Perturbation Theory Hamiltonians

Background

In our representation of our Hamiltonian, we have

$$\mathrm{H}^{(1)}=\sum_{ijk}\frac{1}{2}\frac{\partial g_{ij}}{\partial Q_k}\,p_i\,Q_k\,p_j+\frac{1}{6}\frac{\partial^3 V}{\partial Q_i\,Q_j\,Q_k}\,Q_i\,Q_j\,Q_k$$

then if we ask for element of this

$$\begin{aligned}\langle n|\,\mathrm{H}^{(1)}\,|m\rangle&=\langle n|\,\sum_{ijk}\frac{1}{2}\frac{\partial g_{ij}}{\partial Q_k}\,p_i\,Q_k\,p_j+\frac{1}{6}\frac{\partial^3 V}{\partial Q_i\,Q_j\,Q_k}\,Q_i\,Q_j\,Q_k\,|m\rangle\\&=\sum_{ijk}\frac{1}{2}\frac{\partial g_{ij}}{\partial Q_k}\langle n|\,p_i\,Q_k\,p_j\,|m\rangle+\frac{1}{6}\frac{\partial^3 V}{\partial Q_i\,Q_j\,Q_k}\langle n|\,Q_i\,Q_j\,Q_k\,|m\rangle\end{aligned}$$

we realize that we need to get representations of the operators $p\,Q\,p$ and $Q\,Q\,Q$

The form that these operator representations should take may not be entirely obvious.

A 2D Example

The first thing we should do is consider a 2-dimensional example, e.g. the operator xy. As it turns out, the representation for this in some general basis, $\{\phi\}$, unlike the case of something like x^2+y^2 is unpleasant since it cannot be cleanly separated into some combination of 1D representations.

However, if we set up a direct product basis, i.e. one such that

$$\phi_n=\phi_{n_x}\,\phi_{n_y}$$

this becomes much nicer

In this case we have

$$\begin{aligned}\langle n|\,xy\,|m\rangle&=\langle n_y|\,\langle n_x|\,xy\,|m_x\rangle\,|m_y\rangle\\&=\langle n_x|\,x|m_x\rangle\,\langle n_y|y\,|m_y\rangle\end{aligned}$$

and so if we can set up representations for both x and y, we can take the direct product of those representations and get a total representation

What we *do* need to keep in mind with this is that it will take us from a 2D matrix to a 4D tensor, as we have two quantum numbers $(n_x\,n_y)$ for every n

Representation

What might this look like, then, for a product of harmonic oscillator wavefunction basis?

Let's assume we have N_x wavefunctions in x and N_y in y. This means the representations will be

$$X=\begin{pmatrix} 0 & \sqrt{1} & & & \\ \sqrt{1} & 0 & \sqrt{2} & & \\ & \sqrt{2} & \ddots & \ddots & \\ & & \ddots & & \sqrt{N_x} \\ & & & \sqrt{N_x} & 0 \end{pmatrix}$$

$$Y=\begin{pmatrix} 0 & \sqrt{1} & & & \\ \sqrt{1} & 0 & \sqrt{2} & & \\ & \sqrt{2} & \ddots & \ddots & \\ & & \ddots & & \sqrt{N_y} \\ & & & \sqrt{N_y} & 0 \end{pmatrix}$$

But then what happens when we have our total basis of size $N_x N_y$? Well we can assume that our basis functions are ordered like

$$\begin{aligned} \phi_1 &= \phi_{x=1}\,\phi_{y=1} \\ \phi_2 &= \phi_{x=2}\,\phi_{y=1} \\ &\vdots \\ \phi_{N_x} &= \phi_{x=N_x}\,\phi_{y=1} \\ \phi_{N_x+1} &= \phi_{x=1}\,\phi_{y=2} \\ &\vdots \\ \phi_{N_x N_y} &= \phi_{x=N_x}\,\phi_{y=N_y} \end{aligned}$$

