Matrices Details

The above figure is from the main notes

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  - how do I know the \((p_x, p_y)\) form a set and the \(p_z\) does not? Consider the \(p_z\), does it ever transform onto the \(p_x\) or \(p_y\)? No, so it forms its own subset. Consider the \(p_z\), on an in-plane \(C_3\) rotation it doesn’t transform completely onto itself, we have to combine it with the \(p_z\) to generate the “rotated” orbital, these two must form a set.
  - how are the matrix components for the \((p_x, p_y)\) matrices determined? Here is an example for a \(120^\circ\) rotation of the \(p_x\) and \(p_y\) vectors:

\[
C_3 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}
\]

\[
y = (0,1)
\]

\[
x = (1,0)
\]

\[
\text{unit vector length}=1
\]

\[
\theta = 30^\circ
\]

\[
\theta = 120^\circ
\]

\[
a = 1 \ast \cos 30^\circ = \frac{\sqrt{3}}{2}
\]

\[
b = 1 \ast \sin 30^\circ = -\frac{1}{2}
\]

\[
c = 1 \ast \sin 30^\circ = -\frac{1}{2}
\]

\[
d = 1 \ast \cos 30^\circ = \frac{\sqrt{3}}{2}
\]

\[
D_3
\]

\[
E
\]

\[
C_i^1(z)
\]

\[
C_i^{-1}(z)
\]

\[
C_i^1(a)
\]

\[
C_i^1(b)
\]

\[
C_i^1(c)
\]

<table>
<thead>
<tr>
<th>(D_3)</th>
<th>(E)</th>
<th>(C_i^1(z))</th>
<th>(C_i^{-1}(z))</th>
<th>(C_i^1(a))</th>
<th>(C_i^1(b))</th>
<th>(C_i^1(c))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(B(s))</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(B(p_x,p_y))</td>
<td>(\begin{pmatrix} 1 &amp; 0 \ 0 &amp; 1 \end{pmatrix})</td>
<td>(\begin{pmatrix} -1/2 &amp; \sqrt{3}/2 \ -\sqrt{3}/2 &amp; -1/2 \end{pmatrix})</td>
<td>(\begin{pmatrix} -1/2 &amp; -\sqrt{3}/2 \ \sqrt{3}/2 &amp; 1/2 \end{pmatrix})</td>
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</tr>
<tr>
<td>(B(p_z))</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

\[\textbf{Figure 1}\] different matrix representations of the same symmetry operations

\[\textbf{Figure 2}\] determining \(C_3\) rotation matrix representations

\[\textbf{Figure 3}\] different matrix representations of the same symmetry operations
the easiest way to generate the matrix for the hydrogen atoms is to label each row and column of the “matrix”, the starting position is given first i.e. the row labels, and the final position is given second, i.e. the column labels, Figure 4.

\[
\begin{pmatrix}
A_{11} & A_{12} & A_{13} \\
A_{21} & A_{22} & A_{23} \\
A_{31} & A_{32} & A_{33}
\end{pmatrix}
\]

H\text{a} starts at position 1 and goes to position 2

\[
\begin{pmatrix}
2 \\
1 \\
3
\end{pmatrix}
\rightarrow
\begin{pmatrix}
1 \\
2 \\
3
\end{pmatrix}
\]

Figure 4 different matrix representations of the same symmetry operations