SECOND QUANTIZING OPERATORS - EXAMPLES

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We've seen that we can second quantize a single-particle operator $\hat{\mathcal{A}}$ using creation and annihilation operators to get the multi-particle version:

$$\hat{A}=\sum_{\alpha,\beta}\mathcal{A}_{\alpha\beta}a_{\alpha}^{\dagger}a_{\beta} \tag{1}$$

Using this result, we can get second quantized versions of some common operators. The unit operator is

$$\hat{1}=\sum_{\gamma}\left|\gamma\right\rangle \left\langle \gamma\right| \tag{2}$$

so

$$\left\langle \alpha\left|\hat{1}\right|\beta\right\rangle = \left\langle \alpha\left|\sum_{\gamma}\left|\gamma\right\rangle \left\langle \gamma\right|\right|\beta\right\rangle \tag{3}$$

$$=\sum_{\gamma}\delta_{\alpha\gamma}\delta_{\gamma\beta} \tag{4}$$

$$=\delta_{\alpha\beta} \tag{5}$$

so the multi-particle version is

$$\hat{n}=\sum_{\alpha}a_{\alpha}^{\dagger}a_{\alpha} \tag{6}$$

Since $a_{\alpha}^{\dagger}a_{\alpha}$ is the number operator, it counts the number of particles in state α so $\hat{n}$ gives the total number of particles in the multi-particle state. [I'm still not clear as to whether this result is supposed to apply to states where there are more than one particle in a given momentum state. The derivation of 1 appears to assume that each particle is in a different single-particle state, so it seems safer to assume that $a_{\alpha}^{\dagger}a_{\alpha}$ can return only 0 or 1.]

For the momentum operator (we're still looking at the particle in a box, so momentum states are still discrete) we have

$$\hat{\mathbf{p}}\left|\mathbf{p}\right\rangle = \mathbf{p}\left|\mathbf{p}\right\rangle \tag{7}$$

$$\left\langle \mathbf{q}\left|\hat{\mathbf{p}}\right|\mathbf{p}\right\rangle = \mathbf{p}\left\langle \mathbf{q}\left|\mathbf{p}\right.\right\rangle \tag{8}$$

$$= \mathbf{p}\delta_{\mathbf{qp}} \tag{9}$$

The multi-particle version is therefore

$$\hat{p} = \sum_{\mathbf{q},\mathbf{p}} \mathbf{p}\delta_{\mathbf{qp}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{p}} \tag{10}$$

$$= \sum_{\mathbf{p}} \mathbf{p} a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} \tag{11}$$

We can extend this result to functions of momentum $f(\mathbf{p})$. First, we look at powers of the momentum operator, where we can use induction to prove that $(\hat{\mathbf{p}})^n\left|\mathbf{p}\right\rangle = p^n\left|\mathbf{p}\right\rangle$. We know this is true for $n = 1$ so assume it's true for $n-1$. Then

$$(\hat{\mathbf{p}})^n\left|\mathbf{p}\right\rangle = \hat{\mathbf{p}}(\hat{\mathbf{p}})^{n-1}\left|\mathbf{p}\right\rangle \tag{12}$$

$$= p^{n-1}\hat{\mathbf{p}}\left|\mathbf{p}\right\rangle \tag{13}$$

$$= p^n\left|\mathbf{p}\right\rangle \tag{14}$$

QED. That is, $\left|\mathbf{p}\right\rangle$ is an eigenvector of $(\hat{\mathbf{p}})^n$ with eigenvalue p^n.

Now if the function $f(\hat{\mathbf{p}})$ can be expanded in powers of $\hat{\mathbf{p}}$ then

$$f(\hat{\mathbf{p}}) = f_0 + f_1\hat{\mathbf{p}} + f_2\hat{\mathbf{p}}^2 + \ldots \tag{15}$$

where the f_i are constants. Now$\left|\mathbf{p}\right\rangle$ is an eigenvector of the term $f_i\hat{\mathbf{p}}^i$ in the series with eigenvalue p^i. In other words, we're replacing a series in the operator $\hat{\mathbf{p}}$ with an identical series in its eigenvalue, so

$$f(\hat{\mathbf{p}})\left|\mathbf{p}\right\rangle = f(\mathbf{p})\left|\mathbf{p}\right\rangle \tag{16}$$

$$\left\langle \mathbf{q}\left|f(\hat{\mathbf{p}})\right|\mathbf{p}\right\rangle = f(\mathbf{p})\left\langle \mathbf{q}\left|\mathbf{p}\right.\right\rangle \tag{17}$$

$$= f(\mathbf{p})\,\delta_{\mathbf{qp}} \tag{18}$$

Therefore the second-quantized version of $f(\hat{\mathbf{p}})$ is

$$\hat{A} = \sum_{\mathbf{p}} f(\mathbf{p})\, a_{\mathbf{p}}^{\dagger} a_{\mathbf{p}} \tag{19}$$

$$= \sum_{\mathbf{p}} f(\mathbf{p})\,\hat{n}_{\mathbf{p}} \tag{20}$$

The interpretation is that the operator f acts separately on each particle with the total result being the sum of its values for all particles.

