# SECOND QUANTIZING A SINGLE-PARTICLE OPERATOR

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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.

*Second quantization* is the expression of quantum mechanical states using particles rather than waves. We use creation and annihilation operatorsacting on particle states to make transitions between states. If we have a single-particle operator $\hat{\mathcal{A}}$ we can expand it using two unit operators as follows:

$$\hat{\mathcal{A}} = \sum_{\alpha}|\alpha\rangle\langle\alpha|\hat{\mathcal{A}}\sum_{\beta}|\beta\rangle\langle\beta| \tag{1}$$

$$= \sum_{\alpha,\beta}|\alpha\rangle\mathcal{A}_{\alpha\beta}\langle\beta| \tag{2}$$

where

$$\mathcal{A}_{\alpha\beta}\equiv\left\langle\alpha\left|\hat{\mathcal{A}}\right|\beta\right\rangle \tag{3}$$

Each of the sets $|\alpha\rangle$ and $|\beta\rangle$ are complete, orthonormal sets of states for a single particle. For multi-particle systems, we use the creation and annihilation operators $a_{\mathbf{p}}^{\dagger}$ and $a_{\mathbf{p}}$ to add or subtract particles from a state, so we'd like to know how to define a multi-particle version $\hat{A}$ of the single-particle operator $\hat{\mathcal{A}}$.

The route to this end is a bit complex, so bear with me. Suppose we have a system of $N$ particles. To satisfy the symmetry rules for bosons and fermions, we can write a state of these $N$ particles as

$$|\psi_1,\ldots,\psi_N\rangle=\frac{1}{\sqrt{N!}}\sum_P\xi^P\prod_{i=1}^N\left|\psi_{P(i)}\right\rangle \tag{4}$$

This notation requires a bit of explanation. First, we're assuming that each of the $N$ particles is in a different state and that these states are orthonormal. Only in this case is the normalization factor $\frac{1}{\sqrt{N!}}$. (For example, if we put 2 bosons into the same state $|\psi_1\rangle$, the wave function is $\frac{1}{2}|\psi_1\rangle|\psi_1\rangle$, not $\frac{1}{\sqrt{2}}|\psi_1\rangle|\psi_1\rangle$.) The $P$ refers to a permutation of the integers $1,\ldots,N$, and $P(i)$ is the $i$th integer in the permutation $P$. The product term $\prod_{i=1}^N\left|\psi_{P(i)}\right\rangle$

is a product of $N$ single-particle states in a certain order, where the order of the state in the product determines its spatial coordinate. For example, if $N = 3$ then one permutation is $P = 3,1,2$ so for that permutation

$$\prod_{i=1}^{3} \left|\psi_{P(i)}\right\rangle = \left|\psi_3\left(\mathbf{x}_1\right)\right\rangle \left|\psi_1\left(\mathbf{x}_2\right)\right\rangle \left|\psi_2\left(\mathbf{x}_3\right)\right\rangle \tag{5}$$

The factor $\xi$ is $+1$ for bosons and $-1$ for fermions, and the sum over $P$ sums over all $N!$ possible permutations of the integers $1,\ldots,N$, so the state $|\psi_1,\ldots,\psi_N\rangle$ consists of $N!$ terms, each of which contains a product of $N$ different single particle states. [The fact that the states are all different isn't mentioned in L&B's book, but it seems to me that this is a necessary condition.]

For the purposes of using $P$ as an exponent in $\xi^P$, $P$ can be regarded as the number of swaps of integers in the original sequence $1,\ldots,N$ are required to get the permutation $P$. Thus, to get 3,1,2 from 1,2,3 we swap 1 with 2, then 2 with 3, so there are 2 swaps. Permutations requiring an even (odd) number of swaps are called even (odd) permutations.

Now suppose we have a different $N$-particle state given by

$$|\chi_1,\ldots,\chi_N\rangle = \frac{1}{\sqrt{N!}} \sum_Q \xi^Q \prod_{j=1}^{N} \left|\chi_{Q(j)}\right\rangle \tag{6}$$

The single-particle states $|\chi_i\rangle$ also form a complete orthonormal set, but they could be a different such set from the $|\psi_i\rangle$. If we take the inner product of these two $N$-particle states we get the rather horrible expression

$$\langle\chi_1,\ldots,\chi_N\left|\psi_1,\ldots,\psi_N\right.\rangle = \frac{1}{N!} \sum_{P,Q} \xi^{P+Q} \prod_{i=1}^{N} \left\langle\chi_{Q(i)}\left|\psi_{P(i)}\right.\right\rangle \tag{7}$$

