AMERICAN UNIVERSITY

WASHINGTON, DC

Coefficients of Transformations in Multidimensional Quantum Harmonic Oscillators

Travis J. Volz

Advisor: Nathan Harshman

November 2013

Technical Report No. 2013-6

https://doi.org/10.17606/qa40-h580

Coefficients of Transformations in Multidimensional Quantum Harmonic Oscillators

Travis J. Volz

November 6, 2013

I. Introduction

When one represents a physical system of harmonic oscillators, it is possible to represent the system in many ways. For a system with three degrees of freedom, one could represent a single particle in three dimensions which would be equivalent to three particles in one dimension. The main idea here is that in each case, the total degrees of freedom must be equal for different representations of a given system. There are many other ways that someone can represent a physical system in three dimensions. The system can be represented in Cartesian coordinates, cylindrical coordinates, or spherical coordinates, just to name a few. Then within each of these representations, one could imagine rotating the coordinate systems or scaling them differently. As a result, one specific state of the multidimensional quantum harmonic oscillator can be represented in many different ways. The purpose of this research project is to calculate different coefficients for translating from one representation to another.

II. Computational Approach to Transformation Matrices

Schrödinger's Equation, Hermite Polynomials, and Stationary States

Before we describe the specific methods/thought processes used in this project, we must develop a background language of terms and definitions that will be used when describing the systems and the coefficients. First, it is useful to note that the primary tool to find these coefficients is that of Quantum Mechanics, since the systems modeled are Quantum harmonic oscillators. The technical computing program Mathematica is used to define the functions and computationally intensive integrals that are necessary to find the coefficients, and the High Performance Computing Cluster, Zorro, at American University is often used to do the actual calculations.

To start we must define the Schrödinger equation in one dimension for the stationary states, which is

$$\left(\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{1}{2}k\,x^2\right)\psi(x)=E\,\psi(x) \tag{1}$$

Here, the term in parentheses is the Hamiltonian with the first term being the kinetic energy and the second being the potential energy. On the right hand side, E is the total energy of the system. Stationary state solutions to the harmonic oscillator potential are of the following form,

$$\psi_n(x)=\frac{(\sigma^2\pi)^{-1/4}}{\sqrt{2^n n!}}\mathrm{H}_n\left(\frac{x}{\sigma}\right)e^{-\frac{x^2}{2\sigma^2}} \tag{2}$$

where n is the n^{th} energy level of the harmonic oscillator, $\sigma=\sqrt{\frac{\hbar}{m\omega}}$, and $\mathrm{H}_n(x)$ is the Hermite polynomial of degree n in the variable x, so in our case, the variable is instead $\frac{x}{\sigma}$. One feature that is essential in quantum mechanics is the fact that one cannot know exactly a particle's position and its momentum. The best we can do is to use the wave function squared to find the probability of a particle being found in a specific region. The expectation value is the average if many trials were taken measuring a specific feature of the system. What is meant by stationary state, is that even if these states were left to evolve in time, the expectation values (the value that one would predict) for each observable would be constant throughout all time. The first several Hermite polynomials are shown in Figure 1.

$H_0(x) = 1$	Red
$H_1(x) = 2x$	Orange
$H_2(x) = 4x^2 - 2$	Yellow
$H_3(x) = 8x^3 - 12x$	Green
$H_4(x) = 16x^4 - 48x^2 + 12$	Blue
$H_5(x) = 32x^5 - 160x^3 + 120x$	Violet

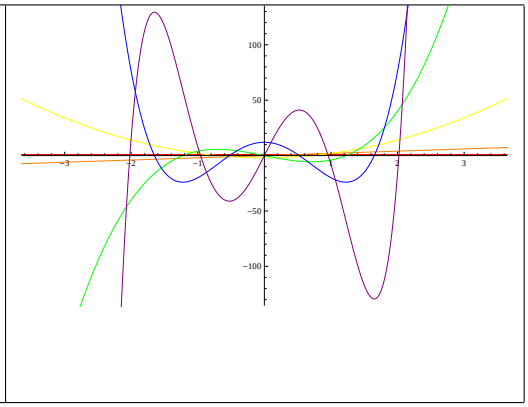


Figure 1:a) The formulas for the first 6 Hermite polynomials. b) The graphs of the first 6 Hermite polynomials

