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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 asumes 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, this map: vectors $\rightarrow$ numbers is a fundamental tool of quantum mechanics.

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,

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

Since

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

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

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

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

that can be linearly combined to produce *any* state vector,

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

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,

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

Observables

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

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

a linear operator

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

For any observable $A(p, q)$ we can construct a set of eigenfunctions

$$
\hat{A}\phi_k(q) = a_k \phi_k(q)
$$

that form an orthonormal basis set. The index/label k may have a continuous set of allowed values, but usually such labels are restricted to a discrete set. The expansion coefficients in

$$
\Psi(q) = \sum_{k=0}^{\infty} c_k \phi_k(q),
$$

provide a representation of Ψ in terms of vectors associated physically with $A(p,q)$.

The Expectation

For a system in a state $\Psi(q)$,

(1) observation of 'q' (a continuous *label*) will see a distribution of values with distribution function $|\Psi(q)|^2$. Since the probability of seeing $a \le q \le b$ is $\int_a^b |\Psi(q)|^2$, the average (*expected*) value for observation of q is

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

just the inter product of the vectors $\Psi(q)$ and $q\Psi(q)$. Similarly,

$$\langle q^2 \rangle = \langle \Psi(q) | q^2 \Psi(q) \rangle,$$
$$\langle q^3 \rangle = \langle \Psi(q) | q^3 \Psi(q) \rangle,$$
$$\cdots$$
$$\langle f(q) \rangle = \langle \Psi(q) | f(q) \Psi(q) \rangle.$$

(2) observation of $A(p,q)$ can only lead to the eigenvalues of the corresponding operator $\hat{A}$. That is, if

$$\hat{A}\phi_k(q) = a_k \phi_k(q), \qquad k = 0, 1, 2, \ldots$$

then only the values $a_0, a_1, a_2, \ldots$ can be observed. If

$$\Psi(q) = \sum_{k=0}^{\infty} c_k \phi_k(q),$$

then the probability of seeing a_k is $|c_k|^2$. Thus the average (*expected*) value for $A(p,q)$ is

$$\langle A \rangle = \sum_{k=0}^{\infty} |c_k|^2 a_k.$$

Since direct calculation gives

$$\begin{aligned}\langle\Psi|\hat{A}\,\Psi\rangle &= \langle\sum_n c_m\phi_m(q)|\hat{A}\sum_n c_n\phi_n(q)\rangle = \langle\sum_n c_m\phi_m(q)|\sum_n c_n a_n\phi_n(q)\rangle\\ &= \sum_{m,n} c_m^* c_n a_n\langle\phi_m|\phi_n\rangle = \sum_{k=0}^{\infty}|c_k|^2 a_k,\end{aligned}$$

the expectation of $A(p,q)$ is

$$\langle A\rangle = \langle\Psi|\hat{A}\,\Psi\rangle,$$

just the inner product of the vectors Ψ and $\hat{A}\,\Psi$. Similarly,

$$\begin{aligned}\langle A^2\rangle &= \langle\Psi|\hat{A}^2\Psi\rangle,\\ \langle A^3\rangle &= \langle\Psi|\hat{A}^3\Psi\rangle,\\ &\cdots\\ \langle f(A)\rangle &= \langle\Psi|f(\hat{A})\Psi\rangle.\end{aligned}$$