We need only one product since we are summing over both permutations $P$ and $Q$, so we get all possible inner products between terms from 4 and 6. For example, if $N = 2$, then for fermions

$$|\psi_1\psi_2\rangle = \frac{1}{\sqrt{2}} \left(\left|\psi_1\left(\mathbf{x}_1\right)\right\rangle \left|\psi_2\left(\mathbf{x}_2\right)\right\rangle - \left|\psi_1\left(\mathbf{x}_2\right)\right\rangle \left|\psi_2\left(\mathbf{x}_1\right)\right\rangle\right) \tag{8}$$

$$|\chi_1\chi_2\rangle = \frac{1}{\sqrt{2}} \left(\left|\chi_1\left(\mathbf{x}_1\right)\right\rangle \left|\chi_2\left(\mathbf{x}_2\right)\right\rangle - \left|\chi_1\left(\mathbf{x}_2\right)\right\rangle \left|\chi_2\left(\mathbf{x}_1\right)\right\rangle\right) \tag{9}$$

On the RHS, we can form inner products only between single-particle states that use the same spatial coordinate and, since $\left\langle\chi_i\left(\mathbf{x}_1\right)\left|\psi_j\left(\mathbf{x}_1\right)\right.\right\rangle = \left\langle\chi_i\left(\mathbf{x}_2\right)\left|\psi_j\left(\mathbf{x}_2\right)\right.\right\rangle$ (since we're integrating over all space on both sides, the integration coordinate doesn't matter) we get

$$\langle\chi_1\chi_2|\psi_1\psi_2\rangle = \frac{1}{2}\left[2\langle\chi_1|\psi_1\rangle\langle\chi_2|\psi_2\rangle - 2\langle\chi_1|\psi_2\rangle\langle\chi_2|\psi_1\rangle\right] \tag{10}$$

$$= \langle\chi_1|\psi_1\rangle\langle\chi_2|\psi_2\rangle - \langle\chi_1|\psi_2\rangle\langle\chi_2|\psi_1\rangle \tag{11}$$

For any given permutation of the $\psi_i$ or $\chi_i$, the position coordinates can be distributed among the $N$ single-particle states in $N!$ ways. If we choose a permutation $Q$ for $|\chi_1,\ldots,\chi_N\rangle$ and $P$ for $|\psi_1,\ldots,\psi_N\rangle$, then the product $\prod_{i=1}^{N}\left\langle\chi_{Q(i)}\middle|\psi_{P(i)}\right\rangle$ occurs $N!$ times because of the $N!$ ways of assigning positions. For example, for $N=2$, we can choose $Q=1,2$ and $P=1,2$ so that

$$\prod_{i=1}^{2}\left\langle\chi_{Q(i)}\middle|\psi_{P(i)}\right\rangle = \langle\chi_1|\psi_1\rangle\langle\chi_2|\psi_2\rangle \tag{12}$$

This combination can occur with $\chi_1$ and $\psi_1$ functions of $\mathbf{x}_1$ and $\chi_2$ and $\psi_2$ functions of $\mathbf{x}_2$ or $\chi_1$ and $\psi_1$ functions of $\mathbf{x}_2$ and $\chi_2$ and $\psi_2$ functions of $\mathbf{x}_1$. In general, for any pairing of $\chi_i$ states with $\psi_i$ states, there are $N!$ ways of distributing the position coordinates, each of which gives the same product of single-particle inner products. We can rewrite this by always ordering the $\chi_i$ states in their original order $1,\ldots,N$ and pairing this ordering with each permutation $P$ of $\psi_i$ states. That is

$$\langle\chi_1,\ldots,\chi_N|\psi_1,\ldots,\psi_N\rangle = \frac{1}{N!}\sum_P \xi^P N!\prod_{i=1}^{N}\left\langle\chi_i\middle|\psi_{P(i)}\right\rangle \tag{13}$$

$$= \sum_P \xi^P \prod_{i=1}^{N}\left\langle\chi_i\middle|\psi_{P(i)}\right\rangle \tag{14}$$

For fermions (with $\xi=-1$) this is actually the definition of the determinant of a matrix (we'll accept this mathematical result):

$$\langle\chi_1,\ldots,\chi_N|\psi_1,\ldots,\psi_N\rangle_{\text{fermions}} = \begin{vmatrix} \langle\chi_1|\psi_1\rangle & \langle\chi_1|\psi_2\rangle & \cdots & \langle\chi_1|\psi_N\rangle \\ \langle\chi_2|\psi_1\rangle & \langle\chi_2|\psi_2\rangle & \cdots & \langle\chi_2|\psi_N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\chi_N|\psi_1\rangle & \langle\chi_N|\psi_2\rangle & \cdots & \langle\chi_N|\psi_N\rangle \end{vmatrix} \tag{15}$$