and so when we look at our total array, it will look like

$$X\,Y=\begin{pmatrix} X_{11}\;Y_{11} & X_{12}\;Y_{11} & \ldots & X_{1N_x}\,Y_{11} & X_{11}\;Y_{12} & \ldots & X_{1N_x}\;Y_{1N_y} \\ X_{21}\;Y_{11} & X_{22}\;Y_{11} & & & & & \vdots \\ \vdots & & \ddots & \vdots & & & \\ X_{N_x1}\;Y_{11} & & \ldots & X_{N_xN_x}\;Y_{11} & & & \\ X_{11}\;Y_{21} & & & \ddots & & & \\ \vdots & & & & & & \\ & & & & & & \\ X_{N_x1}\;Y_{N_y1} & & \ldots & & & & X_{N_xN_x}\;Y_{N_yN_y} \end{pmatrix}$$

which we could rewrite as

$$X\,Y=\begin{pmatrix} X\,Y_{11} & X\,Y_{12} & \ldots & X\,Y_{1N_y} \\ X\,Y_{21} & X\,Y_{22} & & \\ \vdots & & \ddots & \vdots \\ \mathrm{XY}_{N_y1} & & \ldots & X\,Y_{N_yN_y} \end{pmatrix}$$

which is the Kronecker product of the matrices X and Y, or in more standard notation

$$X\,Y = X \otimes Y$$

The ND case follows the same pattern, being

$$X = X_1 \otimes X_2 \otimes \ldots \otimes X_N$$

Representation of $\mathrm{H}^{(1)}$

With all this in place, we can now think about how we will handle just the second part of $\mathrm{H}^{(1)}$

$$\sum_{ijk} \frac{\partial^3 V}{\partial Q_i \, Q_j \, Q_k} Q_i \, Q_j \, Q_k$$

as we've shown previously, we can get a full tensor representation of the derivatives, i.e.

$$(V_{Q^3})_{ijk} = \frac{\partial^3 V}{\partial Q_i \, Q_j \, Q_k}$$

This term has dimension $(M,\ M,\ M)$ where M is the total number of coordinates in our system.

The question, then, is what to do with Q^3?

Here we need to decide how many quanta of excitation we will allow to be in each of our modes. We will let this be N_i. This means our basis elements look like

$$\phi_n = \prod_{i=1}^{M} \varphi_{n_i}$$

and we have a total basis size of

$$N = \prod_{i=1}^{M} N_i$$

and so we expect that $\mathrm{H}^{(1)}$ should be have dimension $(N,\ N)$

Thus we expect to have representation of QQQ that has dimension $(M,\ M,\ M,\ N,\ N)$, which can of course get memory intensive *very* quickly unless we can control the size of N or by computing individual elements of $\mathrm{H}^{(1)}$, like

$$\begin{aligned}\left(\mathrm{H}^{(1)}\right)_{n,m} &= \left(\mathrm{H}^{(1)}\right)_{n_{x_1}\, n_{x_2}\, \ldots\, n_{x_M}, m_{x_1}\, m_{x_2}\, \ldots\, m_{x_M}} \\ &= V_{Q^3} \odot \left(Q^3{}_{\ldots\,\mathrm{nm}}\right)\end{aligned}$$

where the $\odot$ is telling us to contract the axes of V_{Q^3} with the first three axes of Q^3

But, saving that for another day, we're still left with the question of how to represent Q^3, given that for $M > 3$ the indices $i,\ j,\ k$ don't cover the full set of combinations of axes.

In this case, we can think of this as

$$Q^3 = Q^3 \ I^{(M-3)}$$

and so we end up having

$$Q^3 = I_{N_1} \otimes I_{N_2} \otimes \ldots \otimes Q_i \otimes I_{N_{i+1}} \otimes \ldots \otimes Q_j \otimes I_{N_{j+1}} \otimes \ldots \ Q_k \otimes I_{N_{k+1}} \otimes \ldots \mathrm{I}_{N_M}$$

which is a truly massive tensor

On the other hand, it is also an extremely *sparse* tensor, and so by using sparse matrix methods we can end up storing very little of it, if we decide that we *do* want to do a direct calculation of the tensor.

