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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

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

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

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

The vector  $\mathbf{v}$  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  $\phi(x)$ :

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

All predictions of quantum mechanics can be written as an inner product of two vectors.

That is, the map

2 vectors  $\rightarrow$  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,

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

## 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,  $q_1, \dots, q_f, p_1, \dots, p_f$  if there are  $f$  degrees of freedom in the system. Quantum mechanics associates with each classical observable

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

an Hermitian linear operator

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

An operator

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

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

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

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

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

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  $\Psi$  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,

$$\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle \quad (2)$$

Here are some examples of this:

(i) Observation of ‘ $q$ ’ (a continuous *label*). Suppose we define

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

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

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

Thus  $|\Psi(q)|^2$  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  $|\Psi(q)|^2$ . 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

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

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

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

Similarly,

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

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

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