For bosons, the equivalent structure is called the *permanent* of a matrix. A permanent is the same as a determinant except all the minus signs are replaced by plus signs. It doesn't seem to have its own notation so we'll just write it as 'perm'.

$$\left\langle \chi_1,\ldots,\chi_N \middle| \psi_1,\ldots,\psi_N \right\rangle_{\text{bosons}} = \text{perm}\begin{bmatrix} \langle \chi_1|\psi_1\rangle & \langle \chi_1|\psi_2\rangle & \ldots & \langle \chi_1|\psi_N\rangle \\ \langle \chi_2|\psi_1\rangle & \langle \chi_2|\psi_2\rangle & \ldots & \langle \chi_2|\psi_N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \chi_N|\psi_1\rangle & \langle \chi_N|\psi_2\rangle & \ldots & \langle \chi_N|\psi_N\rangle \end{bmatrix} \tag{16}$$

Now we can apply a creation operator $a_\phi^\dagger$ to the state $|\psi_1,\ldots,\psi_N\rangle$ (as far as I can tell, the state $\phi$ can be any state, including one that is a linear combination of the $\psi_i$). This gives

$$a_\phi^\dagger |\psi_1,\ldots,\psi_N\rangle = |\phi,\psi_1,\ldots,\psi_N\rangle \tag{17}$$

If we want to discover the action of an annihilation operator, things are a bit more complicated, since we can choose to annihilate a linear combination of the basis states rather than just a single basis state. Again, as far as I can tell, this annihilation operation works only on the original $N$-particle state $|\psi_1,\ldots,\psi_N\rangle$. We want to find $a_\phi|\psi_1,\ldots,\psi_N\rangle$ so we take the inner product with some other state $|\chi_1,\ldots,\chi_{N-1}\rangle$ (we use an $N-1$ particle state so that the number of particles match up on both sides):

$$\left\langle \chi_1,\ldots,\chi_{N-1} \middle| a_\phi \middle| \psi_1,\ldots,\psi_N \right\rangle = \left\langle \psi_1,\ldots,\psi_{N-1} \middle| a_\phi^\dagger \middle| \chi_1,\ldots,\chi_N \right\rangle^* \tag{18}$$

$$= \left\langle \psi_1,\ldots,\psi_N \middle| \phi,\chi_1,\ldots,\chi_{N-1} \right\rangle^* \tag{19}$$

$$= \begin{vmatrix} \langle \psi_1|\phi\rangle & \langle \psi_1|\chi_1\rangle & \ldots & \langle \psi_1|\chi_{N-1}\rangle \\ \langle \psi_2|\phi\rangle & \langle \psi_2|\chi_1\rangle & \ldots & \langle \psi_2|\chi_{N-1}\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \psi_N|\phi\rangle & \langle \psi_N|\chi_1\rangle & \ldots & \langle \psi_N|\chi_{N-1}\rangle \end{vmatrix}_\xi^* \tag{20}$$

where the subscript $\xi$ on the determinant means to use the permanent if we're talking about bosons so that $\xi = 1$. From here on, I mean 'determinant or permanent' whenever I say 'determinant'. We can expand the determinant about the first column to get

$$\left\langle \chi_1,\ldots,\chi_{N-1} \middle| a_\phi \middle| \psi_1,\ldots,\psi_N \right\rangle = \sum_{k=1}^{N} \xi^{k-1} \langle \psi_k|\phi\rangle^* \left\langle \psi_1,\ldots(\text{no }\psi_k),\ldots,\psi_N \middle| \chi_1,\ldots,\chi_{N-1} \right\rangle^* \tag{21}$$

$$= \sum_{k=1}^{N} \xi^{k-1} \langle \phi|\psi_k\rangle \left\langle \chi_1,\ldots,\chi_{N-1} \middle| \psi_1,\ldots(\text{no }\psi_k),\ldots,\psi_N \right\rangle \tag{22}$$

where the state $|\psi_1, \ldots (\text{no } \psi_k), \ldots, \psi_N\rangle$ is the state $|\psi_1, \ldots, \psi_{N-1}\rangle$ without $\psi_k$. The clever thing about this form is that we made no assumptions about the state $|\chi_1, \ldots, \chi_{N-1}\rangle$ so we can remove it from both sides to get

$$a_\phi |\psi_1, \ldots, \psi_N\rangle = \sum_{k=1}^{N} \xi^{k-1} \langle\phi|\psi_k\rangle |\psi_1, \ldots (\text{no } \psi_k), \ldots, \psi_N\rangle \tag{23}$$

