

Hamiltonian

Hamiltonian (Operator)

Total energy of a single particle in motion
under a potential energy $V(x, y, z)$

$$E = \frac{1}{2m} (\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2) + V(x, y, z) \quad \text{Total energy}$$

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}, \quad \hat{p}_y = -i\hbar \frac{\partial}{\partial y}, \quad \hat{p}_z = -i\hbar \frac{\partial}{\partial z},$$

$$\Rightarrow \hat{H} = \frac{1}{2m} \left(\left(-i\hbar \frac{\partial}{\partial x} \right)^2 + \left(-i\hbar \frac{\partial}{\partial y} \right)^2 + \left(-i\hbar \frac{\partial}{\partial z} \right)^2 \right) + V(x, y, z)$$

$$= -\frac{\hbar}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x, y, z)$$

$$= -\frac{\hbar}{2m} \nabla^2 + V(x, y, z) \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Schrödinger eq.

$$-\frac{\hbar}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V\psi = E\psi$$

$$\Rightarrow \hat{H}\psi = E\psi$$

$$-\frac{\hbar}{2m} \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + V\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

$$\Rightarrow \hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

Eigen value and Eigen function

$$\hat{A}(x)f(x) = af(x) \quad \text{Eigen value equation}$$

a : Eigen value (Constant)

$f(x)$: Eigen vector

It's a special vector that does not change direction at all even if it is transformed with an operator.

$$\hat{H}\psi = E\psi$$

The eigenvalue of operators corresponds to measured values when observing quantum systems.

Why?

Eigen value and expectation value

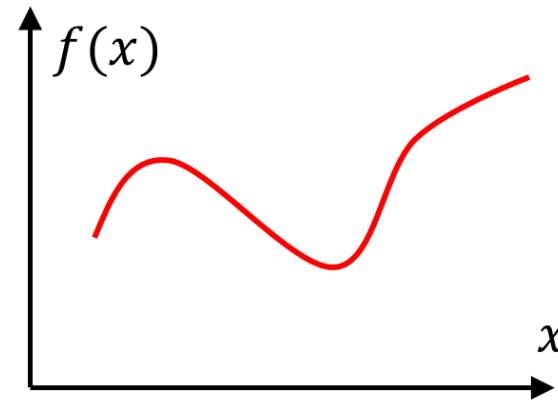
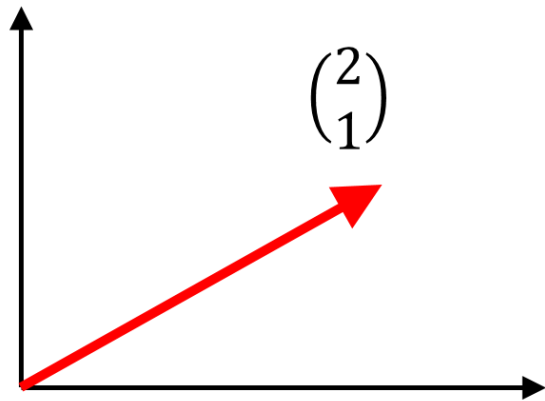
When ψ is an eigen function of \hat{A} , the expected value $\langle A \rangle$ of the physical quantity A calculated from ψ is equal to the eigenvalue a .

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^*(x) [\hat{A} \psi(x)] dx = \int_{-\infty}^{\infty} \psi^*(x) a \psi(x) dx = a \int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx = a$$

$$\langle A \rangle = \langle \psi(x) | \hat{A} | \psi(x) \rangle = \langle \psi(x) | \hat{A} \psi(x) \rangle = a \langle \psi(x) | \psi(x) \rangle = a$$

Wave function can be regarded as vector

If you choose a basis set appropriately, you can express a function in the vector form.



$$f(x) = a_0\phi_0(x) + a_1\phi_1(x) + a_2\phi_2(x) + \dots$$

$$f(x) = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \end{pmatrix}$$

$$\psi(x) = g(x) + i h(x)$$

$$g(x) \rightarrow (j_0, j_1, j_2, \dots, j_n, \dots)$$

$$h(x) \rightarrow (k_0, k_1, k_2, \dots, k_n, \dots)$$

$$a_n = j_n + i k_n$$

Relationship between wave functions and vectors

$$\psi(a) = \int \delta(x-a)\psi(x)dx$$

It is exactly the dot product of a function. In other words, this expression can be expressed as follows.

$$\psi(a) = \langle \delta(x-a) | \psi \rangle$$

Meaning that a particle is definitely found
at the coordinates $x = a$.

