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Vector Space Language

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A Vector Space Language for Quantum Mechanics

References

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The inner product

Given two vectors in 3D, we can construct a *number* by forming the dot (scalar) product

$$\boldsymbol{w} \cdot \boldsymbol{v} = v_x w_x + v_y w_y + v_z w_z.$$

In n dimensions where $\boldsymbol{v}$ would have components $v_1, v_2, \ldots v_n$, this product becomes

$$\boldsymbol{w} \cdot \boldsymbol{v} = \sum_{i=1}^{n} v_i w_i.$$

The vector $\boldsymbol{v}$ can be thought of as a *function* $v(i)$ for which the independent variable i only assumes integer values. From this it is a small step to picturing a function of a *continuous* variable x, $v(x)$, as a vector with an infinite number of components. The extension of the dot product is

$$\int_{-\infty}^{\infty} w(x)\, v(x)\, dx.$$

If $w(x)$ and $v(x)$ are *complex* functions, it is natural to introduce a complex conjugation in such a way as to make the product of a vector with itself be a real number. Hence we define the *inner product* of two functions $\psi(x)$ and $\phi(x)$,

$$\boxed{\langle \psi(x) | \phi(x) \rangle = \int_{-\infty}^{\infty} \psi(x)^* \, \phi(x)\, dx.}$$

All predictions of quantum mechanics can be written as an inner product of two vectors. That is, the map

$$2 \text{ vectors} \rightarrow \text{a number}$$

is a fundamental tool of quantum mechanics.

Basis sets

Along with this definition of the inner product of two vectors, we can import the jargon of vector analysis into quantum mechanics. A wave function $\Psi(x)$ is a *state vector*. A *normalized* state vector is simply a *unit* vector,

$$\langle \Psi(x) | \Psi(x) \rangle = 1.$$

An *orthonormal basis set* is a set of vectors $\{\phi_n(x)\}_{n=0}^{\infty}$ for which

$$\langle \phi_m(x) | \phi_n(x) \rangle = \begin{cases} 0, & \text{if } m \neq n \text{ (orthogonality)} \\ 1, & \text{if } m = n \text{ (normalization)} \end{cases}$$

and for which *any* state vector can be represented

$$\Psi(x) = \sum_{n=0}^{\infty} c_n \phi_n(x).$$

The expansion coefficients $\{c_n\}_{n=0}^{\infty}$ can be determined from

$$c_n = \langle \phi_n(x) | \Psi(x) \rangle.$$

Since the column matrix

$$\Psi = \begin{bmatrix} c_1 \\ c_2 \\ c_2 \\ \vdots \\ \vdots \end{bmatrix}$$

provides the same information as $\Psi(x)$, this matrix will also be called (and thought of as) "a vector". If

$$\Phi(x) = \sum_{k=0}^{\infty} d_k \phi_k(x)$$

represents a different vector, the inner product reduces to

$$\begin{aligned}\langle\Phi|\Psi\rangle &= \int_{-\infty}^{\infty} \Phi(x)^* \, \Psi(x)\, dx \\ &= \sum_{m,n=0}^{\infty} d_m^* c_n \int_{-\infty}^{\infty} \phi_m(x)^* \, \phi_n(x)\, dx \\ &= \sum_{k=0}^{\infty} d_k^* c_k.\end{aligned}$$

This may also be written as a matrix product,

$$\langle\Phi|\Psi\rangle = [\, d_1, d_2, \cdots]^* \begin{bmatrix} c_1 \\ c_2 \\ c_2 \\ \vdots \end{bmatrix}.$$

Hermitian operators

Since a measuring apparatus behaves like a classical object, "observables" come from classical mechanics: position, velocity, energy, angular momentum,. . ..
These quantities are usually expressed in terms of *canonically conjugate* coordinates and momenta, $q_1, \ldots, q_f, p_1, \ldots, p_f$ if there are f degrees of freedom in the system. Quantum mechanics associates with each classical observable

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

an Hermitian linear operator

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

An operator

$$\hat{A} \text{ is } \textit{Hermitian} \quad \Longleftrightarrow \quad \langle\psi|\hat{A}\phi\rangle = \langle\hat{A}\psi|\phi\rangle \text{ for all } \psi, \phi.$$

The Hermiticity of the Hamiltonian $\hat{H}$ guarantees that

$$\langle\Psi(x,t)|\Psi(x,t)\rangle = \langle\Psi(x,0)|\Psi(x,0)\rangle$$

at all t. Thus time evolution leads to a *rotation* of the state vector in the (vector) space of possible states.