Explicit Form

There is also a mild complication that we haven't dealt with here, either, which is that sometimes we won't have three distinct indices. That is sometimes we'll have $Q_x\, Q_y\, Q_z$ but other times we might have $Q_x\, Q_y\, Q_x$. These terms will have different representations:

$$
\begin{gathered}
Q_x\, Q_y\, Q_z \Rightarrow\; Q_x \otimes Q_y \otimes Q_z \\
Q_x\, Q_y\, Q_x \Rightarrow {Q_x}^2 \otimes Q_y
\end{gathered}
$$

where that ${Q_x}^2$ term is, as usual, a matrix power of the representation of Q_x, not a direct term wise multiplication.

This can also make indexing something of a challenge to think about. Let's consider three modes (we'll call them x, y, and z) and in each of these we put up to 1 quantum of excitation.

Then if we're asking for QQQ_{nm} we are really asking for this tensor

$$
\begin{aligned}
\mathrm{QQQ}_{nm} &= \begin{pmatrix}
\begin{pmatrix} (Q_x\, Q_x\, Q_x)_{nm} & (Q_x\, Q_x\, Q_y)_{nm} & (Q_x\, Q_x\, Q_z)_{nm} \\ (Q_x\, Q_y\, Q_x)_{nm} & (Q_x\, Q_y\, Q_y)_{nm} & (Q_x\, Q_y\, Q_z)_{nm} \\ (Q_x\, Q_z\, Q_x)_{nm} & (Q_x\, Q_z\, Q_y)_{nm} & (Q_x\, Q_z\, Q_z)_{nm} \end{pmatrix} \\
\begin{pmatrix} (Q_y\, Q_x\, Q_x)_{nm} & (Q_y\, Q_x\, Q_y)_{nm} & (Q_y\, Q_x\, Q_z)_{nm} \\ (Q_y\, Q_y\, Q_x)_{nm} & (Q_y\, Q_y\, Q_y)_{nm} & (Q_y\, Q_y\, Q_z)_{nm} \\ (Q_y\, Q_z\, Q_x)_{nm} & (Q_y\, Q_z\, Q_y)_{nm} & (Q_y\, Q_z\, Q_z)_{nm} \end{pmatrix} \\
\begin{pmatrix} (Q_z\, Q_x\, Q_x)_{nm} & (Q_z\, Q_x\, Q_y)_{nm} & (Q_z\, Q_x\, Q_z)_{nm} \\ (Q_z\, Q_y\, Q_x)_{nm} & (Q_z\, Q_y\, Q_y)_{nm} & (Q_z\, Q_y\, Q_z)_{nm} \\ (Q_z\, Q_z\, Q_x)_{nm} & (Q_z\, Q_z\, Q_y)_{nm} & (Q_z\, Q_z\, Q_z)_{nm} \end{pmatrix}
\end{pmatrix} \\
&= \begin{pmatrix}
\begin{pmatrix} \left({Q_x}^3\right)_{nm} & \left({Q_x}^2\, Q_y\right)_{nm} & \left({Q_x}^2\, Q_z\right)_{nm} \\ \left({Q_x}^2\, Q_y\right)_{nm} & \left(Q_x\, {Q_y}^2\right)_{nm} & (Q_x\, Q_y\, Q_z)_{nm} \\ \left({Q_x}^2\, Q_z\right)_{nm} & (Q_x\, Q_z\, Q_y)_{nm} & \left(Q_x\, {Q_z}^2\right)_{nm} \end{pmatrix} \\
\begin{pmatrix} \left({Q_x}^2\, Q_y\right)_{nm} & \left(Q_x\, {Q_y}^2\right)_{nm} & (Q_y\, Q_x\, Q_z)_{nm} \\ \left(Q_x\, {Q_y}^2\right)_{nm} & \left({Q_y}^3\right)_{nm} & \left({Q_y}^2\, Q_z\right)_{nm} \\ (Q_y\, Q_z\, Q_x)_{nm} & \left({Q_y}^2\, Q_z\right)_{nm} & \left(Q_y\, {Q_z}^2\right)_{nm} \end{pmatrix} \\
\begin{pmatrix} \left({Q_x}^2\, Q_z\right)_{nm} & (Q_z\, Q_x\, Q_y)_{nm} & \left(Q_x\, {Q_z}^2\right)_{nm} \\ (Q_z\, Q_y\, Q_x)_{nm} & \left({Q_y}^2\, Q_z\right)_{nm} & \left(Q_y\, {Q_z}^2\right)_{nm} \\ \left(Q_x\, {Q_z}^2\right)_{nm} & \left(Q_y\, {Q_z}^2\right)_{nm} & \left({Q_z}^3\right)_{nm} \end{pmatrix}
\end{pmatrix}
\end{aligned}
$$

