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Operators in Quantum Machanics

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The Observables of Quantum Mechanics

Observables

Since a measuring apparatus behaves like a *classical* object, "observables" come from classical mechanics: position, velocity, energy, angular momentum, ...

Observables are usually expressed in terms of *canonically conjugate coordinates* and *momemta*, $q_1, \ldots, q_f, p_1, \ldots, p_f$, $f =$ the number of degrees of freedom in the system.

Quantum mechanics associates with each classical observable

$$q_i, \quad \frac{p_i}{m}, \quad H = \frac{\vec{p}^2}{2m} + V(\vec{r}), \quad \vec{L} = \vec{r} \times \vec{r}, \ \ldots$$

a linear operator

$$\hat{q}_i, \quad \frac{\hat{p}_i}{m}, \quad \hat{H}, \quad \hat{\vec{L}}, \ \ldots$$

with *linearity* meaning that

$$\hat{A}\,(\alpha\,\psi + \beta\,\phi) = \alpha\,\hat{A}\,\psi + \beta\,\hat{A}\,\phi$$

for all numbers α, β, vectors ψ, ϕ.

Classical correspondence

How do we know what the operators are?

(1) Most observables have a classical analogue. In this case a formal rule for constructing operators can be given:

Let the *Poisson bracket* of two functions $A(p,q)$, $B(p,q)$ be

$$\{A(p,q),\, B(p,q)\} \stackrel{\text{def}}{=} \sum_{i=1}^{f} \left[\frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} - \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i}\right]$$

and the *commutator* of two operators $\hat{A}$, $\hat{B}$ be

$$[\hat{A},\, \hat{B}] \stackrel{\text{def}}{=} \hat{A}\,\hat{B} - \hat{B}\,\hat{A}$$

The rule is the correspondence

$$[\hat{A},\, \hat{B}] \quad \longleftrightarrow \quad -i\hbar\, \{A(p,q),\, B(p,q)\}$$

between commutators and Poisson brackets.

(2) This identification doesn't work for quantities, such as the "intrinsic spin" of an elementary particle, for which there is no classical analogue. The spin operators are identified by invoking an "analogy" with normal angular momentum and by making suitable "abstract extensions" of the quantum mechanical rules.

The algebraic representation

Only the algebraic structure of the commutator algebra is important. Since all observables can be built upon p, q, it suffices to identify the commutators between the p and q variables. Since

$$\{p_j, p_k\} = 0; \quad \{q_j, q_k\} = 0; \quad \{p_j, q_k\} = \delta_{jk} = \begin{cases} 1, & \text{if } j = k, \\ 0, & \text{if } j \neq k, \end{cases}$$

we have the abstract rules

$$[\hat{p}_j, \hat{p}_k] = 0; \quad [\hat{q}_j, \hat{q}_k] = 0; \quad [\hat{p}_j, \hat{q}_k] = -i\hbar\delta_{jk}\hat{1} \tag{1}$$

The commutator of any pair of operators can be deduced from these rules.

The simplest example

A one-dimensional harmonic oscillator has a Hamiltonian

$$H = \frac{1}{2m}\left[p^2 + m^2\omega^2 q^2\right],$$

or, quantum mechanically,

$$\hat{H} = \frac{1}{2m}\left[\hat{p}^2 + m^2\omega^2 \hat{q}^2\right]. \tag{2}$$

Insight into the algebraic structure of $\hat{H}$ comes from examining the operators

$$\hat{a} \stackrel{\text{def}}{=} \frac{\hat{p} - im\omega\hat{q}}{\sqrt{2m\hbar\omega}}, \qquad \hat{a}^\dagger \stackrel{\text{def}}{=} \frac{\hat{p} + im\omega\hat{q}}{\sqrt{2m\hbar\omega}}. \tag{3}$$

These are just a linear transformation of $\hat{p}$ and $\hat{q}$, so we only need to know $\hat{a}$ and $\hat{a}^\dagger$ to fix

$$\hat{p} = \sqrt{\frac{m\hbar\omega}{2}}\,(\hat{a}^\dagger + \hat{a}) \quad \text{and} \quad \hat{q} = -i\sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}^\dagger - \hat{a}). \tag{4}$$

A description of a system in terms of $\hat{a}$ and $\hat{a}^\dagger$ operators is equivalent to a description in terms of $\hat{p}$ and $\hat{q}$ operators.

