Chem. 540
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Dirac bra-ket notation

The symbol $|n\rangle$ (or $|\Psi_n\rangle$) is called a "ket" and denotes the state described by the wavefunction Ψ_n. The complex conjugate of the wavefunction, Ψ_n^*, is denoted by the "bra" $\langle n|$ (or $\langle \Psi_n|$). The ket denotes a state in the most abstract form, without reference to a particular representation.

When we put a bra together with a ket, with an operator in the middle, we imply integration over all space:

$$\int d\mathbf{r}\,\Psi_n^*(\mathbf{r})\hat{A}\Psi_m(\mathbf{r}) \equiv \langle \Psi_n|\hat{A}|\Psi_m\rangle \quad \text{or} \quad \langle n|\hat{A}|m\rangle$$

Leaving out the operator implies the identity operator, i.e.,

$$\langle \Psi_m|\Psi_n\rangle \equiv \int d\mathbf{r}\,\Psi_m^*(\mathbf{r})\Psi_n(\mathbf{r}) = \langle \Psi_n|\Psi_m\rangle^*$$

$\langle \Psi_m|\Psi_n\rangle$ is the amplitude for a particle in state Ψ_n to be also in state Ψ_m. This is also known as the overlap of these two states.

In this notation, the condition for an operator to be hermitian is

$$\langle \Psi_m|\hat{A}|\Psi_n\rangle = \langle \Psi_n|\hat{A}|\Psi_m\rangle^*.$$

Remarks

$\langle \Phi_n|\Phi_m\rangle$ is a scalar (i.e., a number).

$|\Phi_m\rangle\langle \Phi_n|$ is an operator, because it can operate on $|\Psi\rangle$ to give

$$\left(|\Phi_m\rangle\langle \Phi_n|\right)|\Psi\rangle = \alpha|\Phi_m\rangle, \qquad \alpha = \langle \Phi_n|\Psi\rangle$$

$\hat{P}_n \equiv |\Phi_n\rangle\langle \Phi_n|$ is a projection operator. It gives the component of a state along $|\Phi_n\rangle$.

The sum of all projection operators onto all states of an orthonormal complete set gives the identity operator.

Position and momentum states

$|x\rangle$ is the state of a particle located precisely at position *x*. Therefore, the momentum of the system is completely uncertain.

$|p\rangle$ is the state of a particle with momentum precisely equal to *p*. Therefore, the position of the particle is completely uncertain.

$\langle x|p\rangle$ is the amplitude for a particle in a state of precisely defined momentum *p* to be at position *x*. Since the position of such a particle is completely uncertain, the probability of finding the particle at *x* should be independent of *x*, i.e., any position is equally probable:

$$|\langle x|p\rangle|^2 \text{ independent of } x.$$

Using similar arguments, the momentum of a particle in state $|x\rangle$ is completely uncertain, and thus we conclude

$$|\langle p|x\rangle|^2 \text{ independent of } p.$$

Therefore, since the above two probabilities are equal, it follows

$$|\langle x|p\rangle|^2 = \text{constant.}$$

$|x\rangle$ is an eigenstate of the position operator with eigenvalue *x*. This is so because any measurement of the position of the particle in state $|x\rangle$ should yield the result *x*. Thus,

$$\hat{x}|x\rangle = x|x\rangle$$

Similarly, $|p\rangle$ is an eigenstate of the momentum operator with eigenvalue *p*:

$$\hat{p}|p\rangle = p|p\rangle$$

$\langle x|\Psi_n\rangle$ is the amplitude that a particle in state $|\Psi_n\rangle$ will be found at position *x*. Therefore,

$$\langle x|\Psi_n\rangle \equiv \Psi_n(x)$$

The normalization condition becomes $\int dx |\langle x|\Psi_n\rangle|^2 = 1$

Note that since $|\langle x|p\rangle|^2$ = constant., the wavefunctions for momentum states cannot be normalized to 1.

The two-slit experiment in Dirac notation

$|s\rangle \equiv$ state of the electron as it leaves the source (beam)

$\langle k|s\rangle =$ amplitude for an electron in state $|s\rangle$ to go through hole *k*.

$\langle x|k\rangle =$ amplitude for an electron coming out of hole *k* to end up at *x*.

Since we are summing amplitudes,

$$\langle x|s\rangle = \langle x|1\rangle\langle 1|s\rangle + \langle x|2\rangle\langle 2|s\rangle .$$

Note: the object $|1\rangle\langle 1| + |2\rangle\langle 2|$ plays the role of the identity operator.

$|k\rangle\langle k|$ is a projection operator that projects on the state of hole *k*.