SECOND QUANTIZING A SINGLE-PARTICLE OPERATOR

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog and include the title or URL of this post in your comment.

Post date: 25 Jul 2023.

Second quantization is the expression of quantum mechanical states using particles rather than waves. We use creation and annihilation operators acting 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 ith 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 ξ 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 Lancaster & Blundell's book, but it seems to me that this is a necessary condition.]

For the purposes of using P as an exponent in ξ^P, P can be regarded as the number of swaps of integers in the original sequence $1,\ldots,N$ that 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. For bosons, ξ^P is always 1, while for fermions, ξ^P is +1 if P is even and -1 if P is odd.

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

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

Here Q also represents a permutation. I've used a different symbol so that we can treat P and Q as two different permutations.

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

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

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 $\left\langle\chi_i\left(\mathbf{x}_1\right)\middle|\psi_j\left(\mathbf{x}_1\right)\right\rangle =$

$\langle\chi_i(\mathbf{x}_2)|\psi_j(\mathbf{x}_2)\rangle$ (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 ψ_i or χ_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 $\prod_{i=1}^{N}\langle\chi_{Q(i)}|\psi_{P(i)}\rangle$ 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

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

This combination can occur with χ_1 and ψ_1 functions of $\mathbf{x}_1$ and χ_2 and ψ_2 functions of $\mathbf{x}_2$ or χ_1 and ψ_1 functions of $\mathbf{x}_2$ and χ_2 and ψ_2 functions of $\mathbf{x}_1$. In general, for any pairing of χ_i states with ψ_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 χ_i states in their original order $1,\ldots,N$ and pairing this ordering with each permutation P of ψ_i states. That is

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

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

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'.

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

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 ϕ can be any state, including one that is a linear combination of the ψ_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):

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

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

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

where the subscript ξ 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

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

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

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 ψ_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. 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 α 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 ξ^{k-1} which eliminates the other ξ^{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 ξ^{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

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

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

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

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 ψ_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 $|\alpha\rangle$). The last line follows from 31. 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 β, 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

Pingback: Second quantizing operators - examples
Pingback: Second quantizing the tight-binding hamiltonian