A vector representing "a state where a particle is definitely present at the coordinates x " is defined as $|x\rangle$.

$$\psi(x) = \langle x | \psi \rangle$$

The wave function is composed of coefficients when expressing the original state of this particle only by the combination of basis vectors having the value of "position where the particle exists".

What is a wave function

If you do unitary transformation, you should be able to evaluate the same state from another viewpoint, and the expression by wave functions is only one view of the state. Therefore, this wave function sometimes is called the "coordinate display" of the state.

In addition, it is possible to take a viewpoint such as "momentum display" expressed in terms of the value criterion of how much momentum to have, "particle number display" to extract particle properties from the state vector, and the like.

The physical quantity is represented by a matrix

Momentum vector:

$$|p_0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad |p_1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \quad |p_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \dots$$

$$\begin{pmatrix} p_0 & 0 & 0 & \dots \\ 0 & p_1 & 0 & \dots \\ 0 & 0 & p_2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} = p_0 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \quad \text{Momentum } p_0, p_1, p_2, \dots$$

$$\hat{A}|p_0\rangle = p_0|p_0\rangle$$

Unitary transformation: all vectors rotate in the same way while maintaining the positional relationship of all vectors in the complex vector space.

$$\hat{A}|p_0\rangle = p_0|p_0\rangle \Rightarrow U\hat{A}|p_0\rangle = p_0U|p_0\rangle \Rightarrow U\hat{A}U^{-1}U|p_0\rangle = p_0U|p_0\rangle$$

$$H|p'_0\rangle = p_0|p'_0\rangle \quad H = U\hat{A}U^{-1}$$

Hermitian

$$H^\dagger = (U\hat{A}U^{-1})^\dagger = (U\hat{A}\cdot U^{-1})^\dagger = (U^{-1})^\dagger (U\hat{A})^\dagger = (U^\dagger)^\dagger \hat{A}^\dagger U^\dagger = U\hat{A}U^{-1} = H$$

Unitary transformation: $U^{-1} = U^\dagger$ \hat{A} : Real diagonal matrix

$$\langle \phi | H | \psi \rangle = \int \phi^*(x) H \psi(x) dx$$
$$|\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \end{pmatrix} \quad \langle \phi | = (\phi_0^* \quad \phi_1^* \quad \phi_2^* \quad \dots)$$

$$\langle \phi | H | \psi \rangle^* = \langle \psi | H | \phi \rangle$$

$$\left(\sum_{i,j} \phi_i^* H_{ij} \psi_j \right)^* = \sum_{i,j} \phi_i H_{ij}^* \psi_j^* = \sum_{i,j} \phi_i H_{ji} \psi_j^* = \sum_{i,j} \psi_j^* H_{ji} \phi_i = \sum_{i,j} \psi_i^* H_{ij} \phi_j$$

$$\left(\int \phi^* H \psi dx \right)^* = \int \psi^* H \phi dx$$

Properties of eigen function and eigen values

(i) Eigen values for Hermitian operators are real.

$$\hat{A}\psi = a\psi \quad \Rightarrow \quad \int \psi^* \hat{A}\psi dv = a \int \psi^* \psi dv$$

ψ^* From the left side

$$\Rightarrow \int (\hat{A}\psi)^* \psi dv = a^* \int \psi \psi^* dv$$

c.c.

$$\int \psi^* \hat{A}\psi dv = \int (\hat{A}\psi)^* \psi dv = \int \psi \hat{A}^* \psi^* dv = \int \psi \hat{A} \psi^* dv$$

Hermitian

$$\Rightarrow 0 = (a - a^*) \int \psi^* \psi dv$$

$$\Rightarrow a = a^* \quad \text{Real}$$

Properties of eigen function and eigen values

(ii) Eigen functions of any Hermitian operator with different eigen values are orthogonal function.

$$\hat{A}\psi_1 = a_1\psi_1 \quad \Rightarrow \quad \int \psi_2^* \hat{A}\psi_1 dv = a_1 \int \psi_2^* \psi_1 dv$$