Then the question is: what is nm?

To answer this we need to think about how our total Hamiltonian is structured. A given element of this looks like

$$\langle n|\,\mathrm{H}\,|m\rangle = \langle n|\,\mathrm{T}\,|m\rangle + \langle n|\,\mathrm{V}\,|m\rangle$$

and keeping in mind that our basis is the direct product of the basis sets

$$\Phi_x = \{|0\rangle_x,\ |1\rangle_x\}$$
$$\Phi_y = \{|0\rangle_y,\ |1\rangle_y\}$$
$$\Phi_z = \{|0\rangle_z,\ |1\rangle_z\}$$

so our overall basis is

$$\Phi = \{|0\rangle_x|0\rangle_y|0\rangle_z,\ |1\rangle_x|0\rangle_y|0\rangle_z,\ |0\rangle_x|1\rangle_y|0\rangle_z,\ |0\rangle_x|0\rangle_y|1\rangle_z,$$
$$|1\rangle_x|1\rangle_y|0\rangle_z,\ |1\rangle_x|0\rangle_y|1\rangle_z,\ |0\rangle_x|1\rangle_y|1\rangle_z,\ |1\rangle_x|1\rangle_y|1\rangle_z,\}$$

and then n refers to one of these basis functions and m to another, i.e. (removing the redundant subscripts)

$$\Phi_n = |n_x\rangle\,|n_y\rangle\,|n_z\rangle$$

So overall

$$\mathrm{QQQ}_{nm} = \langle n_x|\,\langle n_y|\,\langle n_z| \begin{pmatrix} \begin{pmatrix} (Q_x^3) & (Q_x^2\,Q_y) & (Q_x^2\,Q_z) \\ (Q_x^2\,Q_y) & (Q_x\,Q_y^2) & (Q_x\,Q_y\,Q_z) \\ (Q_x^2\,Q_z) & (Q_x\,Q_z\,Q_y) & (Q_x\,Q_z^2) \end{pmatrix} \\ \begin{pmatrix} (Q_x^2\,Q_y) & (Q_x\,Q_y^2) & (Q_y\,Q_x\,Q_z) \\ (Q_x\,Q_y^2) & (Q_y^3) & (Q_y^2\,Q_z) \\ (Q_y\,Q_z\,Q_x) & (Q_y^2\,Q_z) & (Q_y\,Q_z^2) \end{pmatrix} \\ \begin{pmatrix} (Q_x^2\,Q_z) & (Q_z\,Q_x\,Q_y) & (Q_x\,Q_z^2) \\ (Q_z\,Q_y\,Q_x) & (Q_y^2\,Q_z) & (Q_y\,Q_z^2) \\ (Q_x\,Q_z^2) & (Q_y\,Q_z^2) & (Q_z^3) \end{pmatrix} \end{pmatrix} |m_x\rangle\,|m_y\rangle\,|m_z\rangle$$

this is a real pain to show in full, so we'll just focus on the three types of terms in the middle block

