# Expectation value:

In quantum mechanics, the **expectation value** is the predicted mean value of the result (measurement) of an experiment. Despite the name, it is not the most probable value of a measurement. It is a fundamental concept in all areas of quantum physics.

## Operational definition

Quantum physics shows an inherent statistical behavior: The measured outcome of an experiment will generally not be the same if the experiment is repeated several times. Only the statistical mean of the measured values, averaged over a large number of runs of the experiment, is a repeatable quantity. Quantum theory does not, in fact, predict the result of individual measurements, but only their statistical mean. This predicted mean value is called the *expectation value*.

While the computation of the mean value of experimental results is very much the same as in classical statistics, its mathematical representation in the formalism of quantum theory differs significantly from classical measure theory.

## Formalism in quantum mechanics

In quantum theory, an experimental setup is described by the observable $A$ to be measured, and the state $\sigma$ of the system. The expectation value of $A$ in the state $\sigma$ is denoted as $\langle A\rangle_\sigma$.

Mathematically, $A$ is a self-adjoint operator on a Hilbert space. In the most commonly used case in quantum mechanics, $\sigma$ is a pure state, described by a normalized Vector $\psi$ in the Hilbert space. The expectation value of $A$ in the state $\psi$ is defined as

$$\langle A\rangle_\psi = \langle\psi|A|\psi\rangle. \qquad (1)$$

If dynamics is considered, either the vector $\psi$ or the operator $A$ is taken to be time-dependent, depending on whether the Schrödinger picture or Heisenberg picture is used. The time-dependence of the expectation value does not depend on this choice, however.

If $A$ has a complete set of eigenvectors $\phi_j$, with eigenvalues $a_j$, then (1) can be expressed as

$$\langle A\rangle_\psi = \sum_j a_j |\langle \psi|\phi_j\rangle|^2 \qquad (2)$$

This expression is similar to the arithmetic mean, and illustrates the physical meaning of the mathematical formalism: The eigenvalues $a_j$ are the possible outcomes of the experiment, and their corresponding coefficient $|\langle \psi|\phi_j\rangle|^2$ is the probability that this outcome will occur; it is often called the *transition probability*.

A particularly simple case arises when $A$ is a projection, and thus has only the eigenvalues 0 and 1. This physically corresponds to a "yes-no" type of experiment. In this case, the expectation value is the probability that the experiment results in "1", and it can be computed as

(3) $$\langle A\rangle_\psi = \|A\psi\|^2.$$

In quantum theory, also operators with non-discrete spectrum are in use, such as the position operator $Q$ in quantum mechanics. This operator does not have eigenvalues, but has a completely continuous spectrum. In this case, the vector $\psi$ can be written as a complex-valued function $\psi(x)$ on the spectrum of $Q$ (usually the real line). For the expectation value of the position operator, one then has the formula

(4) $$\langle Q\rangle_\psi = \int x\,|\psi(x)|^2\,dx.$$

A similar formula holds for the momentum operator $P$, in systems where it has continuous spectrum.

All the above formulae are valid for pure states $\sigma$ only. Prominently in thermodynamics, also *mixed states* are of importance; these are described by a positive trace-class operator $\rho = \sum_i \rho_i |\psi_i\rangle\langle\psi_i|$, the *statistical operator* or *density matrix*. The expectation value then can be obtained as

(5) $$\langle A\rangle_\rho = \mathrm{Trace}(\rho A) = \sum_i \rho_i \langle\psi_i|A|\psi_i\rangle = \sum_i \rho_i \langle A\rangle_{\psi_i}.$$

# General formulation

In general, quantum states $\sigma$ are described by positive normalized linear functional on the set of observables, mathematically often taken to be a C* algebra. The expectation value of an observable $A$ is then given by

(6) $\langle A \rangle_\sigma = \sigma(A)$.

If the algebra of observables acts irreducibly on a Hilbert space, and if $\sigma$ is a *normal functional*, that is, it is continuous in the ultraweak topology, then it can be written as

$$\sigma(\cdot) = \mathrm{Trace}(\rho \cdot)$$

with a positive trace-class operator $\rho$ of trace 1. This gives formula (5) above. In the case of a pure state, $\rho = |\psi\rangle\langle\psi|$ is a projection onto a unit vector $\psi$. Then $\sigma = \langle\psi| \cdot \ \psi\rangle$, which gives formula (1) above.