Next, we will take a look at the first 6 stationary states of the harmonic oscillator as in equation (2). In this case, n gives the number of nodes, so the first one is labeled $n = 0$ and so on, similar to the Hermite polynomials. Notice that $\psi_n(x)$ is a Hermite polynomial multiplied by a Gaussian. Therefore even though the Hermite polynomials would go to infinity as $x \to \pm\infty$, since they are multiplied by a Gaussian that goes to 0 more quickly, so the net result is the wave function going to 0 at the edges. This is essential, because as noted above, the squared wave function gives the probability density and we know that the probability must be 1 of finding the particle somewhere. Therefore

$$\int_{-\infty}^{\infty} |\psi_n|^2 dx = 1$$

In the graph below, I have shifted the stationary states up so they are at their correct energy levels (looking more like the energies of a classical particle in a harmonic oscillator). Namely, on the graph $E_n = \hbar\omega(n + \frac{1}{2})$, where we have let $\hbar = 1$ and $\omega = 1$ to scale the graphs.

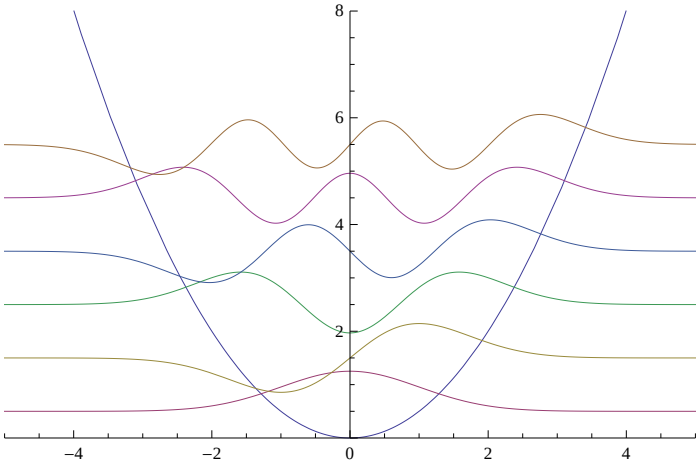


Figure 2: The first 6 energy levels of the quantum harmonic oscillator, shifted to their respective locations on the graph.

Components of a general state.

A general wave function or state, can be comprised of a combination of the stationary states discussed above. Since each of the stationary states satisfy the Schrödinger equation, and since it is a linear homogeneous system of equations, we know that any linear combination of stationary states will also satisfy the Schrödinger equation. Therefore, in general, we can construct any state $\Psi(x)$ as the sum of stationary states, notated as follows

$$\Psi(x) = \sum_{n=0}^{\infty} c_n \psi_n(x) \tag{3}$$

where c_n is a complex number representing the amount of each stationary state $\psi_n(x)$ in $\Psi(x)$. Likewise, if we instead know $\Psi(x)$, we can decompose it into the components. First let us multiply both sides of equation (3) by $\psi^*_{n'}(x)$ and then take the integral with respect to x. Equation (3) then becomes

$$\int_{-\infty}^{\infty} \psi_{n'}^*(x)\Psi(x)\ \mathrm{d}x = \int_{-\infty}^{\infty} \sum_{n=0}^{\infty} c_n \psi_{n'}^*(x)\psi_n(x)\ \mathrm{d}x \tag{4}$$

Note, that since n' is not in the sum, the sum can be taken outside. Also since each of the stationary states are mutually orthogonal, when their product is integrated from negative infinity to infinity, it becomes the Kronecker Delta, $\delta_{n'n}$. The equation therefore becomes

$$\int_{-\infty}^{\infty} \psi_{n'}^*(x)\Psi(x)\ \mathrm{d}x = c_{n'} \tag{5}$$

This means that we can find the component of each stationary state in $\Psi(x)$ simply by doing the above integral.

Stationary States in Two Dimensions, x and y.

Let us now imagine multiplying a stationary state in one direction by one in another. This seems reasonable since each state is completely independent and normalized so the multiplication should preserve normalization. Therefore let us define:

$$\psi_{n_x n_y}(x, y) = \psi_{n_x}(x)\psi_{n_y}(y) \tag{6}$$

Similarly to the one dimensional case, we can express any state, $\Psi(x, y)$, which may or may not be a superposition of many stationary states, as

$$\Psi(x, y) = \sum_{n_x, n_y} c_{n_x n_y}\psi_{n_x n_y}(x, y) \tag{7}$$

where $c_{n_x n_y}$ is the weight of the $\psi_{n_x n_y}(x, y)$ stationary state in the state $\Psi(x, y)$. Once again, analogously, we can find the coefficients from equation (7) like in we did for the one dimensional case in equation (5) as

$$c_{n_x n_y} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi_{n_x n_y}^*(x, y)\Psi(x, y)\ \mathrm{d}x\ \mathrm{d}y \tag{8}$$

Rotating a Wave Function.