Since

$$\langle\phi|\hat{a}\psi\rangle = \langle\hat{a}^\dagger\phi|\hat{\psi}\rangle, \quad \text{all } \phi, \psi,$$

the $\hat{a}$, $\hat{a}^\dagger$ are not Hermitian.* Direct calculation gives

$$\begin{aligned}\hbar\omega\,\hat{a}^\dagger\hat{a} =& \frac{1}{2m}\,(\hat{p} + im\omega\hat{q})\,(\hat{p} - im\omega\hat{q}) \\ =& \frac{1}{2m}\,\left(\hat{p}^2 + m^2\omega^2\hat{q}^2 + im\omega\,[\hat{q},\hat{p}]\right) \\ =& \hat{H} - \frac{1}{2}\,\hbar\omega\hat{1}\end{aligned} \tag{5}$$

and

$$\hbar\omega\,\hat{a}\hat{a}^\dagger = \hat{H} + \frac{1}{2}\,\hbar\omega\hat{1} \tag{6}$$

from which it follows that

$$[\hat{a},\,\hat{a}^\dagger] = \hat{1}. \tag{7}$$

Suppose that we know the ground state eigenvector ϕ_0 and

$$\hat{H}\,\phi_0 = E_0\,\phi_0. \tag{8}$$

If

$$\varphi_n \stackrel{\text{def}}{=} (\hat{a}^\dagger)^n\,\phi_0 \tag{9}$$

then

$$\hat{H}\,\varphi_n = \hbar\omega\,(\hat{a}^\dagger\hat{a} + \frac{1}{2})\,\varphi_n = \hbar\omega\,(\hat{a}^\dagger\hat{a} + \frac{1}{2})\,\hat{a}^\dagger\varphi_{n-1}$$

But (7) $\Rightarrow$

$$(\hat{a}^\dagger\hat{a} + \frac{1}{2})\,\hat{a}^\dagger = a^\dagger\,(\hat{a}\hat{a}^\dagger + \frac{1}{2}) = a^\dagger\,(\hat{a}^\dagger\hat{a} + \frac{3}{2}),$$

* In fact, $\hat{a}^\dagger$ is the *Hermitian conjugate* of $\hat{a}$ (and *vice versa*).

so

$$\begin{aligned}
\hat{H}\,\varphi_n &= \hbar\omega\,\hat{a}^\dagger\,(\hat{a}^\dagger\hat{a} + \frac{3}{2})\,\varphi_{n-1} \\
&= \hbar\omega\,(\hat{a}^\dagger)^2\,(\hat{a}^\dagger\hat{a} + \frac{5}{2})\,\varphi_{n-2} \\
&\vdots \\
&= \hbar\omega\,(\hat{a}^\dagger)^n\,(\hat{a}^\dagger\hat{a} + n + \frac{1}{2})\,\varphi_0 \\
&= (\hat{a}^\dagger)^n\,(\hat{H} + n\hbar\omega)\,\phi_0 \\
&= (\hat{a}^\dagger)^n\,(E_0 + n\hbar\omega)\,\phi_0 \\
&= (E_0 + n\hbar\omega)\,(\hat{a}^\dagger)^n\,\phi_0 \\
&= (E_0 + n\hbar\omega)\,\varphi_n \qquad (10)
\end{aligned}$$

That is, φ_n is an eigenfunction of $\hat{H}$ with eigenvalue $E_0 + n\hbar\omega$. For this reason, $\hat{a}^\dagger$ is often called a *raising* operator or a *creation* (of an excitation) operator. Conversely, (6) $\Rightarrow$

$$\hat{a}\,\varphi_n = \hat{a}\hat{a}^\dagger\,\varphi_{n-1} = \left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2}\right)\varphi_{n-1} = \left(\frac{E_0}{\hbar\omega} + n - \frac{1}{2}\right)\varphi_{n-1}, \qquad (11)$$

so $\hat{a}$ is a *lowering*, or *destruction* operator.

