EIGENFUNCTIONS OF POSITION AND MOMENTUM; UNIT OPERATORS

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There are a few results that will be used frequently in quantum theory that I think it's worth collecting together and explaining in full.

First, we'll revisit the eigenfunctions of the position and momentum operators. In the earlier post, we showed that the eigenfunctions of the position operator are delta functions and we wrote

$$|x_0\rangle = \delta(x - x_0) \tag{1}$$

Strictly speaking this equation gives the position space representation of the eigenfunction. More precisely, we should just say that $|x_0\rangle$ is an eigenfunction of the position operator $\hat{x}$ and leave it at that. In order to write it as a 'proper' function (that is, a function we can use in calculations such as integrals), we need to specify the space we're using and then write $|x_0\rangle$ in that space, as we did above for position space.

For momentum, we've seen that the eigenfunctions are

$$|p_0\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip_0 x/\hbar} \tag{2}$$

The normalizations of both the position and momentum eigenfunctions give us more delta functions:

$$\langle x_1 | x_0 \rangle = \int \delta(x - x_1)\, \delta(x - x_0)\, dx \tag{3}$$

$$= \delta(x_1 - x_0) \tag{4}$$

$$\langle p_1 | p_0 \rangle = \frac{1}{2\pi\hbar} \int e^{i(p_0 - p_1)x/\hbar} dx \tag{5}$$

$$= \delta(p_0 - p_1) \tag{6}$$

Given a complete basis set of states, we can define a set of projection operators each of which projects a function onto the basis vector that defines the projection operator. A projection operator has the form

$$\hat{P} \equiv |\alpha\rangle\langle\alpha| \tag{7}$$

so that applying it to a state $|\psi\rangle$ gives

$$\hat{P}|\psi\rangle = \langle\alpha|\psi\rangle|\alpha\rangle \tag{8}$$

Note that this is a completely general expression; we can choose *any* basis states $|\alpha\rangle$ (they could be the eigenstates of position or momentum, or the discrete set of states for some system such as the states of the infinite square well or harmonic oscillator) and the projection operator gives the component of $|\psi\rangle$ 'along' that basis vector. In practice, to do calculations we usually express $|\psi\rangle$ in position or momentum space (or in matrix form if it's a spin state) but in this formula, $|\psi\rangle$ is just an abstract symbol representing some arbitrary state.

For a complete set of discrete basis states we can define the *unit operator*

$$1 \equiv \sum_{\alpha} |\alpha\rangle\langle\alpha| \tag{9}$$

or for a continuous set of basis states

$$1 \equiv \int d\alpha\, |\alpha\rangle\langle\alpha| \tag{10}$$

This works because it's just like expressing a 3-d vector as a sum of its components in some basis, such as rectangular coordinates

$$\mathbf{v} = v_x\hat{\mathbf{x}} + v_y\hat{\mathbf{y}} + v_z\hat{\mathbf{z}} \tag{11}$$

Since the basis consisting of the states $|\alpha\rangle$ is complete, we can write any other state in terms of that basis set. We're using the projection operator for each basis state to project out the new state onto each of the basis states in turn, then adding up the result:

$$|\psi\rangle = \sum_{\alpha} |\alpha\rangle\langle\alpha|\psi\rangle \tag{12}$$

or

$$|\psi\rangle = \int d\alpha\, |\alpha\rangle\langle\alpha|\psi\rangle \tag{13}$$

Example 1. Armed with these results, it's worth looking at Example 3.6 in Lancaster & Blundell in a bit more detail. In that example, they extend the creation-annihilation operator representation to cases where the momentum (and hence the energy) states merge into a continuum. In that case, the commutation relation for the operators becomes

$$\left[a_{\mathbf{p}}, a_{\mathbf{q}}^{\dagger}\right] = \delta^{(3)}(\mathbf{p}-\mathbf{q}) \tag{14}$$

L&B are dealing with a 3-d particle in a box with periodic boundary conditions (rather than requiring the wave function to be zero outside the box), so the momentum eigenstate $|\mathbf{p}\rangle$ is just a plane wave so that its position space representation is

$$\langle \mathbf{x} | \mathbf{p} \rangle = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{p}\cdot\mathbf{x}} \tag{15}$$

where $\mathcal{V}$ is the volume of the box.

They begin with a one-particle state

$$\langle \mathbf{p} | \mathbf{p}' \rangle = \left\langle \hat{a}_{\mathbf{p}}^{\dagger} 0 \middle| \hat{a}_{\mathbf{p}'}^{\dagger} 0 \right\rangle \tag{16}$$

$$= \left\langle 0 \middle| \hat{a}_{\mathbf{p}} \hat{a}_{\mathbf{p}'}^{\dagger} \middle| 0 \right\rangle \tag{17}$$