Let us now suppose that we wished to rotate a wave function about the origin by θ. We would need to transform each point (x, y) to a new point, say (x', y'). It can be shown that from the properties of trigonometry, if we wish to rotate a point (x, y) about the origin by θ, we can multiply the point by the following matrix to obtain the new coordinate in the old coordinate system:

$$\begin{pmatrix} \cos(\theta) & \text{-}\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x' \\ y' \end{pmatrix} \tag{9}$$

For example, if the point (1,0) is rotated by $\pi/4$, we would obtain the new point

$$\begin{pmatrix} \cos(\pi/2) & \text{-}\sin(\pi/2) \\ \sin(\pi/2) & \cos(\pi/2) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} \end{pmatrix}$$

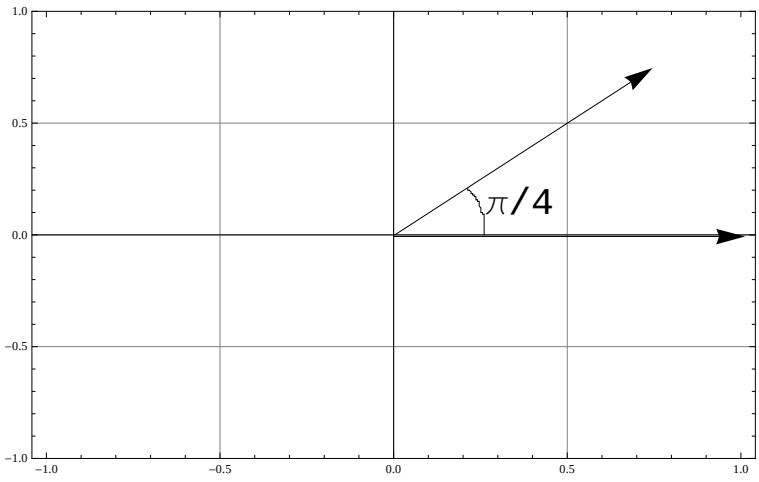
Let us call this matrix in equation (9) of coordinate rotation, T. There is another simple transformation that one could imagine doing in 2 dimensions. For this new transformation, lets call it $\bar{T}$, we could imagine rotating the axes of the coordinate system by θ. We would then look at what the coordinates of the old (unmoved) point in the new coordinate system would be. To find this new point, $(\tilde{x}, \tilde{y})$, we multiply $\bar{T}$ by (x, y), which is defined as follows:

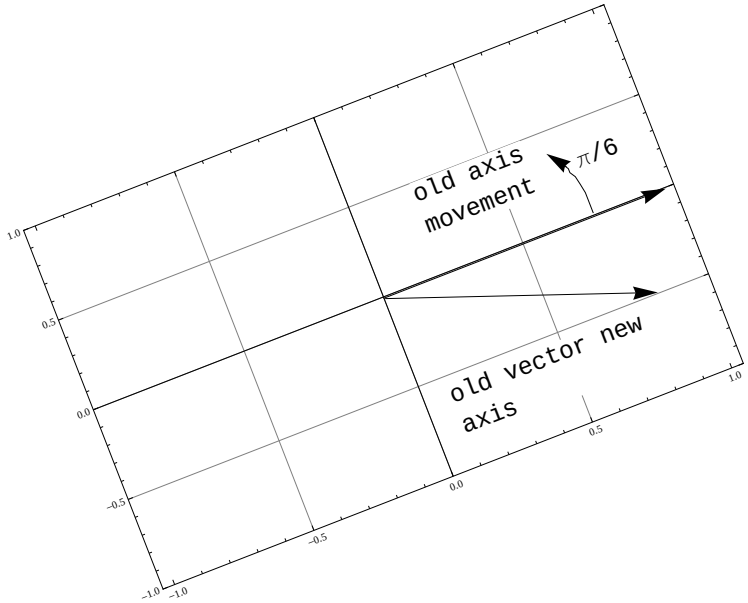
$$\begin{pmatrix} \cos(\theta) & \sin(\theta) \\ \text{-}\sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix} \tag{10}$$

Again, for example, lets suppose that we rotate the coordinate system by $\pi/6$. We can find the new coordinates of $(1, 0)$ as follows:

$$\begin{pmatrix} \cos(\pi/6) & \sin(\pi/6) \\ \text{-}\sin(\pi/6) & \cos(\pi/6) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix}$$

The examples are illustrated below:





The reason we discussed the rotation matrices above is so that we can apply the rotations to the wave functions. Let us therefore define

$$\phi_{\nu_x\nu_y}(x,y) = \psi_{n_xn_y}\left(\bar{T}\begin{pmatrix} x \\ y \end{pmatrix}\right) \tag{11}$$

This new wave function $\phi_{\nu_x\nu_y}(x,y)$ is simply the original wave function rotated about the origin in the $x-y$ plane by θ as defined in the matrix $\bar{T}$. Our new goal is to find the components of the wave functions of the form $\psi_{n_xn_y}(x,y)$ that make up each rotated state $\phi_{\nu_x\nu_y}(x,y)$. We can define this in the way that we found the components of the total wave function $\Psi(x,y)$ as in equation (8). In this case, we will substitute $\phi_{\nu_x\nu_y}(x,y)$ in for $\Psi(x,y)$, giving us

$$c_{n_xn_y}^{\nu_x\nu_y} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi_{n_xn_y}^*(x,y)\phi_{\nu_x\nu_y}(x,y)\ \mathrm{d}x\ \mathrm{d}y \tag{12}$$

One very important point to notice, is that due to the symmetries of the quantum harmonic oscillator, each state $\psi_{n_xn_y}(x,y)$ that is present in the rotated state $\phi_{\nu_x\nu_y}(x,y)$ will have the property that $N = n_x + n_y = \nu_x + \nu_y$. We therefore only have to calculate N integrals as in (12) to find all of the possible components $c_{n_xn_y}^{\nu_x\nu_y}$ of the rotated state $\phi_{\nu_x\nu_y}(x,y)$ in terms of the original states $\psi_{n_xn_y}(x,y)$. For example if $n_x = 0$ and $n_y = 0$, the total is zero and thus we see that both ν_x and ν_y must also be zero. This also makes intuitive sense, because the $\psi_{00}(x,y)$ state is rotationally symmetric about the origin so it shouldn't matter how much the states are rotated, they must always be 0 0.

Since $\phi_{\nu_x\nu_y}(x,y)$ is only made up of the $\psi_{n_xn_y}(x,y)$ parts that have the above property described, we could imagine writing each state in terms of its components. For example, lets take $\phi_{20}(x,y)$ for some arbitrary rotation of θ. We know that it will be of the form

$$\phi_{20}(x,y) = a\psi_{02}(x,y) + b\psi_{11}(x,y) + c\psi_{20}(x,y) \tag{13}$$

for some constants a, b, and c. A very important property that restricts these constants is the fact that $\mid a \mid^2 + \mid b \mid^2 + \mid c \mid^2 = 1$. This is required by normalization as noted above. Therefore the probability of finding the particle in some state must be 1, while the probability, in this example, for finding it in the $\psi_{02}(x,y)$ would be $\mid a \mid^2$. The absolute value or magnitude signs here are important, because the constants may be imaginary and thus we must take a times its complex conjugate, in symbols written as $\mid a \mid^2 = a^* a$. This is very useful, because that quantity is always real and thus the probability of finding a particle in a given state is also always real.

The constants, a, b, and c in the above example will all depend on θ. It would then make sense if we could find a succinct way to express these factors. We would want to find all of the factors $c_{n_1 n_2}^{\nu_1 \nu_2}$ and write them in a compact form. A way to do this is to represent all of the factors in matrix form. Let us look at a simple state first then we can generalize it to larger states. Let us write the components for the state with $N = n_x + n_y = \nu_x + \nu_y = 1$ in a matrix. This matrix would be

$$\begin{pmatrix} c_{n_1 n_2}^{\nu_1 \nu_2} & c_{n_1 n_2}^{\nu_1 \nu_2} \\ c_{n_1 n_2}^{\nu_1 \nu_2} & c_{n_1 n_2}^{\nu_1 \nu_2} \end{pmatrix} \rightarrow \begin{pmatrix} c_{0\,1}^{0\,1} & c_{0\,1}^{1\,0} \\ c_{1\,0}^{0\,1} & c_{1\,0}^{1\,0} \end{pmatrix}$$

If we now write the general rotated state $\phi_{10}(x,y)$ as a vector, we would be able to multiply it by the above matrix to obtain the components of $\psi_{01}(x,y)$ and $\psi_{10}(x,y)$ in the state $\phi_{10}(x,y)$. To follow the convention above as you go down a column vector, first you have the 01 state and then the 10 state. In general, you would start with the $n, 0$ state at the top of the column vector, then the $n-1, 1$ then all the way to the $0, n$ state at the bottom of the column vector. In the actual column vector would go the components of the original state in each of the stationary states. In this case, the state is solely the $\phi_{10}(x,y)$ state, which can be written as

$$(0)\phi_{01}(x,y) + (1)\phi_{10}(x,y) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Therefore to find the components in the $\psi_{01}(x,y)$ and $\psi_{10}(x,y)$ states we take the product

$$\begin{pmatrix} c_{0\,1}^{0\,1} & c_{0\,1}^{1\,0} \\ c_{1\,0}^{0\,1} & c_{1\,0}^{1\,0} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} c_{0\,1}^{1\,0} \\ c_{1\,0}^{1\,0} \end{pmatrix}$$