If $\langle\phi_0|\phi_0\rangle = 1$,

$$E_0 = \langle\phi_0|\hat{H}\,\phi_0\rangle = \tfrac{1}{2m}[\underbrace{\langle\hat{p}\,\phi_0\,|\,\hat{p}\,\phi_0\rangle}_{\geq 0} + m^2\omega^2\,\underbrace{\langle\hat{q}\,\phi_0\,|\,\hat{q}\,\phi_0\rangle}_{\geq 0}]$$

i.e., $E_0 \;\geq\; 0$. If follows that the *lowering* operation cannot proceed indefinitely. Thus $\hat{a}\,\phi_0 = 0$. In this case (5) $\Rightarrow$

$$\hat{H}\phi_0 = \hbar\omega\,\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\,\hbar\omega\right)\,\phi_0 = \frac{1}{2}\hbar\omega\,\phi_0$$

and

$$E_n = (n + \frac{1}{2})\,\hbar\omega, \quad n = 1, 2, \ldots$$

With this result, (11) $\Rightarrow$

$$\hat{a}\,\varphi_n = n\,\varphi_{n-1}$$

whence

$$
\begin{aligned}
n^2\langle\varphi_{n-1}|\varphi_{n-1}\rangle =&\langle\hat{a}\varphi_n|\hat{a}\varphi_n\rangle = \langle\varphi_n|\hat{a}^\dagger\hat{a}\varphi_n\rangle \\
=&\langle\varphi_n|\left(\frac{\hat{H}}{\hbar\omega}+\frac{1}{2}\right)\varphi_n\rangle = n\,\langle\varphi_n|\varphi_n\rangle
\end{aligned} \tag{12}
$$

If

$$
\phi_n \overset{\text{def}}{=} \frac{1}{\sqrt{n!}}\varphi_n, \tag{13}
$$

then (12) gives

$$
\langle\phi_n|\phi_n\rangle = \langle\phi_{n-1}|\phi_{n-1}\rangle.
$$

All the ϕ_n are normalized if ϕ_0 is normalized.

These rules determine the results of any observation on the harmonic oscillator. If, for example, we measure q for a system in the state

$$
\Psi(t) = \frac{1}{\sqrt{2}}\left[\phi_0\, e^{-iE_0t/\hbar} - i\phi_1\, e^{-iE_1t/\hbar}\right],
$$

(4) $\Rightarrow$ we expect to see

$$
\begin{aligned}
\langle q\rangle_t =&\langle\Psi(t)|\hat{q}\,\Psi(t)\rangle \\
=&-\frac{i}{2}\sqrt{\frac{\hbar}{2m\omega}}\,\langle\phi_0\, e^{-iE_0t/\hbar} - i\phi_1\, e^{-iE_1t/\hbar}|(\hat{a}^\dagger-\hat{a})\,[\phi_0\, e^{-iE_0t/\hbar} - i\phi_1\, e^{-iE_1t/\hbar}]\rangle \\
=&-\frac{i}{2}\sqrt{\frac{\hbar}{2m\omega}}\,\langle\phi_0\, e^{-iE_0t/\hbar} - i\phi_1\, e^{-iE_1t/\hbar}| \\
&\qquad \phi_1\, e^{-iE_0t/\hbar} - i\sqrt{2}\,\phi_2\, e^{-iE_1t/\hbar} + i\phi_0\, e^{-iE_1t/\hbar}\rangle \\
=&-\frac{i}{2}\sqrt{\frac{\hbar}{2m\omega}}\left[+ie^{-i\omega t}+ie^{i\omega t}\right] \\
=&\sqrt{\frac{\hbar}{2m\omega}}\,\cos\omega t
\end{aligned}
$$

Explicit representations

(1) Schrödinger's original 'correspondence' was

$$
\hat{p}_i = \frac{\hbar}{i}\frac{\partial}{\partial q_i}, \qquad \hat{q}_i = q_i, \qquad i = 1,\ldots,f,
$$

with the implicit assumption that the functions operated on are functions of q. Equation (1) is satisfied since

$$[\hat{p},\hat{q}]f(q) = \frac{\hbar}{i}\frac{\partial}{\partial q}[q\, f(q)] - q\,\frac{\hbar}{i}\frac{\partial}{\partial q}f(q) = \frac{\hbar}{i}f(q) = -i\hbar\, f(q).$$

This representation corresponds to "wave mechanics".

(2) A very similar representation is produced by

$$\hat{p} = p, \qquad \hat{q} = -\frac{\hbar}{i}\frac{\partial}{\partial p_i}$$

with operators operating on functions of p. This gives a "momentum representation" for quantum mechanics.

