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Introduction

! The essential function of physical theory is to make quantitative predictions about experiments.

`preparation`	***representation*** →	$\vert\Psi(t_1)\rangle$	
↓		↓	
`evolution`	***specification of dynamics***	$i\hbar\frac{d}{dt}\vert\Psi\rangle = \mathbf{H}\vert\Psi\rangle$	1
↓		↓	
`measurement`	← ***prediction***	$\vert\langle i\vert\mathbf{O}\vert\Psi(t_2)\rangle\vert^2$	

Most of the subtlety and wonder of quantum physics stems from the rules for ***representation*** and ***prediction***. Nevertheless, we'll spend most of the year developing tools to analyze quantum ***dynamics***.

Thinking clearly about quantum mechanics requires a thorough understanding of the basic physical principles, plus a firm command of linear algebra. In order to foster our quantum intuitions, we will initially restrict our attention to finite-dimensional systems.

Basic postulates for an isolated quantum system

- Physical states are represented by vectors Ψ in a complex Hilbert space.
- Dynamics are specified by Hermitian operators **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 $|\mathbf{P}_i\Psi|^2$.

Dirac notation for quantum states

States may be written as 'ket'

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

or ‘bra’

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

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

Bras and kets are related by Hermitian conjugation:

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

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

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

One typically drops one of the vertical bars and writes $\langle\Psi_a|\Psi_b\rangle$. Normalized states satisfy $\langle\Psi|\Psi\rangle = 1$.

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

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

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

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

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

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

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

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

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

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

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

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

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

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,

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

The outer product of any vector with itself is a projection operator:

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

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

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

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:

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

Accordingly,

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

as noted above.

The Measurement postulate

The point of writing down a physical 'state' is to represent mathematically everything we know about the preparation of a given system. In quantum mechanics, it happens that the most efficient and complete way to do this is by choosing a normalized vector in a complex Hilbert space (or in some situations a density matrix, as we'll see later). Sometimes in the course of events however we may decide that we somehow manage to obtain new and reliable information about the system, so quantum theory must also tell us how to *update* our mathematical description accordingly. Ideally the update rules should take maximal advantage of this new information in 'conditioning' the quantum state, but they should never tell us to make unjustified alterations of it. In this sense, quantum measurement theory plays an analogous role to that of Bayesian Inference in classical physics. Quantum states represent what we know about a system; when we learn something new (by whatever means) we need to update the state. We will eventually see how quantum measurement theory allows us to do this in great generality, even (optimally) taking into account uncertainties we may have about the accuracy of information.

Traditional quantum measurement theory deals with orthogonal projection measurements. The effect of an ideal orthogonal measurement is to determine which of a given set of mutually-exclusive propositions is true. Some simple examples of such sets of propositions could be:

- The particle is at position x_0, the particle is at position x_1, the particle is at position x_2,

…

- The particle has momentum p_0, the particle has momentum p_1, the particle has momentum p_2, …
- The atom is in its ground state, the atom is in its excited state.
- The rotor has one unit of angular momentum, the rotor has two units of angular momentum, …
- The photon has left-circular polarization, the photon has right-circular polarization.
- …

In quantum measurement theory, mutually-exclusive propositions correspond to orthogonal projectors (projection operators) on the system state space. Two projectors $\mathbf{P}_a$, $\mathbf{P}_b$ are orthogonal if

$$\mathbf{P}_a \mathbf{P}_b |\Psi\rangle = 0 \qquad 22$$

for ***every*** state $|\Psi\rangle$ in the Hilbert space. For simplicity, one often writes $\mathbf{P}_a \mathbf{P}_b = 0$.

A “complete” or “exhaustive” set of propositions is a set for which at least one proposition must be true. Correspondingly, we define a *complete set of orthogonal projectors* to be a set $\{\mathbf{P}_0, \mathbf{P}_1, \mathbf{P}_2, \dots\}$ such that

$$\sum_i \mathbf{P}_i = \mathbf{1}. \qquad 23$$

Note that by this definition, the number of projectors in a complete orthogonal set must be $\leq$ the dimension of the Hilbert space.

