SECOND QUANTIZING OPERATORS - EXAMPLES

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Reference: Tom Lancaster and Stephen J. Blundell, *Quantum Field Theory for the Gifted Amateur*, (Oxford University Press, 2014), Section 4.2.

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:

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

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

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

so

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

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

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

so the multi-particle version is

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

Since $a^{\dagger}_{\alpha} a_{\alpha}$ 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 $a^{\dagger}_{\alpha} a_{\alpha}$ 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

$$\begin{aligned} \left\langle \mathbf{q} \middle| \hat{V} \middle| \mathbf{p} \right\rangle &= \frac{1}{\mathcal{V}} \int d^3x\, e^{i\mathbf{q}\cdot\mathbf{x}} V(\mathbf{x})\, e^{-i\mathbf{p}\cdot\mathbf{x}} && (22) \\ &= \frac{1}{\mathcal{V}} \int d^3x\, e^{-i(\mathbf{p}-\mathbf{q})\cdot\mathbf{x}} V(\mathbf{x}) && (23) \\ &\equiv \tilde{V}_{\mathbf{p}-\mathbf{q}} && (24) \end{aligned}$$

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

$$\begin{aligned} \hat{H} &= E_0 \sum_{i=1}^{3} a_i^\dagger a_i + W\left[a_1^\dagger a_2 - a_1^\dagger a_3 + a_2^\dagger a_1 + a_2^\dagger a_3 - a_3^\dagger a_1 + a_3^\dagger a_2\right] && (26) \\ &\equiv T + V && (27) \end{aligned}$$

where 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.

$$\begin{aligned} V|100\rangle &= W(|010\rangle - |001\rangle) && (28) \\ V|010\rangle &= W(|100\rangle + |001\rangle) && (29) \\ V|001\rangle &= W(-|100\rangle + |010\rangle) && (30) \end{aligned}$$

We can write the hamiltonian as a matrix

$$\begin{aligned} \hat{H} &= T+V & (31)\\ &= E_0\begin{bmatrix} 1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1 \end{bmatrix} + W\begin{bmatrix} 0 & 1 & -1\\ 1 & 0 & 1\\ -1 & 1 & 0 \end{bmatrix} & (32) \end{aligned}$$

In this form, for example, 28 would be written as

$$V|100\rangle = W\begin{bmatrix} 0 & 1 & -1\\ 1 & 0 & 1\\ -1 & 1 & 0 \end{bmatrix}\begin{bmatrix} 1\\ 0\\ 0 \end{bmatrix} = W\begin{bmatrix} 0\\ 1\\ -1 \end{bmatrix} \quad (33)$$

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

$$E = E_0+W,\ E_0+W,\ E_0-2W \quad (34)$$

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

$$|\Omega\rangle = \frac{1}{\sqrt{3}}\left(|100\rangle - |010\rangle + |001\rangle\right) \quad (35)$$

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

$$\frac{1}{\sqrt{2}}\left(-|100\rangle + |001\rangle\right),\ \frac{1}{\sqrt{2}}\left(|100\rangle + |010\rangle\right) \quad (36)$$