(3) It is also possible to introduce matrices that satisfy (1). These are the most common representations in practice. For the harmonic oscillator, for example, (11) $\Rightarrow$

$$\hat{a}\,\varphi_n = \varphi_{n-1} \quad \Rightarrow \quad \hat{a}\,\phi_n = \sqrt{n}\,\phi_{n-1}$$

whence

$$\begin{aligned}
[\hat{a}]_{mn} =&\langle\phi_m|\hat{a}\,\phi_n\rangle = \sqrt{n}\,\delta_{m,n-1}\\
=&\langle\hat{a}^\dagger\,\phi_m|\phi_n\rangle = \langle\phi_n|\hat{a}^\dagger\,\phi_m\rangle^* = [\hat{a}^\dagger]^*_{nm}\\
[\hat{a}^\dagger]_{mn} =&\sqrt{m}\,\delta_{n,m-1}\\
[\hat{q}]_{mn} =&-i\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{m}\,\delta_{n,m-1} - \sqrt{n}\,\delta_{m,n-1}\right) && (14)\\
[\hat{p}]_{mn} =&\sqrt{\frac{m\hbar\omega}{2}}\left(\sqrt{m}\,\delta_{n,m-1} + \sqrt{n}\,\delta_{m,n-1}\right) && (15)
\end{aligned}$$

The identifications (14) and (15) satisfy (1). These can be used to calculate

$$\begin{aligned}
\frac{1}{2}m\omega^2[\hat{q}^2]_{mn} =&\frac{1}{4}\left[-\sqrt{m(m-1)}\,\delta_{m,n+2} + (2n+1)\delta_{mn} - \sqrt{n(n-1)}\,\delta_{m+2,n}\right]\\
\frac{1}{2m}[\hat{p}^2]_{mn} =&\frac{1}{4}\left[\sqrt{m(m-1)}\,\delta_{m,n+2} + (2n+1)\delta_{mn} + \sqrt{n(n-1)}\,\delta_{m+2,n}\right]\\
[\hat{H}]_{mn} =&(n+\frac{1}{2})\,\hbar\omega\,\delta_{mn}
\end{aligned}$$

Energy eigenstates in the Schrödinger Representation

In this representation,

$$\hat{a} \to \frac{\frac{\hbar}{i}\frac{\partial}{\partial q} - im\omega q}{\sqrt{2m\hbar\omega}}, \qquad \hat{a}^\dagger \to \frac{\frac{\hbar}{i}\frac{\partial}{\partial q} + im\omega q}{\sqrt{2m\hbar\omega}}. \tag{16}$$

If we replace

$$q \to x = \sqrt{\frac{\hbar}{m\omega}}\, q,$$

a dimensionless coordinate, then (16) is equivalent to

$$\hat{a} \to \frac{-i}{\sqrt{2}}\left(\frac{\partial}{\partial x} + x\right), \qquad \hat{a}^\dagger \to \frac{-i}{\sqrt{2}}\left(\frac{\partial}{\partial x} - x\right). \tag{17}$$

Since

$$\hat{a}\, f = \frac{-i}{\sqrt{2}}\left(\frac{\partial}{\partial x} + x\right) f = \frac{-i}{\sqrt{2}}\, e^{-\frac{1}{2}x^2}\frac{\partial}{\partial x}\left[e^{\frac{1}{2}x^2} f\right],$$

(16) is equivalent to

$$\hat{a} \to \frac{-i}{\sqrt{2}}\, e^{-\frac{1}{2}x^2}\frac{\partial}{\partial x}\left[e^{\frac{1}{2}x^2}\ \ \cdot\right]; \qquad \hat{a}^\dagger \to \frac{-i}{\sqrt{2}}\, e^{\frac{1}{2}x^2}\frac{\partial}{\partial x}\left[e^{-\frac{1}{2}x^2}\ \ \cdot\right] \tag{18}$$

The ground state is fixed by

$$\hat{a}\,\phi_0 = 0,$$

or

$$0 = \frac{\partial}{\partial x}\left[e^{\frac{1}{2}x^2}\phi_0(x)\right] \tag{19}$$

which has the general solution

$$\phi_0(x) = C\, e^{-\frac{1}{2}x^2}.$$

Using x (rather than q) for normalization fixes

$$\phi_0(x) = \frac{1}{\sqrt[4]{\pi}}\, e^{-\frac{1}{2}x^2} \tag{20}$$

The n^{th} excited state can be calculated from (13) and (18):

$$\begin{aligned}\phi_n(x) =& \frac{1}{\sqrt{n!}} \left(\hat{a}^\dagger\right)^n \phi_0(x) \\ =& \frac{1}{\sqrt{n!}} \left(\frac{-i}{\sqrt{2}}\right)^n e^{\frac{1}{2}x^2} \frac{\partial^n}{\partial x^n} \left(e^{-\frac{1}{2}x^2} \phi_0(x)\right) \\ =& \frac{1}{\sqrt{\sqrt{\pi}\, n!}} \left(\frac{-i}{\sqrt{2}}\right)^n e^{\frac{1}{2}x^2} \frac{\partial^n}{\partial x^n} \left(e^{-x^2}\right)\end{aligned}$$

