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 $\hat{o}$, and we take them as a given. 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, our goal is to 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. In the prompt for problem 1, 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 $\psi_\alpha, \psi_\beta, \psi_\gamma$. In the problem prompt, you are only asked to find one column of this matrix: the column corresponding to acting with $\hat{O}$ on the multi-particle basis state with two particles in orbital a, one particle in orbital b, and no particles in orbital c. One of the steps in this problem is finding expressions for the multi-particle basis states (similar to what happened in line 2). Note that we are working with bosons here and in problem 1 of the homework.

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 $\psi_\alpha, \psi_\beta, \psi_\gamma$. In problem 1 of the homework, you will follow this same procedure to show the equivalence of the first and second quantized methods but with three orbitals and three particles.