We can now use the relation 14 to get

$$\hat{a}_{\mathbf{p}} \hat{a}_{\mathbf{p}'}^{\dagger} = \delta^{(3)} \left(\mathbf{p} - \mathbf{p}' \right) + \hat{a}_{\mathbf{p}'}^{\dagger} \hat{a}_{\mathbf{p}} \tag{18}$$

and since $\hat{a}_{\mathbf{p}} |0\rangle = 0$ we get

$$\langle \mathbf{p} | \mathbf{p}' \rangle = \left\langle 0 \middle| \delta^{(3)} \left(\mathbf{p} - \mathbf{p}' \right) \middle| 0 \right\rangle \tag{19}$$

$$= \delta^{(3)} \left(\mathbf{p} - \mathbf{p}' \right) \tag{20}$$

Now we want to get the position space version of the state $|\mathbf{p}\rangle$. From 1 (generalized to 3-d) we see that

$$\phi_{\mathbf{p}}(\mathbf{x}) \equiv \langle \mathbf{x} | \mathbf{p} \rangle \tag{21}$$

$$= \int d^3\mathbf{x}' \langle \mathbf{x} | \mathbf{x}' \rangle \langle \mathbf{x}' | \mathbf{p} \rangle \tag{22}$$

$$= \int d^3\mathbf{x}' \delta^{(3)} \left(\mathbf{x} - \mathbf{x}' \right) \langle \mathbf{x}' | \mathbf{p} \rangle \tag{23}$$

so if we can write $|\mathbf{p}\rangle$ as a function of $\mathbf{x}'$ then the expression $\langle \mathbf{x} | \mathbf{p} \rangle$ picks out the precise position $\mathbf{x}$ that we're interested in. Using a set of momentum basis states $|\mathbf{q}\rangle$ we can transform $|\mathbf{x}\rangle$ using the unit operator 13:

$$|\mathbf{x}\rangle = \int d^3\mathbf{q} \, |\mathbf{q}\rangle \langle \mathbf{q} | \mathbf{x} \rangle \tag{24}$$

$$= \int d^3\mathbf{q} \, |\mathbf{q}\rangle \langle \mathbf{x} | \mathbf{q} \rangle^* \tag{25}$$

$$= \int d^3\mathbf{q} \, \phi_{\mathbf{q}}^*(\mathbf{x}) \, |\mathbf{q}\rangle \tag{26}$$

Therefore

$$\langle\mathbf{x}| = \int d^3\mathbf{q}\phi_{\mathbf{q}}(\mathbf{x})\langle\mathbf{q}| \tag{27}$$

$$\langle\mathbf{x}|\mathbf{p}\rangle = \int d^3\mathbf{q}\phi_{\mathbf{q}}(\mathbf{x})\langle\mathbf{q}|\mathbf{p}\rangle \tag{28}$$

$$= \int d^3\mathbf{q}\phi_{\mathbf{q}}(\mathbf{x})\delta^{(3)}(\mathbf{q}-\mathbf{p}) \tag{29}$$

$$= \phi_{\mathbf{p}}(\mathbf{x}) \tag{30}$$

Example 2. We can apply the same arguments to a 2-particle state. Start with

$$\langle\mathbf{p}'\mathbf{q}'|\mathbf{pq}\rangle = \left\langle 0\left|\hat{a}_{\mathbf{p}'}\hat{a}_{\mathbf{q}'}\hat{a}^\dagger_{\mathbf{q}}\hat{a}^\dagger_{\mathbf{p}}\right|0\right\rangle \tag{31}$$

From commutation relations 14 we get

$$\hat{a}_{\mathbf{p}'}\hat{a}_{\mathbf{q}'}\hat{a}^\dagger_{\mathbf{q}}\hat{a}^\dagger_{\mathbf{p}} = \hat{a}_{\mathbf{p}'}\left(\delta^{(3)}(\mathbf{q}-\mathbf{q}')+\hat{a}^\dagger_{\mathbf{q}}\hat{a}_{\mathbf{q}'}\right)\hat{a}^\dagger_{\mathbf{p}} \tag{32}$$

$$= \delta^{(3)}(\mathbf{q}-\mathbf{q}')\left(\delta^{(3)}(\mathbf{p}-\mathbf{p}')+\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}'}\right)+\hat{a}_{\mathbf{p}'}\hat{a}^\dagger_{\mathbf{q}}\hat{a}_{\mathbf{q}'}\hat{a}^\dagger_{\mathbf{p}} \tag{33}$$

$$= \delta^{(3)}(\mathbf{q}-\mathbf{q}')\left(\delta^{(3)}(\mathbf{p}-\mathbf{p}')+\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}'}\right)+ \left(\delta^{(3)}(\mathbf{q}-\mathbf{p}')+\hat{a}^\dagger_{\mathbf{q}}\hat{a}_{\mathbf{p}'}\right)\left(\delta^{(3)}(\mathbf{p}-\mathbf{q}')+\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{q}'}\right) \tag{34}$$

Applying $\hat{a}_{\mathbf{p}}|0\rangle = 0$ we get

$$\langle\mathbf{p}'\mathbf{q}'|\mathbf{pq}\rangle = \delta^{(3)}(\mathbf{q}-\mathbf{q}')\delta^{(3)}(\mathbf{p}-\mathbf{p}')+\delta^{(3)}(\mathbf{q}-\mathbf{p}')\delta^{(3)}(\mathbf{p}-\mathbf{q}') \tag{35}$$