Formula (22.11.17) in Abramowitz and Stegun identifies the Hermite polynomials in terms of a derivative of the form shown in this equation,

$$e^{-x^2} * H_n(x) = (-1)^n \frac{\partial^n}{\partial x^n} \left[e^{-x^2}\right]$$

so

$$\phi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\, n!}} \left(\frac{i}{\sqrt{2}}\right)^n H_n(x)\, e^{-\frac{1}{2}x^2}$$

The i factors in this expression reflect the (arbitrary) choice of phases for the energy eigenfunctions. Removing the i's gives the simpler expression

$$\phi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\, n!}} \frac{1}{2^{n/2}} H_n(x)\, e^{-\frac{1}{2}x^2}, \qquad n = 0, 1, \ldots \tag{21}$$

State space

The objects on which the 'linear operators of quantum mechanics' operate are vectors in some vector space. The vector space is often ∞-dimensional. Two general types of vectors are used.

(1) Continuous vectors: $\psi(q_1, \ldots, q_f)$.
For continuous vectors, an *inner product* is defined by

$$\langle\phi|\psi\rangle = \int \cdots \int dq_1 \cdots dq_f\, \phi(q_1, \ldots, q_f)^* \psi(q_1, \ldots, q_f),$$

normalization means

$$\langle\psi|\psi\rangle = 1,$$

and $|\psi(q_1, \ldots, q_f)|^2$ gives the probability density for observing '$q_1, \ldots, q_f$'.

(2) Discrete vectors: Suppose

$$\hat{A}\, v_n(q_1,\ldots,q_f) = a_n\, v_n(q_1,\ldots,q_f), \quad n = 1,2,\ldots$$

If $\hat{A}$ is Hermitian, the $\{v_n\}$ can be chosen to form an orthonormal basis set, i.e.,

$$\langle v_m | v_n \rangle = \delta_{mn},$$

and any continuous vector $\psi(q_1,\ldots,q_f)$ can be represented

$$\psi(q_1,\ldots,q_f) = \sum_{n=1}^{\infty} c_n\, v_n(q_1,\ldots,q_f). \tag{16}$$

This gives a matrix representation for ψ: $c_1, c_2, \ldots$ are components in the directions $v_1, v_2, \ldots$.

If $\psi = \sum_n c_n\, v_n$ and $\phi = \sum_m d_m\, v_m$,

$$\langle \phi | \psi \rangle = \sum_{m,n} d_m^* c_n \langle v_m | v_n \rangle = \sum_n d_n^* c_n.$$

The inner product becomes a matrix product, the analogue of a 'dot' product in 3D. Normalization now means

$$\sum_n |c_n|^2 = 1$$

and $|c_n|^2$ gives the probability that observation of A will yield a_n.

Equation(16) is actually a rule for a changing from a discrete $c_1, c_2, \ldots$ representation of the state to a continuous $\psi(q_1,\ldots,q_f)$ a representation,

$$\{c_n\} \to \psi(q_1,\ldots,q_f)$$

The inverse relation

$$c_n = \langle v_n | \psi \rangle = \int\cdots\int dq_1 \cdots dq_f\, v_n(q_1,\ldots,q_f)^* \psi(q_1,\ldots,q_f), \tag{17}$$

is the rule for transforming in the other direction.

The $v_n(q_1,\ldots,q_f)$ in (16) may be thought of as the transforming matrix or linear operator for a $n \to q_1,\ldots,q_f$ transformation. In this spirit, the $v_n(q_1,\ldots,q_f)^*$ in (17) represents the tranforming matrix for the $q_1,\ldots,q_f \to n$ transformation. In these cases the transformation is between a continuous and a discrete representation. There are analogous transformations between different continuous representations and between different discrete representations.