$$\langle n_x|\,\langle n_y|\,\langle n_z|\;Q_y^3\;|m_x\rangle\,|m_y\rangle\,|m_z\rangle = \langle n_y|\;Q_y^3\;|m_y\rangle\,\langle n_x|m_x\rangle\,\langle n_z|m_z\rangle$$
$$\langle n_x|\,\langle n_y|\,\langle n_z|\;Q_x^2\,Q_y\;|m_x\rangle\,|m_y\rangle\,|m_z\rangle = \langle n_x|\;Q_x^2\;|m_x\rangle\,\langle n_y|\;Q_y\;|m_y\rangle\,\langle n_z|m_z\rangle$$
$$\langle n_x|\,\langle n_y|\,\langle n_z|\;Q_x\,Q_y^2\;|m_x\rangle\,|m_y\rangle\,|m_z\rangle = \langle n_x|\;Q_x\;|m_x\rangle\,\langle n_y|\;Q_y^2\;|m_y\rangle\,\langle n_z|m_z\rangle$$
$$\langle n_x|\,\langle n_y|\,\langle n_z|\;Q_y^2\,Q_z\;|m_x\rangle\,|m_y\rangle\,|m_z\rangle = \langle n_y|\;Q_y^2\;|m_y\rangle\,\langle n_z|\;Q_z\;|m_z\rangle\,\langle n_x|m_x\rangle$$
$$\langle n_x|\,\langle n_y|\,\langle n_z|\;Q_y\,Q_z^2\;|m_x\rangle\,|m_y\rangle\,|m_z\rangle = \langle n_y|\;Q_y\;|m_y\rangle\,\langle n_z|\;Q_z^2\;|m_z\rangle\,\langle n_x|m_x\rangle$$
$$\langle n_x|\,\langle n_y|\,\langle n_z|\;Q_y\,Q_x\,Q_z\;|m_x\rangle\,|m_y\rangle\,|m_z\rangle = \langle n_x|\;Q_x\;|m_x\rangle\,\langle n_y|\;Q_y\;|m_y\rangle\,\langle n_z|\;Q_z\;|m_z\rangle$$

and assuming that x, y, and z all have the same representation for Q this means the whole tensor is

$$\mathrm{QQQ}_{nm}=\begin{pmatrix}\begin{pmatrix} Q^3{}_{n_x\,m_x}\,\delta_{n_y\,m_y}\,\delta_{n_z\,m_z} & Q^2{}_{n_x\,m_x}\,Q_{n_y\,m_y}\,\delta_{n_z\,m_z} & Q^2{}_{n_x\,m_x}\,Q_{n_z\,m_z}\,\delta_{n_y\,m_y} \\ Q^2{}_{n_x\,m_x}\,Q_{n_y\,m_y}\,\delta_{n_z\,m_z} & Q_{n_x\,m_x}\,Q^2{}_{n_y\,m_y}\,\delta_{n_z\,m_z} & Q_{n_x\,m_x}\,Q_{n_y\,m_y}\,Q_{n_z\,m_z} \\ Q^2{}_{n_x\,m_x}\,Q_{n_z\,m_z}\,\delta_{n_y\,m_y} & Q_{n_x\,m_x}\,Q_{n_y\,m_y}\,Q_{n_z\,m_z} & Q_{n_x\,m_x}\,Q^2{}_{n_z\,m_z}\,\delta_{n_y\,m_y}\end{pmatrix} \\ \begin{pmatrix} Q^2{}_{n_x\,m_x}\,Q_{n_y\,m_y}\,\delta_{n_z\,m_z} & Q_{n_x\,m_x}\,Q^2{}_{n_y\,m_y}\,\delta_{n_z\,m_z} & Q_{n_x\,m_x}\,Q_{n_y\,m_y}\,Q_{n_z\,m_z} \\ Q_{n_x\,m_x}\,Q^2{}_{n_y\,m_y}\,\delta_{n_z\,m_z} & Q^3{}_{n_y\,m_y}\,\delta_{n_x\,m_x}\,\delta_{n_z\,m_z} & Q^2{}_{n_y\,m_y}\,Q_{n_z\,m_z}\,\delta_{n_x\,m_x} \\ Q_{n_x\,m_x}\,Q_{n_y\,m_y}\,Q_{n_z\,m_z} & Q^2{}_{n_y\,m_y}\,Q_{n_z\,m_z}\,\delta_{n_x\,m_x} & Q_{n_y\,m_y}\,Q^2{}_{n_z\,m_z}\,\delta_{n_x\,m_x}\end{pmatrix} \\ \begin{pmatrix} Q^2{}_{n_x\,m_x}\,Q_{n_z\,m_z}\,\delta_{n_y\,m_y} & Q_{n_x\,m_x}\,Q_{n_y\,m_y}\,Q_{n_z\,m_z} & Q_{n_x\,m_x}\,Q^2{}_{n_z\,m_z}\,\delta_{n_y\,m_y} \\ Q_{n_x\,m_x}\,Q_{n_y\,m_y}\,Q_{n_z\,m_z} & Q^2{}_{n_y\,m_y}\,Q_{n_z\,m_z}\,\delta_{n_x\,m_x} & Q_{n_y\,m_y}\,Q^2{}_{n_z\,m_z}\,\delta_{n_x\,m_x} \\ Q_{n_x\,m_x}\,Q^2{}_{n_z\,m_z}\,\delta_{n_y\,m_y} & Q_{n_y\,m_y}\,Q^2{}_{n_z\,m_z}\,\delta_{n_x\,m_x} & Q^3{}_{n_z\,m_z}\,\delta_{n_x\,m_x}\,\delta_{n_y\,m_y}\end{pmatrix}\end{pmatrix}$$

