CAS PY 452 — Quantum Physics II

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Discussion Notes
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Equivalence of first and second quantization for two particles and two orbitals

First quantization: Consider the system where there are two orbitals a, b and two particles. The single particle basis states are $\psi_a(x), \psi_b(x)$, and the single-particle operator $\hat{o}(x)$ operates as,

$$\hat{o}(x)\psi_a(x) = o_{aa}\psi_a(x) + o_{ba}\psi_b(x), \qquad \hat{o}(x)\psi_b(x) = o_{ab}\psi_a(x) + o_{bb}\psi_b(x). \tag{1}$$

The values $o_{aa}, o_{ba}, o_{ab}, o_{bb}$ are the matrix elements of the single-particle operator $\hat{o}$. The multi-particle basis states are,

$$\psi_\alpha(x_1, x_2) = \psi_a(x_1)\psi_a(x_2), \quad \psi_\beta(x_1, x_2) = \frac{1}{\sqrt{2}}\left(\psi_a(x_1)\psi_b(x_2) + \psi_a(x_2)\psi_b(x_1)\right), \quad \psi_\gamma(x_1, x_2) = \psi_b(x_1)\psi_b(x_2). \tag{2}$$

In the first quantization, we can calculate the matrix elements of the operator $\hat{O} = \hat{o}(x_1) + \hat{o}(x_2)$ in terms of the basis states $\psi_\alpha, \psi_\beta, \psi_\gamma$. The notation $\hat{o}(x_1)$ means that this operator only acts on coordinate x_1 and leaves wave-functions in terms of x_2 alone. We want to find the matrix elements only corresponding to one basis state, so that's what we'll do here with the basis state $\psi_\alpha(x_1, x_2)$. To find the matrix elements, we act on $\psi_\alpha(x_1, x_2)$ with the operator $\hat{O}$ and then express the resulting wave-function in terms of the basis states $\psi_\alpha, \psi_\beta, \psi_\gamma$:

$$\begin{aligned}
\hat{O}[\psi_\alpha(x_1, x_2)] &= \hat{o}(x_1)[\psi_\alpha(x_1, x_2)] + \hat{o}(x_2)[\psi_\alpha(x_1, x_2)] = \hat{o}(x_1)[\psi_a(x_1)\psi_a(x_2)] + \hat{o}(x_2)[\psi_a(x_1)\psi_a(x_2)] \\
&= \psi_a(x_2)\hat{o}(x_1)[\psi_a(x_1)] + \psi_a(x_1)\hat{o}(x_2)[\psi_a(x_2)] \\
&= \psi_a(x_2)(o_{aa}\psi_a(x_1) + o_{ba}\psi_b(x_1)) + \psi_a(x_1)(o_{aa}\psi_a(x_2) + o_{ba}\psi_b(x_2)) \\
&= 2o_{aa}\psi_a(x_1)\psi_a(x_2) + o_{ba}(\psi_a(x_2)\psi_b(x_1) + \psi_a(x_1)\psi_b(x_2)) \\
&= 2o_{aa}\psi_\alpha(x_1, x_2) + \sqrt{2}o_{ba}\psi_\beta(x_1, x_2) + 0\psi_\gamma(x_1, x_2).
\end{aligned} \tag{3}$$

In the last line, we factored our expression in terms of the basis states $\psi_\alpha, \psi_\beta, \psi_\gamma$ The matrix elements in this multi-particle basis are then $2o_{aa}$, $\sqrt{2}o_{ba}$, 0. We could write this as a column in a matrix like so:

$$\begin{pmatrix} 2o_{aa} & \cdot & \cdot \\ \sqrt{2}o_{ba} & \cdot & \cdot \\ 0 & \cdot & \cdot \end{pmatrix}. \tag{4}$$

Here, the dots are the matrix elements that we do not know yet; we would find these matrix elements by computing $\hat{O}\psi_\beta$ and $\hat{O}\psi_\gamma$ and then factoring the results in terms of $\psi_\alpha, \psi_\beta, \psi_\gamma$. Note that we are working with bosons here.

Second quantization: Now, we work in the second-quantized notation, so our basis states are $|2,0\rangle$, $|1,1\rangle$, and $|0,2\rangle$. The operator $\hat{O}$ is expressed as,

$$\hat{O} = \hat{a}_a^\dagger o_{aa}\hat{a}_a + \hat{a}_b^\dagger o_{ba}\hat{a}_a + \hat{a}_a^\dagger o_{ab}\hat{a}_b + \hat{a}_b^\dagger o_{bb}\hat{a}_b, \tag{5}$$

in the second quantization. To compute matrix elements, we use the rules $\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle$, $\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$, and $\hat{a}\,|0\rangle = 0$. Similarly to before, we act on $|2,0\rangle$ with $\hat{O}$ and then factor in terms of basis states,

$$\begin{aligned}
\hat{O}\,|2,0\rangle &= \hat{a}_a^\dagger o_{aa}\hat{a}_a\,|2,0\rangle + \hat{a}_b^\dagger o_{ba}\hat{a}_a\,|2,0\rangle + \hat{a}_a^\dagger o_{ab}\hat{a}_b\,|2,0\rangle + \hat{a}_b^\dagger o_{bb}\hat{a}_b\,|2,0\rangle = \sqrt{2}o_{aa}\hat{a}_a^\dagger\,|1,0\rangle + \sqrt{2}o_{ba}\hat{a}_b^\dagger\,|1,0\rangle + 0 + 0 \\
&= \sqrt{2}\times\sqrt{2}o_{aa}\,|2,0\rangle + \sqrt{2}o_{ba}\,|1,1\rangle + 0\,|0,2\rangle\,.
\end{aligned} \tag{6}$$

Here we see that we are able to re-produce the same matrix elements from the first quantization where the basis states $|2,0\rangle\,, |1,1\rangle\,, |0,2\rangle$ correspond to $\psi_\alpha, \psi_\beta, \psi_\gamma$.