nothing really changes. For example, if we consider the expectation value of a fixed Hermitian operator $\hat{A}$,

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi(0)|\hat{A}|\psi(0)\rangle,$$

the expectation value is frozen in time. For this reason, energy eigenstates are also called "stationary states."

Since the Schrödinger equation is linear, and we know the solution for each stationary state, it is easy to write down the general solution.

If $|\psi(0)\rangle = \sum_n c_n |\psi_n\rangle$ and $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$,

then $|\psi(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar}|\psi_n\rangle$

Since the Schrödinger equation is linear (while the equations of motion of a classical dynamical system can be nonlinear) it seems, contrary to expectations, that quantum dynamics is easier to analyze than classical dynamics. The catch is that finding the eigenvalues and eigenstates of $\hat{H}$ can be a difficult problem.

The general solution to the Schrodinger solution can be expressed as

$$|\psi(t)\rangle = \sum_n |\psi_n\rangle e^{-iE_nt/\hbar} c_n = \sum_n |\psi_n\rangle e^{-iE_nt/\hbar}\langle\psi_n|\psi(0)\rangle$$

or $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$

where the time evolution operator $\hat{U}(t)$ for time interval $[0,t]$ is $\hat{U}(t) = \sum_n |\psi_n\rangle e^{-iE_nt/\hbar}\langle\psi_n|$

while the Hamiltonian is $\hat{H} = \sum_n |\psi_n\rangle E_n \langle\psi_n|$.

Thus we may write:

$$\hat{U}(t) = \exp(-i\hat{H}t/\hbar).$$

The meaning of this equality is clear in the basis in which $\hat{H}$ and $\hat{U}(t)$ are both diagonal. For a general basis, we may think of $\hat{U}(t)$ as defined by its (convergent) power series expansion

$$\exp(-i\hat{H}t/\hbar) = \sum_{r=0}^{\infty} \frac{1}{r!}\left(\frac{-it}{\hbar}\right)^r \hat{H}^r.$$

We note that $\hat{U}(t)$ also solves a version of the Schrödinger equation, since

$$\hat{U}(t+dt) = \exp(-i\hat{H}dt/\hbar)\exp(-i\hat{H}t/\hbar)$$
$$= [\hat{I} - i\hat{H}dt/\hbar]\,\hat{U}(t)$$

$$\Rightarrow \frac{d}{dt}\hat{U}(t) = -\frac{i}{\hbar}\hat{H}\hat{U}(t) \quad \text{with initial condition } \hat{U}(0) = \hat{I}$$

We also note that

$$\hat{U}(t_2)\,\hat{U}(t_1) = \hat{U}(t_2+t_1),$$

– time evolution for time t_2+t_1 is equivalent to evolution for time t_1 followed by evolution for time t_2.

It may seem strange that energy eigenstates are stationary irrespective of the value of E_n, as normally we expect a more energetic state to move faster than a less energetic state. To recover the expected connection between energy and speed of motion we should consider an initial state that is a superposition of energy eigenstates with distinct eigenvalues, a "nonstationary state."

Consider for example a simple model of an atom, with just two energy levels: the ground state $|g\rangle$ with energy E_g and the excited state $|e\rangle$ with energy E_e, where $\omega = (E_e - E_g)/\hbar$.

E_e —— $|e\rangle$

E_g —— $|g\rangle$

The Hamiltonian for this system is

$$\hat{H} = E_g |g\rangle\langle g| + E_e |e\rangle\langle e|$$

and the corresponding time evolution operator is

$$\hat{U}(t) = e^{-iE_g t/\hbar} |g\rangle\langle g| + e^{-iE_e t/\hbar} |e\rangle\langle e|.$$

Thus, if the initial state is $|\psi(0)\rangle = a|g\rangle + b|e\rangle$, the state at time t is

$$|\psi(t)\rangle = a e^{-iE_g t/\hbar} |g\rangle + b e^{-iE_e t/\hbar} |e\rangle$$

$$= e^{-iE_g t/\hbar} \left(a|g\rangle + b e^{-i\omega t} |e\rangle \right)$$

(where $e^{-iE_g t/\hbar}$ is a physically irrelevant overall phase).

Consider the orthonormal basis

$$|+\rangle = \frac{1}{\sqrt{2}} \left(|g\rangle + |e\rangle \right)$$

$$|-\rangle = \frac{1}{\sqrt{2}} \left(|g\rangle - |e\rangle \right)$$

Note that

$$\langle + | + \rangle = \langle - | - \rangle = 1$$

$$\langle - | + \rangle = \langle + | - \rangle = 0$$

Suppose the atom is prepared in the state $|+\rangle$ at time $t = 0$. After time t the state becomes

$$|\psi(t)\rangle = (\text{phase}) \frac{1}{\sqrt{2}} \left(|g\rangle + e^{-i\omega t} |e\rangle \right).$$

Suppose that at time t a measurement is performed that projects onto the basis $\{ |+\rangle, |-\rangle \}$

The outcome $+$ occurs with probability

$$P(+) = |\langle + | \psi(t) \rangle|^2 = \left| \frac{1}{2} (\langle g| + \langle e|) \left(|g\rangle + e^{-i\omega t} |e\rangle \right) \right|^2$$

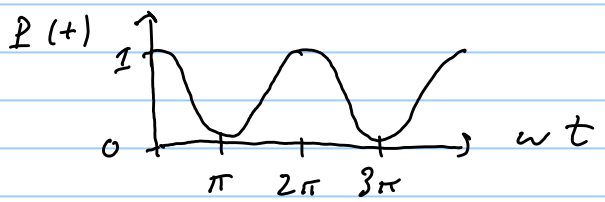
$$= \left| \frac{1}{2} (1 + e^{-i\omega t}) \right|^2 = \frac{1}{4} (1 + 1 + e^{-i\omega t} + e^{i\omega t})$$

$$= \frac{1}{2} (1 + \cos \omega t) = \cos^2(\omega t/2)$$

and the $-$ outcome occurs with probability

$$P(-) = |\langle -|\psi(t)\rangle|^2 = \frac{1}{2}(1-\cos\omega t) = \sin^2(\omega t/2)$$

An experimentalist can verify this prediction by performing repeated experiments in which $|+\rangle$ is prepared and the $\{|+\rangle, |-\rangle\}$ projective measurement is performed after time t. For each value of t, the experiment is repeated enough times to estimate $P(+)$ with high statistical confidence. Then plotting $P(+)$ as a function of t she finds:



$P(+)$ oscillates with period $2\pi/\omega$ between $P(+) = 1$ and $P(-) = 0$

Thus when the energy difference $E_e - E_g$ is larger the oscillation is faster.