For example, the hamiltonian for a single free particle is $\hat{H}=\hat{\mathbf{p}}^2/2m$ so the hamiltonian for a collection of free particles is

$$\hat{H}=\sum_{\mathbf{p}}\frac{\mathbf{p}^2}{2m}\hat{n}_{\mathbf{p}} \tag{21}$$

The potential energy is usually given as a function of position, so using the momentum eigenfunction $|\mathbf{p}\rangle=\frac{1}{\sqrt{\mathcal{V}}}e^{-i\mathbf{p}\cdot\mathbf{x}}$ (where $\mathcal{V}$ is the volume of the box) we have from 1

$$\left\langle\mathbf{q}\left|\hat{V}\right|\mathbf{p}\right\rangle=\frac{1}{\mathcal{V}}\int d^3x\,e^{i\mathbf{q}\cdot\mathbf{x}}V(\mathbf{x})\,e^{-i\mathbf{p}\cdot\mathbf{x}} \tag{22}$$

$$=\frac{1}{\mathcal{V}}\int d^3x\,e^{-i(\mathbf{p}-\mathbf{q})\cdot\mathbf{x}}V(\mathbf{x}) \tag{23}$$

$$\equiv\tilde{V}_{\mathbf{p}-\mathbf{q}} \tag{24}$$

The potential can then be second quantized as

$$\hat{V}=\sum_{\mathbf{p},\mathbf{q}}\tilde{V}_{\mathbf{p}-\mathbf{q}}a^\dagger_{\mathbf{p}}a_{\mathbf{q}} \tag{25}$$

Example. Suppose we have a 3 state system with a hamiltonian

$$\hat{H}=E_0\sum_{i=1}^{3}a_i^\dagger a_i+W\left[a_1^\dagger a_2-a_1^\dagger a_3+a_2^\dagger a_1+a_2^\dagger a_3-a_3^\dagger a_1+a_3^\dagger a_2\right] \tag{26}$$

$$\equiv T+V \tag{27}$$

where W and E_0 are constants, T is the kinetic energy (the first term) and V is the potential energy (the second term). T is diagonal but V is not; we can see the effect of V on the basis states $|100\rangle$, $|010\rangle$ and $|001\rangle$ by observing that $a_1^\dagger a_2|010\rangle=|100\rangle$ (annihilate state 2 and create state 1), $a_1^\dagger a_2|100\rangle=0$ (no particle in state 2 so annihilation of state 2 produces 0) and so on.

$$V|100\rangle=W(|010\rangle-|001\rangle) \tag{28}$$

$$V|010\rangle=W(|100\rangle+|001\rangle) \tag{29}$$

$$V|001\rangle=W(-|100\rangle+|010\rangle) \tag{30}$$

We can write the hamiltonian as a matrix

$$\hat{H} = T + V \tag{31}$$

$$= E_0 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + W \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & 1 \\ -1 & 1 & 0 \end{bmatrix} \tag{32}$$

Each element in the hamiltonian matrix is given by the matrix element between two states. For example, $\left\langle 100 \middle| \hat{H} \middle| 010 \right\rangle$ is found by substituting for $\hat{H}$ from 26 and using the actions of the creation and annihilation operators.

$$\left\langle 100 \middle| \hat{H} \middle| 010 \right\rangle = \left\langle 100 \middle| E_0 \sum_{i=1}^{3} a_i^\dagger a_i \middle| 010 \right\rangle + \left\langle 100 \middle| W \left[a_1^\dagger a_2 - a_1^\dagger a_3 + a_2^\dagger a_1 + a_2^\dagger a_3 - a_3^\dagger a_1 + a_3^\dagger a_2 \right] \middle| 010 \right\rangle \tag{33}$$

The kinetic energy term gives zero, since it requires us to annihilate a particular particle and then create the same particle again. This gives a non-zero result only for particle 2, but this state is orthogonal to $|100\rangle$. Thus we'd get

$$\left\langle 100 \middle| E_0 \sum_{i=1}^{3} a_i^\dagger a_i \middle| 010 \right\rangle = E_0 \langle 100 | 010 \rangle = 0 \tag{34}$$

The potential energy term is worked out in a similar fashion.

In this form 28 would be written as

$$V|100\rangle = W \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & 1 \\ -1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = W \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix} \tag{35}$$

Finding the energies and eigenstates of this hamiltonian means we need to find the eigenvalues and eigenvectors of $\hat{H}$, which turn out to be

$$E = E_0 + W,\ E_0 + W,\ E_0 - 2W \tag{36}$$

The ground state $|\Omega\rangle$ (assuming $W > 0$) has energy $E_0 - 2W$ and its eigenvector is

$$|\Omega\rangle = \frac{1}{\sqrt{3}} \left(|100\rangle - |010\rangle + |001\rangle \right) \tag{37}$$

The other energy level $E_0 + W$ is doubly degenerate and its 2-d space of eigenvectors is spanned by

$$\frac{1}{\sqrt{2}}\left(-|100\rangle+|001\rangle\right),\ \frac{1}{\sqrt{2}}\left(|100\rangle+|010\rangle\right) \tag{38}$$