which looks imposing, but really ends up being quite simple. If, for instance, we have

$$\begin{matrix} n_x=1 & m_x=0 \\ n_y=0 & m_y=1 \\ n_z=1 & m_z=1 \end{matrix}$$

based on ordering our basis as

$$\Phi=\{|0\rangle_x\,|0\rangle_y\,|0\rangle_z,\ |1\rangle_x\,|0\rangle_y\,|0\rangle_z,\ |0\rangle_x\,|1\rangle_y\,|0\rangle_z,\ |0\rangle_x\,|0\rangle_y\,|1\rangle_z,$$
$$|1\rangle_x\,|1\rangle_y\,|0\rangle_z,\ |1\rangle_x\,|0\rangle_y\,|1\rangle_z,\ |0\rangle_x\,|1\rangle_y\,|1\rangle_z,\ |1\rangle_x\,|1\rangle_y\,|1\rangle_z,\}$$

we get

$$\mathrm{QQQ}_{65}=\begin{pmatrix}\begin{pmatrix} Q^3{}_{10}\,\delta_{01}\,\delta_{11} & Q^2{}_{10}\,Q_{01}\,\delta_{11} & Q^2{}_{10}\,Q_{11}\,\delta_{01} \\ Q^2{}_{10}\,Q_{01}\,\delta_{11} & Q_{10}\,Q^2{}_{01}\,\delta_{11} & Q_{10}\,Q_{01}\,Q_{11} \\ Q^2{}_{10}\,Q_{11}\,\delta_{01} & Q_{10}\,Q_{01}\,Q_{11} & Q_{10}\,Q^2{}_{11}\,\delta_{01}\end{pmatrix} \\ \begin{pmatrix} Q^2{}_{10}\,Q_{01}\,\delta_{11} & Q_{10}\,Q^2{}_{01}\,\delta_{11} & Q_{10}\,Q_{01}\,Q_{11} \\ Q_{10}\,Q^2{}_{01}\,\delta_{11} & Q^3{}_{01}\,\delta_{10}\,\delta_{11} & Q^2{}_{01}\,Q_{11}\,\delta_{10} \\ Q_{10}\,Q_{01}\,Q_{11} & Q^2{}_{01}\,Q_{11}\,\delta_{10} & Q_{01}\,Q^2{}_{11}\,\delta_{10}\end{pmatrix} \\ \begin{pmatrix} Q^2{}_{10}\,Q_{11}\,\delta_{01} & Q_{10}\,Q_{01}\,Q_{11} & Q_{10}\,Q^2{}_{11}\,\delta_{01} \\ Q_{10}\,Q_{01}\,Q_{11} & Q^2{}_{01}\,Q_{11}\,\delta_{10} & Q_{01}\,Q^2{}_{11}\,\delta_{10} \\ Q_{10}\,Q^2{}_{11}\,\delta_{01} & Q_{01}\,Q^2{}_{11}\,\delta_{10} & Q^3{}_{11}\,\delta_{10}\,\delta_{01}\end{pmatrix}\end{pmatrix}$$