**Example 1.** Suppose we have a 3-boson system and

$$|\phi\rangle = \frac{\sqrt{2}}{3}|\psi_1\rangle + \frac{\sqrt{6}}{3}|\psi_2\rangle + \frac{1}{3}|\psi_3\rangle \tag{24}$$

Then

$$\langle\phi|\psi_1\rangle = \frac{\sqrt{2}}{3} \tag{25}$$

$$\langle\phi|\psi_2\rangle = \frac{\sqrt{6}}{3} \tag{26}$$

$$\langle\phi|\psi_3\rangle = \frac{1}{3} \tag{27}$$

so

$$a_\phi |\psi_1\psi_2\psi_3\rangle = \frac{\sqrt{2}}{3}|\psi_2\psi_3\rangle + \frac{\sqrt{6}}{3}|\psi_1\psi_3\rangle + \frac{1}{3}|\psi_1\psi_2\rangle \tag{28}$$

Now suppose we apply a creation operator:

$$a_\alpha^\dagger a_\phi |\psi_1, \ldots, \psi_N\rangle = \sum_{k=1}^{N} \xi^{k-1} \langle\phi|\psi_k\rangle a_\alpha^\dagger |\psi_1, \ldots (\text{no } \psi_k), \ldots, \psi_N\rangle \tag{29}$$

$$= \sum_{k=1}^{N} \xi^{k-1} \langle\phi|\psi_k\rangle |\alpha, \psi_1, \ldots (\text{no } \psi_k), \ldots, \psi_N\rangle \tag{30}$$

For the fermion case, we can swap $\alpha$ with all the states $\psi_1, \ldots, \psi_{k-1}$ and since swapping rows in a determinant changes the sign, this results in a factor of $\xi^{k-1}$ which eliminates the other $\xi^{k-1}$ (since $\xi^{2(k-1)} = 1$ always), so we get the final form

$$a_\alpha^\dagger a_\phi |\psi_1, \ldots, \psi_N\rangle = \sum_{k=1}^{N} \langle\phi|\psi_k\rangle |\psi_1, \ldots, \psi_{k-1}, \alpha, \psi_{k+1}, \ldots, \psi_N\rangle \tag{31}$$

For bosons, swapping columns in a permanent makes no difference to the result and since $\xi = 1$ in this case we can just ignore the $\xi^{k-1}$ factor.

After all this, we can get back to our original operator $\hat{\mathcal{A}}$. Since it's a single-particle operator, we can assume that its multi-particle equivalent's effect on a multi-particle state is the sum of the single-particle operator's effects on each individual particle within the state. That is, from 2 the inner product of the state $\langle\beta|$ is taken with each $|\psi_k\rangle$ in turn and the result summed over $k$. Calling the multi-particle operator $\hat{A}$ we have

$$\hat{A}|\psi_1,\ldots,\psi_N\rangle = \sum_k \sum_{\alpha,\beta} |\alpha\rangle \mathcal{A}_{\alpha\beta} \langle\beta|\psi_k\rangle |\psi_1,\ldots(\text{no } \psi_k),\ldots,\psi_N\rangle \tag{32}$$

$$= \sum_{\alpha,\beta} \mathcal{A}_{\alpha\beta} \langle\beta|\psi_k\rangle |\psi_1,\ldots,\psi_{k-1},\alpha,\psi_{k+1},\ldots,\psi_N\rangle \tag{33}$$

$$= \sum_{\alpha,\beta} \mathcal{A}_{\alpha\beta} a_\alpha^\dagger a_\beta |\psi_1,\ldots,\psi_N\rangle \tag{34}$$

In the second line we inserted the state $|\alpha\rangle$ into $|\psi_1,\ldots(\text{no } \psi_k),\ldots,\psi_N\rangle$ at the position occupied by $\psi_k$ since $\hat{\mathcal{A}}$ is a single-particle operator so it operates on the same coordinate throughout (that is $\langle\beta|$ operates on the same coordinate as $|\alpha\rangle$). Therefore the multi-particle operator is

$$\hat{A} = \sum_{\alpha,\beta} \mathcal{A}_{\alpha\beta} a_\alpha^\dagger a_\beta \tag{35}$$

We can think of this as the operator looking for a particle (or component of a particle) in each state $\beta$, removing that particle and operating on it with the single-particle operator $\hat{\mathcal{A}}$ and then reinserting the particle in state $|\alpha\rangle$.

## PINGBACKS

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