

## 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  $\hat{A}$  using creation and annihilation operators to get the multi-particle version:

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

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

$$\hat{1} = \sum_{\gamma} |\gamma\rangle \langle \gamma| \quad (2)$$

so

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

$$= \sum_{\gamma} \delta_{\alpha\gamma} \delta_{\gamma\beta} \quad (4)$$

$$= \delta_{\alpha\beta} \quad (5)$$

so the multi-particle version is

$$\hat{n} = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \quad (6)$$

Since  $a_{\alpha}^{\dagger} a_{\alpha}$  is the number operator, it counts the number of particles in state  $\alpha$  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

$$\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle \quad (7)$$

$$\langle \mathbf{q}|\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}\langle \mathbf{q}|\mathbf{p}\rangle \quad (8)$$

$$= \mathbf{p}\delta_{\mathbf{qp}} \quad (9)$$

The multi-particle version is therefore

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

$$= \sum_{\mathbf{p}} \mathbf{p}a_{\mathbf{p}}^{\dagger}a_{\mathbf{p}} \quad (11)$$

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  $(\hat{\mathbf{p}})^n|\mathbf{p}\rangle = p^n|\mathbf{p}\rangle$ . We know this is true for  $n = 1$  so assume it's true for  $n - 1$ . Then

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

$$= p^{n-1}\hat{\mathbf{p}}|\mathbf{p}\rangle \quad (13)$$

$$= p^n|\mathbf{p}\rangle \quad (14)$$

QED. That is,  $|\mathbf{p}\rangle$  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

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

where the  $f_i$  are constants. Now  $|\mathbf{p}\rangle$  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

$$f(\hat{\mathbf{p}})|\mathbf{p}\rangle = f(\mathbf{p})|\mathbf{p}\rangle \quad (16)$$

$$\langle \mathbf{q}|f(\hat{\mathbf{p}})|\mathbf{p}\rangle = f(\mathbf{p})\langle \mathbf{q}|\mathbf{p}\rangle \quad (17)$$

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

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

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

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

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

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

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

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

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

$$\equiv \tilde{V}_{\mathbf{p}-\mathbf{q}} \quad (24)$$

The potential can then be second quantized as

$$\hat{V} = \sum_{\mathbf{p}, \mathbf{q}} \tilde{V}_{\mathbf{p}-\mathbf{q}} a_{\mathbf{p}}^{\dagger} a_{\mathbf{q}} \quad (25)$$

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

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

$$\equiv T + V \quad (27)$$

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.

$$V |100\rangle = W (|010\rangle - |001\rangle) \quad (28)$$

$$V |010\rangle = W (|100\rangle + |001\rangle) \quad (29)$$

$$V |001\rangle = W (-|100\rangle + |010\rangle) \quad (30)$$

We can write the hamiltonian as a matrix

$$\hat{H} = T + V \quad (31)$$

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

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

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

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

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