assuming we're working with harmonic oscillator wavefunctions, this gives us

$$Q=\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad Q^2=\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{3}{2} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{5}{2} \end{pmatrix} \quad Q^3=\begin{pmatrix} 0 & \frac{3}{2\sqrt{2}} & 0 \\ \frac{3}{2\sqrt{2}} & 0 & 3 \\ 0 & 3 & 0 \end{pmatrix}$$

and so

$$Q_{10}=\frac{1}{\sqrt{2}} \qquad Q_{11}=0 \qquad Q_{01}=\frac{3}{\sqrt{2}}$$

$$Q^2{}_{10}=0 \qquad Q^2{}_{11}=\frac{3}{2} \qquad Q^2{}_{01}=0$$

$$Q^3{}_{10}=\frac{3}{\sqrt{2}} \qquad Q^3{}_{11}=0 \qquad Q^3{}_{01}=\frac{3}{\sqrt{2}}$$

and so

$$\mathrm{QQQ}_{65}=\begin{pmatrix} \begin{pmatrix} \frac{3}{2\sqrt{2}}\,\delta_{01}\,\delta_{11} & 0*\frac{1}{\sqrt{2}}\,\delta_{11} & 0*0\,\delta_{01} \\ 0*\frac{1}{\sqrt{2}}\,\delta_{11} & \frac{1}{\sqrt{2}}*0\,\delta_{11} & \frac{1}{\sqrt{2}}*\frac{1}{\sqrt{2}}*0 \\ 0*0\,\delta_{01} & \frac{1}{\sqrt{2}}*\frac{1}{\sqrt{2}}*0 & \frac{1}{\sqrt{2}}*\frac{3}{2}\,\delta_{01} \end{pmatrix} \\ \begin{pmatrix} 0*\frac{1}{\sqrt{2}}\,\delta_{11} & \frac{1}{\sqrt{2}}*0\,\delta_{11} & \frac{1}{\sqrt{2}}*\frac{1}{\sqrt{2}}*0 \\ \frac{1}{\sqrt{2}}*0\,\delta_{11} & \frac{3}{2\sqrt{2}}\,\delta_{10}\,\delta_{11} & 0*0\,\delta_{10} \\ \frac{1}{\sqrt{2}}*\frac{1}{\sqrt{2}}*0 & 0*0\,\delta_{10} & \frac{1}{\sqrt{2}}\,\frac{3}{2}\,\delta_{10} \end{pmatrix} \\ \begin{pmatrix} 0*0\,\delta_{01} & \frac{1}{\sqrt{2}}*\frac{1}{\sqrt{2}}*0 & \frac{1}{\sqrt{2}}*\frac{3}{2}\,\delta_{01} \\ \frac{1}{\sqrt{2}}*\frac{1}{\sqrt{2}}*0 & 0*0\,\delta_{10} & \frac{1}{\sqrt{2}}*\frac{3}{2}\,\delta_{10} \\ \frac{1}{\sqrt{2}}*\frac{3}{2}\,\delta_{01} & \frac{1}{\sqrt{2}}*\frac{3}{2}\,\delta_{10} & 0\,\delta_{10}\,\delta_{01} \end{pmatrix} \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{pmatrix}$$

And so looked like a very large tensor turns out to be identically 0. This is a pretty common phenomenon with these and if we are trying to be very computationally efficient we can use selection rules to guide which terms we actually need to consider.