SECOND QUANTIZING OPERATORS - EXAMPLES

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:

\[
\hat{A} = \sum_{\alpha,\beta} A_{\alpha\beta} a^\dagger_{\alpha} a_{\beta}
\]  

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

\[
\hat{1} = \sum_{\gamma} |\gamma\rangle \langle \gamma|
\]  

so

\[
\langle \alpha | \hat{1} | \beta \rangle = \langle \alpha | \sum_{\gamma} |\gamma\rangle \langle \gamma| \beta \rangle
\]

\[
= \sum_{\gamma} \delta_{\alpha\gamma} \delta_{\gamma\beta}
\]

\[
= \delta_{\alpha\beta}
\]

so the multi-particle version is

\[
\hat{n} = \sum_{\alpha} a^\dagger_{\alpha} a_{\alpha}
\]

Since \( a^\dagger_{\alpha} a_{\alpha} \) 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 \( \hat{n} \) 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

\[ \hat{p} |p\rangle = p |p\rangle \]  
\[ \langle q | \hat{p} | p \rangle = p \langle q | p \rangle \]  
\[ = p \delta_{qp} \]  

The multi-particle version is therefore

\[ \hat{p} = \sum_{q,p} p \delta_{qp} a_q^\dagger a_p \]  
\[ = \sum_{p} p a_p^\dagger a_p \]  

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

\[ (\hat{p})^n |p\rangle = \hat{p} (\hat{p})^{n-1} |p\rangle \]  
\[ = p^{n-1} \hat{p} |p\rangle \]  
\[ = p^n |p\rangle \]  

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

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

\[ f(\hat{p}) = f_0 + f_1 \hat{p} + f_2 (\hat{p})^2 + \ldots \]  

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

\[ f(\hat{p}) |p\rangle = f(\hat{p}) |p\rangle \]  
\[ \langle q | f(\hat{p}) | p \rangle = f(\hat{p}) \langle q | p \rangle \]  
\[ = f(\hat{p}) \delta_{qp} \]  

Therefore the second-quantized version of \( f(\hat{p}) \) is
\[ \hat{A} = \sum_p f(p) a_p^\dagger a_p \]  
\[ = \sum_p f(p) \hat{n}_p \]  
\[ (19) \]

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 \( \hat{H} = \hat{p}^2 / 2m \) so the hamiltonian for a collection of free particles is

\[ \hat{H} = \sum_p \frac{\hat{p}_p^2}{2m} \hat{n}_p \]  
\[ (20) \]

The potential energy is usually given as a function of position, so using the momentum eigenfunction \( |p\rangle = \frac{1}{\sqrt{V}} e^{-i\hat{p} \cdot \hat{x}} \) (where \( V \) is the volume of the box) we have from (19)

\[ \langle q | \hat{V} | p \rangle = \frac{1}{V} \int d^3x e^{i\hat{q} \cdot \hat{x}} V(x) e^{-i\hat{p} \cdot \hat{x}} \]  
\[ = \frac{1}{V} \int d^3x e^{-i(\hat{p} - \hat{q}) \cdot \hat{x}} V(x) \]  
\[ = \hat{V}_{p-q} \]  
\[ (22) \]

The potential can then be second quantized as

\[ \hat{V} = \sum_{p,q} \hat{V}_{p-q} a_p^\dagger a_q \]  
\[ (23) \]

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

\[ \hat{H} = E_0 \sum_{i=1}^3 a_i^\dagger a_i + W \left[ a_1^\dagger a_2 - a_1^\dagger a_3 + a_2^\dagger a_1 + a_2^\dagger a_3 - a_3^\dagger a_1 + a_3^\dagger a_2 \right] \]  
\[ = T + V \]  
\[ (24) \]

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), \( a_1^\dagger a_2 |001\rangle = 0 \) (no particle in state 2 so annihilation of state 2 produces 0) and so on.
\[ V |100 \rangle = W (|010 \rangle - |001 \rangle) \] (28)
\[ V |010 \rangle = W (|100 \rangle + |001 \rangle) \] (29)
\[ V |001 \rangle = W (-|100 \rangle + |010 \rangle) \] (30)

We can write the Hamiltonian as a matrix

\[ \hat{H} = T + V \] (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)

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

\[ V |100 \rangle = W \begin{bmatrix} 0 & 1 & -1 \\ 1 & 0 & 1 \\ -1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = W \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix} \] (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

\[ E = E_0 + W, \ E_0 + W, \ E_0 - 2W \] (34)

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

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

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

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