$A$ is assumed to be a self-adjoint operator. In the general case, its spectrum will neither be entirely discrete nor entirely continuous. Still, one can write $A$ in a spectral decomposition,

$$A = \int a \, \mathrm{d}P(a)$$

with a projector-valued measure $P$. For the expectation value of $A$ in a pure state $\sigma = \langle\psi| \cdot \ \psi\rangle$, this means

$$\langle A \rangle_\sigma = \int a \ \mathrm{d}\langle\psi|P(a)\psi\rangle ,$$

which may be seen as a common generalization of formulas (2) and (4) above.

In non-relativistic theories of finitely many particles (quantum mechanics, in the strict sense), the states considered are generally normal. However, in other areas of quantum theory, also non-normal states are in use: They appear, for example. in the form of KMS states in quantum statistical mechanics of infinitely extended media and as charged states in quantum field theory. In these cases, the expectation value is determined only by the more general formula (6).

# Example in configuration space

As an example, let us consider a quantum mechanical particle in one spatial dimension, in the configuration space representation. Here the Hilbert space is $\mathcal{H} = L^2(\mathbb{R})$, the space of square-integrable functions on the real line. Vectors $\psi \in \mathcal{H}$ are represented by functions $\psi(x)$, called wave functions. The scalar product is given by $\langle\psi_1|\psi_2\rangle = \int \psi_1(x)^* \psi_2(x) \, \mathrm{d}x$. The wave functions have a direct interpretation as a probability distribution:

$$p(x)dx = \psi^*(x)\psi(x)dx$$

gives the probability of finding the particle in an infinitesimal interval of length $dx$ about some point $x$.

As an observable, consider the position operator $Q$, which acts on wave functions $\psi$ by

$$(Q\psi)(x) = x\psi(x).$$

The expectation value, or mean value of measurements, of $Q$ performed on a very large number of *identical* independent systems will be given by

$$\langle Q \rangle_\psi = \langle \psi | Q\psi \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x\, \psi(x)\, \mathrm{d}x = \int_{-\infty}^{\infty} x\, p(x)\, \mathrm{d}x.$$

The expectation value only exists if the integral converges, which is not the case for all vectors $\psi$. This is because the position operator is unbounded, and $\psi$ has to be chosen from its domain of definition.

In general, the expectation of any observable can be calculated by replacing $Q$ with the appropriate operator. For example, to calculate the average momentum, one uses the momentum operator *in configuration space*, $P = -i\hbar\, d/dx$. Explicitly, its expectation value is

$$\langle P \rangle_\psi = -i\hbar \int_{-\infty}^{\infty} \psi^*(x)\, \frac{d\psi}{dx}(x)\, \mathrm{d}x.$$

Not all operators in general provide a measureable value. An operator that has a pure real expectation value is called an observable and its value can be directly measured in experiment.

# 2nd topic:

The **Ehrenfest theorem**, named after Paul Ehrenfest, the Austrian physicist and mathematician, relates the time derivative of the expectation value for a quantum mechanical operator to the commutator of that operator with the Hamiltonian of the system. It is

$$\frac{d}{dt}\langle A \rangle = \frac{1}{i\hbar}\langle [A, H] \rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle$$

where A is some QM operator and $\langle A \rangle$ is its expectation value. Ehrenfest's theorem is obvious in the Heisenberg picture of quantum mechanics, where it is just the expectation value of the Heisenberg equation of motion.

Ehrenfest's theorem is closely related to Liouville's theorem from Hamiltonian mechanics, which involves the Poisson bracket instead of a commutator. In fact, it is a rule of thumb that a theorem

in quantum mechanics which contains a commutator can be turned into a theorem in classical mechanics by changing the commutator into a Poisson bracket and multiplying by $i\hbar$. This causes the operator expectation values to obey their corresponding classical equations of motion provided the Hamiltonian is at most quadratic in the coordinates and momenta. Otherwise, the equations still may hold approximately, provided fluctuations are small.

# Derivation

Suppose some system is presently in a quantum state $\Phi$. If we want to know the instantaneous time derivative of the expectation value of A, that is, by definition

$$\frac{d}{dt}\langle A\rangle = \frac{d}{dt}\int \Phi^* A\Phi \, dx^3 = \int \left(\frac{\partial \Phi^*}{\partial t}\right) A\Phi \, dx^3 + \int \Phi^* \left(\frac{\partial A}{\partial t}\right) \Phi \, dx^3 + \int \Phi^* A \left(\frac{\partial \Phi}{\partial t}\right)$$
$$= \int \left(\frac{\partial \Phi^*}{\partial t}\right) A\Phi \, dx^3 + \left\langle \frac{\partial A}{\partial t} \right\rangle + \int \Phi^* A \left(\frac{\partial \Phi}{\partial t}\right) \, dx^3,$$

where we are integrating over all space. If we apply the Schrödinger equation, we find that

$$\frac{\partial \Phi}{\partial t} = \frac{1}{i\hbar} H\Phi$$

and

$$\frac{\partial \Phi^*}{\partial t} = \frac{-1}{i\hbar}\Phi^* H^* = \frac{-1}{i\hbar}\Phi^* H.$$