If $\hat{A}$ has a set of eigenvectors, eigenfunctions

$$\hat{A}\phi_k(q) = a_k\phi_k(q), \quad k = 1, 2, \ldots,$$

and $\hat{A}$ is Hermitian, then

$$a_k\langle\phi_\ell|\phi_k\rangle = \langle\phi_\ell|\hat{A}\phi_k\rangle = \langle\hat{A}\phi_\ell|\phi_k\rangle = a_\ell^*\langle\phi_\ell|\phi_k\rangle,$$

or

$$(a_k - a_\ell^*)\langle\phi_\ell|\phi_k\rangle = 0. \tag{1}$$

The $k = \ell$ case of (1) shows that all the eigenvalues of $\hat{A}$ are *real*. If $a_k \neq a_\ell$, (1) shows that all $\langle\phi_\ell|\phi_k\rangle = 0$. That is, the eigenvectors corresponding to *different* eigenvalues must be orthogonal. If there are n (linearly independent) eigenvectors of $\hat{A}$ with the *same* eigenvalue, (1) says nothing. But these vectors define an n-dimensional subspace and *any* set of orthonormal vectors in this subspace is a set of eigenvectors corresponding to the same eigenvalue of $\hat{A}$.

In summary, the Hermiticity of $\hat{A}$ assures us that we can find an orthonormal set of vectors, with each vector an eigenvector of $\hat{A}$ with a real eigenvalue. We argue that this set must be a *basis* set because of "physical completeness", because the set of eigenvectors of $\hat{A}$ exhausts what can be realized physically. The index/label k may have a continuous set of allowed values, but usually such labels are restricted to a discrete set.

The Expectation

In classical mechanics, observation of Q on a system in state p, q gives $Q(p, q)$ with certainty. In quantum mechanics, however, observation of Q on a system in a state Ψ does not necessarily give a definite answer. Repeating the same experiment exactly does not necessarily give the same result. In this case, of course, one can't predict explicitly what will be seen in a measurement. One can, however, predict the *expectation* – the average result which many repetitions of the measurement would give. Explicitly,

$$\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle \tag{2}$$

Here are some examples of this:

(i) Observation of 'q' (a continuous *label*). Suppose we define

$$Q = \begin{cases} 1, & \text{if } a \le q \le b, \\ 0, & \text{otherwise.} \end{cases}$$

The expectation of this Q is just the probability that we will see $a \le q \le b$, so

$$\text{Prob}[a \le q \le b] = \int_a^b dq \, |\Psi(q)|^2 .$$

Thus $|\Psi(t)|^2$ gives the distribution on q. Observation of q itself gives

$$\langle q \rangle = \langle \Psi(q) | \hat{Q} \Psi(q) \rangle = \int_{-\infty}^{\infty} |\Psi(q)|^2 q \, dq,$$

from (2) directly, or from the physical interpretation of $|\Psi(t)|^2$. Similarly,

$$\begin{aligned} \langle q^2 \rangle &= \langle \Psi(q) | \hat{Q}^2 \Psi(q) \rangle = \int_{-\infty}^{\infty} |\Psi(q)|^2 q^2 \, dq, \\ \langle q^3 \rangle &= \langle \Psi(q) | \hat{Q}^3 \Psi(q) \rangle = \int_{-\infty}^{\infty} |\Psi(q)|^2 q^3 \, dq, \\ &\dots \\ \langle f(q) \rangle &= \langle \Psi(q) | f(\hat{Q}) \Psi(q) \rangle = \int_{-\infty}^{\infty} |\Psi(q)|^2 f(q) \, dq. \end{aligned}$$

(ii) observation of a Q for which the corresponding $\hat{Q}$ has discrete eigenvalues. Suppose

$$\hat{Q} \phi_k(q) = \lambda_k \phi_k(q), \qquad k = 0, 1, 2, \dots$$

with $\{\phi_k(q)\}$ an orthonormal basis set. We can represent

$$\Psi(q) = \sum c_k \phi_k(q)$$

The expectation of $Q(p, q)$ is

$$\begin{aligned}
\langle Q \rangle &= \langle \Psi | \hat{Q}\, \Psi \rangle \\
&= \langle \sum_n c_m \phi_m(q) | \hat{Q} \sum_n c_n \phi_n(q) \rangle = \langle \sum_n c_m \phi_m(q) | \sum_n c_n \lambda_n \phi_n(q) \rangle \\
&= \sum_{m,n} c_m^* c_n \lambda_n \langle \phi_m | \phi_n \rangle = \sum |c_k|^2 \lambda_k,
\end{aligned}$$

Similarly,

$$\begin{aligned}
\langle q^2 \rangle &= \langle \Psi(q) | \hat{Q}^2 \Psi(q) \rangle = \sum_{k=0}^{\infty} |c_k|^2 \lambda_k^2, \\
\langle q^3 \rangle &= \langle \Psi(q) | \hat{Q}^3 \Psi(q) \rangle = \sum_{k=0}^{\infty} |c_k|^2 \lambda_k^2, \\
&\dots \\
\langle f(q) \rangle &= \langle \Psi(q) | f(\hat{Q}) \Psi(q) \rangle = \sum_{k=0}^{\infty} |c_k|^2 f(\lambda_k).
\end{aligned}$$

This will hold for *any* $f(q)$ only if the only possible values of Q which can be observed are the eigenvalues $\lambda_1, \lambda_2, \dots$ and the probability of seeing $q = \lambda_k$ is

$$|c_k|^2 = |\langle \phi_k | \Psi \rangle|^2 .$$