To convert to position coordinates, this time we have two independent positions, one for each particle, which we'll call **x** and **y**, so a position state is $|\mathbf{xy}\rangle$. Since the particles are independent, we can represent the compound state as the product of two single-particle states:

$$|\mathbf{p}'\mathbf{q}'\rangle = |\mathbf{p}'\rangle|\mathbf{q}'\rangle \tag{36}$$

where each single-particle state has its own coordinates, independent of the other state. The inner product of two such states is

$$\langle\mathbf{rs}|\mathbf{pq}\rangle = \langle\mathbf{r}|\mathbf{p}\rangle\langle\mathbf{s}|\mathbf{q}\rangle \tag{37}$$

since each particle's coordinates are independent of the other particle.

Using the more familiar wave function representation, we could have something like this:

$$\langle \mathbf{rs} | \mathbf{pq} \rangle = \int d^3\mathbf{x} \int d^3\mathbf{y} \phi^*_{\mathbf{r}}(\mathbf{x}) \phi^*_{\mathbf{s}}(\mathbf{y}) \psi_{\mathbf{p}}(\mathbf{x}) \psi_{\mathbf{q}}(\mathbf{y}) \tag{38}$$

$$= \int d^3\mathbf{x} \phi^*_{\mathbf{r}}(\mathbf{x}) \psi_{\mathbf{p}}(\mathbf{x}) \int d^3\mathbf{y} \phi^*_{\mathbf{s}}(\mathbf{y}) \psi_{\mathbf{q}}(\mathbf{y}) \tag{39}$$

$$= \langle \mathbf{r} | \mathbf{p} \rangle \langle \mathbf{s} | \mathbf{q} \rangle \tag{40}$$

In that case we can write

$$|\mathbf{xy}\rangle = \frac{1}{\sqrt{2!}} \int d^3p' \int d^3q' \left|\mathbf{p}'\right\rangle \left|\mathbf{q}'\right\rangle \left\langle \mathbf{q}' | \mathbf{y} \right\rangle \left\langle \mathbf{p}' | \mathbf{x} \right\rangle \tag{41}$$

$$= \frac{1}{\sqrt{2!}} \int d^3p' \int d^3q' \phi^*_{\mathbf{p}'}(\mathbf{x}) \phi^*_{\mathbf{q}'}(\mathbf{y}) \left|\mathbf{p}'\right\rangle \left|\mathbf{q}'\right\rangle \tag{42}$$

$$\langle \mathbf{xy}| = \frac{1}{\sqrt{2!}} \int d^3p' \int d^3q' \phi_{\mathbf{p}'}(\mathbf{x}) \phi_{\mathbf{q}'}(\mathbf{y}) \left\langle \mathbf{p}'\right| \left\langle \mathbf{q}'\right| \tag{43}$$

$$= \frac{1}{\sqrt{2!}} \int d^3p' \int d^3q' \phi_{\mathbf{p}'}(\mathbf{x}) \phi_{\mathbf{q}'}(\mathbf{y}) \left\langle \mathbf{p}'\mathbf{q}'\right| \tag{44}$$

The $\frac{1}{\sqrt{2!}}$ is there because the double integral extends over all values of both $\mathbf{p}'$ and $\mathbf{q}'$ so it counts the state $|\mathbf{p}'\rangle|\mathbf{q}'\rangle$ twice, once as $|\mathbf{p}'\rangle|\mathbf{q}'\rangle$ and once as $|\mathbf{q}'\rangle|\mathbf{p}'\rangle$. It's a square root because we're dealing with a raw wave function and it's the square modulus of this that must be normalized.

With this, we get, using 35

$$\langle \mathbf{xy} | \mathbf{pq} \rangle = \frac{1}{\sqrt{2!}} \int d^3p' \int d^3q' \phi_{\mathbf{p}'}(\mathbf{x}) \phi_{\mathbf{q}'}(\mathbf{y}) \left\langle \mathbf{p}'\mathbf{q}' | \mathbf{pq} \right\rangle \tag{45}$$

$$= \frac{1}{\sqrt{2}} \left[\phi_{\mathbf{p}}(\mathbf{x}) \phi_{\mathbf{q}}(\mathbf{y}) + \phi_{\mathbf{q}}(\mathbf{x}) \phi_{\mathbf{p}}(\mathbf{y})\right] \tag{46}$$

This is the symmetrized wave function for two identical bosons. Following through the same argument using anticommutators for fermions gives the fermion result

$$\langle \mathbf{xy} | \mathbf{pq} \rangle_{fermion} = \frac{1}{\sqrt{2}} \left[\phi_{\mathbf{p}}(\mathbf{x}) \phi_{\mathbf{q}}(\mathbf{y}) - \phi_{\mathbf{q}}(\mathbf{x}) \phi_{\mathbf{p}}(\mathbf{y})\right] \tag{47}$$