Notice $H = H^*$because the Hamiltonian is hermitian. Placing this into the above equation we have

$$\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\int \Phi^*(AH - HA)\Phi \, dx^3 + \left\langle \frac{\partial A}{\partial t} \right\rangle = \frac{1}{i\hbar}\langle [A,H]\rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle.$$

Often (but not always) the operator A is time independent, so that its derivative is zero and we can ignore the last term.

# General example

For the very general example of a massive particle moving in a potential, the Hamiltonian is simply

$$H(x,p,t) = \frac{p^2}{2m} + V(x,t)$$

where $x$is just the location of the particle. Suppose we wanted to know the instantaneous change in momentum $p$. Using Ehrenfest's theorem, we have

$$\frac{d}{dt}\langle p\rangle = \frac{1}{i\hbar}\langle [p,H]\rangle + \left\langle \frac{\partial p}{\partial t}\right\rangle = \frac{1}{i\hbar}\langle [p,V(x,t)]\rangle$$

since the operator $p$commutes with itself and has no time dependence. By expanding the right-hand-side, replacing *p* by $-i\hbar\nabla$, we get

$$\frac{d}{dt}\langle p\rangle = \int \Phi^* V(x,t)\nabla\Phi \, dx^3 - \int \Phi^*\nabla(V(x,t)\Phi) \, dx^3.$$

After applying the product rule on the second term, we have

$$\begin{aligned}
&\frac{d}{dt}\langle p\rangle = \int \Phi^* V(x,t)\nabla\Phi \, dx^3 - \int \Phi^*(\nabla V(x,t))\Phi \, dx^3 - \int \Phi^* V(x,t)\nabla\Phi \, dx^3 \\
&= -\int \Phi^*(\nabla V(x,t))\Phi \, dx^3 \\
&= \langle -\nabla V(x,t)\rangle = \langle F\rangle,
\end{aligned}$$

but we recognize this as Newton's second law. This is an example of the correspondence principle, the result manifests as Newton's second law in the case of having so many particles that the net motion is given exactly by the expectation value of a single particle.

Similarly we can obtain the instantaneous change in the position expectation value.

$$\begin{aligned}
&\frac{d}{dt}\langle x\rangle = \frac{1}{i\hbar}\langle [x,H]\rangle + \left\langle \frac{\partial x}{\partial t}\right\rangle = \\
&= \frac{1}{i\hbar}\langle [x,\frac{p^2}{2m} + V(x,t)]\rangle + 0 = \frac{1}{i\hbar}\langle [x,\frac{p^2}{2m}]\rangle = \\
&= \frac{1}{i\hbar}\langle [x,\frac{p^2}{2m} + V(x,t)]\rangle = \frac{1}{i\hbar 2m}\langle [x,p]\frac{d}{dp}p^2\rangle = \\
&= \frac{1}{i\hbar 2m}\langle i\hbar 2p\rangle = \frac{1}{m}\langle p\rangle
\end{aligned}$$

This result is again in accord with the classical equation.

# Notes

1. In bra-ket notation

$$\frac{\partial}{\partial t}\langle\phi|x\rangle = \frac{-1}{i\hbar}\langle\phi|\hat{H}|x\rangle = \frac{-1}{i\hbar}\langle\phi|x\rangle H = \frac{-1}{i\hbar}\Phi^* H$$

where $\hat{H}$ is the Hamiltonian operator, and *H* is the Hamiltonian represented in coordinate space (as is the case in the derivation above). In other words, we applied the adjoint operation to the entire Schrödinger equation, which flipped the order of operations for *H* and $\Phi$.

2. Although the expectation value of the momentum $\langle p \rangle$, which is a real-number-valued function of time, will have time dependence, the momentum operator $p$ does not. Rather, the momentum operator is a constant linear operator on the Hilbert space of the system. The time dependence of the expectation value is due to the time evolution of the wavefunction for which the expectation value is calculated. An Ad hoc example of an operator which does have time dependence is $xt^2$, where $x$ is the ordinary position operator and $t$ is just the (non-operator) time