The postulate:

A complete set of orthogonal projectors specifies an exhaustive measurement. For a system prepared in state $|\Psi\rangle$, the probability of the i^{th} outcome is given by

$$\begin{aligned} \Pr(i) &= |\mathbf{P}_i|\Psi\rangle|^2 \\ &= (\mathbf{P}_i|\Psi\rangle)^\dagger \mathbf{P}_i|\Psi\rangle \\ &= \langle\Psi|\mathbf{P}_i^\dagger \mathbf{P}_i|\Psi\rangle \\ &= \langle\Psi|(\mathbf{P}_i)^2|\Psi\rangle \\ &= \langle\Psi|\mathbf{P}_i|\Psi\rangle. \end{aligned} \qquad 24$$

Note that $\sum_i \Pr(i) = 1$ by completeness of the set of projectors.

Furthermore, the state of the system after outcome i has been obtained is given by

$$|\Psi\rangle \mapsto \frac{\mathbf{P}_i|\Psi\rangle}{\sqrt{\langle\Psi|\mathbf{P}_i|\Psi\rangle}}. \qquad 25$$

Later in the course we’ll see that while every complete set of orthogonal projectors specifies a performable measurement, not every performable measurement corresponds to an orthogonal set of projectors! Likewise, more general post-measurement states than (25) are possible.

But for now let’s stick to traditional measurement theory...

Observables and operator moments:

Every physically-meaningful quantity q (energy, position, component of spin, etc.) is is represented by a Hermitian operator $\mathbf{O}_q$. Such operators are typically called "observables." An observable specifies an exhaustive measurement via its spectral decomposition:

$$\mathbf{O}_q = \sum_i \lambda_i^q \mathbf{P}_i^q, \qquad \mathbf{P}_i^q = |i_q\rangle\langle i_q|, \tag{26}$$

where λ_i^q is the i^{th} eigenvalue of $\mathbf{O}_q$ and $|i_q\rangle$ is the corresponding eigenvector:

$$\mathbf{O}_q|i_q\rangle = \lambda_i^q|i_q\rangle. \tag{27}$$

In the case of a degenerate eigenvalue $\bar{\lambda}_i^q$, let $\mathbf{P}_i^q$ be the projector into the corresponding subspace.

Note that since $\mathbf{O}_q$ is Hermitian, all the λ_i^q are real, the $\{\mathbf{P}_i^q\}$ are orthogonal, and $\sum_i \mathbf{P}_i^q = \mathbf{1}$.

It is customary to speak of "measuring" the observable $\mathbf{O}_q$, by which we mean measuring the set $\{\mathbf{P}_i^q\}$ and associating the value $q = \lambda_i^q$ with the occurance of the i^{th} outcome. Note that the expected (average) result for a state $|\Psi\rangle$ is then given by

$$\begin{aligned} \langle q\rangle &= \sum_i \lambda_i^q \langle\Psi|\mathbf{P}_i^q|\Psi\rangle \\ &= \langle\Psi|\mathbf{O}_q|\Psi\rangle \\ &= \langle\mathbf{O}_q\rangle. \end{aligned} \tag{28}$$

Likewise, the variance of q is given by

$$\begin{aligned} \langle q^2\rangle - \langle q\rangle^2 &= \sum_i (\lambda_i^q)^2 \langle\Psi|\mathbf{P}_i^q|\Psi\rangle - \left(\sum_i \lambda_i^q \langle\Psi|\mathbf{P}_i^q|\Psi\rangle\right)^2 \\ &= \left\langle\mathbf{O}_q^2\right\rangle - \langle\mathbf{O}_q\rangle^2 \\ &= \left\langle(\mathbf{O}_q - \langle\mathbf{O}_q\rangle)^2\right\rangle \\ &= \left\langle\mathbf{O}_q^2 - 2\mathbf{O}_q\langle\mathbf{O}_q\rangle + \langle\mathbf{O}_q\rangle^2\right\rangle \\ &= \left\langle\mathbf{O}_q^2\right\rangle - 2\langle\mathbf{O}_q\rangle\langle\mathbf{O}_q\rangle + \langle\mathbf{O}_q\rangle^2 \\ &= (\Delta\mathbf{O}_q)^2. \end{aligned} \tag{29}$$

And so on and so forth for higher moments of q and $\mathbf{O}_q$.