ψ_2^* From the left side

$$\hat{A}\psi_2 = a_2\psi_2 \quad \Rightarrow \quad \int \psi_1^* \hat{A}\psi_2 dv = a_2 \int \psi_1^* \psi_2 dv$$

ψ_1^* From the left side

$$\Rightarrow \int (\hat{A}\psi_1)^* \psi_2 dv = a_1^* \int \psi_1^* \psi_2 dv = a_2 \int \psi_1^* \psi_2 dv$$

$$\int \psi_1^* (A\psi_2) d\tau = \int \psi_2 (A\psi_1)^* d\tau = \left(\int \psi_2^* (A\psi_1) d\tau \right)^*$$

$$\Rightarrow (a_1 - a_2) \int \psi_1^* \psi_2 dv = 0 \quad \Rightarrow \quad \int \psi_1^* \psi_2 dv = 0$$

(iii) Eigen functions of an Hermitian operator form an orthonormal complete system.

$$\psi = c_1\phi_1 + c_2\phi_2 + \cdots + c_n\phi_n + \cdots = \sum_i c_i\phi_i \quad \hat{A}\phi_i = a_i\phi_i$$

$$\int \phi_n^* \psi dv = c_1 \int \phi_n^* \phi_1 dv + c_2 \int \phi_n^* \phi_2 dv + \cdots + c_n \int \phi_n^* \phi_n dv + \cdots$$

$$c_n = \int \phi_n^* \psi dv$$

$$\int \phi_i^* (A\phi_j) d\tau = \int \phi_i^* a_j \phi_j d\tau = a_j \int \phi_i^* \phi_j d\tau = a_j \delta_{ij},$$

(iv) Commutable Hermitian operators have common eigen functions.

$$\hat{A}\hat{B} = \hat{B}\hat{A} \qquad \hat{A}\psi_n^a = a_n\psi_n^a \qquad \text{No degeneracy}$$

$$\Rightarrow \hat{A}(\hat{B}\psi_n^a) = \hat{B}(\hat{A}\psi_n^a) = \hat{B}a_n\psi_n^a = a_n(\hat{B}\psi_n^a)$$

No degeneracy

$$\Rightarrow \hat{B}\psi_n^a = b_n\psi_n^a$$

What does it mean that operators are Hermitian?

In quantum mechanics, it is difficult to grasp intuitively that the wave function is a complex number or the coefficient of the operator is a complex number. But be relieved. **Even though the wave function may be a complex number, when you actually measure the position, momentum or spin of a particle, the needle of the detector always points to a real number.** The complex coordinates of the photosensitive plate do not shine, and it is impossible for a complex current to flow in the galvanometer. **The physical phenomena you actually see always come in real form.**

"The measured value is a real number."

Definite state and probability state for two physical quantities

Quantum state: Probabilistic superposition of eigenstates of physical quantity operators

Physical quantity A $\hat{A}|\phi_i\rangle = a_i|\phi_i\rangle$

Physical quantity B $\hat{B}|\psi_j\rangle = b_j|\psi_j\rangle$

$|\phi_i\rangle = |\psi_j\rangle \Rightarrow$ Definite state: No uncertainty

$|\phi_i\rangle = \sum_j c_j |\psi_j\rangle \Rightarrow$ Probabilistic state: Uncertainty

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

$[\hat{A}, \hat{B}] \neq 0 \Rightarrow$ A and B have no common eigen states.
A and B cannot be observed simultaneously.

$[\hat{A}, \hat{B}] \neq 0 \Rightarrow A$ and B have no common eigen states.

Assuming

$[\hat{A}, \hat{B}] \neq 0 \quad \hat{A}, \hat{B}$: have a common eigen states $|\phi\rangle$.

$$\hat{A}|\phi\rangle = a|\phi\rangle, \quad \hat{B}|\phi\rangle = b|\phi\rangle$$

$$\hat{B}\hat{A}|\phi\rangle = a\hat{B}|\phi\rangle = ab|\phi\rangle, \quad \hat{A}\hat{B}|\phi\rangle = b\hat{A}|\phi\rangle = ba|\phi\rangle$$

$$\Rightarrow \hat{B}\hat{A}|\phi\rangle = \hat{A}\hat{B}|\phi\rangle \Rightarrow [\hat{A}, \hat{B}]|\phi\rangle = 0 \Rightarrow [\hat{A}, \hat{B}] = 0$$

Let's reconsider the uncertainty principle!!