Finally, we see that $\phi_{10}(x,y) = c_{0\,1}^{1\,0}\psi_{01}(x,y) + c_{1\,0}^{1\,0}\psi_{10}(x,y)$, which we could have easily seen from equation (7). Using Mathematica, we can calculate these coefficients by doing the integral in equation (12) for each of them. For a general θ, and we can show that the matrix above is actually equal to

$$\begin{pmatrix} \text{Cos}[\theta] & \text{-Sin}[\theta] \\ \text{Sin}[\theta] & \text{Cos}[\theta] \end{pmatrix}$$

Following are some more matrices of transformations from $\phi_{\nu_1 \nu_2}(x,y)$ to the states $\psi_{n_1 n_2}(x,y)$ given that the dimension of the matrix corresponds to $N+1 = \nu_1 + \nu_2 + 1 = n_1 + n_2 + 1$.

$$\begin{pmatrix} \text{Cos}[\theta]^2 & -\sqrt{2}\text{Cos}[\theta]\text{Sin}[\theta] & \text{Sin}[\theta]^2 \\ \sqrt{2}\text{Cos}[\theta]\text{Sin}[\theta] & \text{Cos}[2\theta] & -\sqrt{2}\text{Cos}[\theta]\text{Sin}[\theta] \\ \text{Sin}[\theta]^2 & \sqrt{2}\text{Cos}[\theta]\text{Sin}[\theta] & \text{Cos}[\theta]^2 \end{pmatrix}$$

$$\begin{pmatrix} \text{Cos}[\theta]^3 & -\sqrt{3}\text{Cos}[\theta]^2\text{Sin}[\theta] & \sqrt{3}\text{Cos}[\theta]\text{Sin}[\theta]^2 & -\text{Sin}[\theta]^3 \\ \sqrt{3}\text{Cos}[\theta]^2\text{Sin}[\theta] & \frac{1}{2}\text{Cos}[\theta](-1+3\text{Cos}[2\theta]) & \frac{1}{4}(\text{Sin}[\theta]-3\text{Sin}[3\theta]) & \sqrt{3}\text{Cos}[\theta]\text{Sin}[\theta]^2 \\ \sqrt{3}\text{Cos}[\theta]\text{Sin}[\theta]^2 & \frac{1}{2}(1+3\text{Cos}[2\theta])\text{Sin}[\theta] & \frac{1}{4}(\text{Cos}[\theta]+3\text{Cos}[3\theta]) & -\sqrt{3}\text{Cos}[\theta]^2\text{Sin}[\theta] \\ \text{Sin}[\theta]^3 & \sqrt{3}\text{Cos}[\theta]\text{Sin}[\theta]^2 & \sqrt{3}\text{Cos}[\theta]^2\text{Sin}[\theta] & \text{Cos}[\theta]^3 \end{pmatrix}$$

$$\begin{pmatrix} \text{Cos}[\theta]^4 & -2\text{Cos}[\theta]^3\text{Sin}[\theta] & \sqrt{6}\text{Cos}[\theta]^2\text{Sin}[\theta]^2 & -2\text{Cos}[\theta]\text{Sin}[\theta]^3 & \text{Sin}[\theta]^4 \\ 2\text{Cos}[\theta]^3\text{Sin}[\theta] & \frac{1}{2}(\text{Cos}[2\theta]+\text{Cos}[4\theta]) & -\frac{1}{2}\sqrt{\frac{3}{2}}\text{Sin}[4\theta] & (1+2\text{Cos}[2\theta])\text{Sin}[\theta]^2 & -2\text{Cos}[\theta]\text{Sin}[\theta]^3 \\ \sqrt{6}\text{Cos}[\theta]^2\text{Sin}[\theta]^2 & \frac{1}{2}\sqrt{\frac{3}{2}}\text{Sin}[4\theta] & \frac{1}{4}(1+3\text{Cos}[4\theta]) & -\frac{1}{2}\sqrt{\frac{3}{2}}\text{Sin}[4\theta] & \sqrt{6}\text{Cos}[\theta]^2\text{Sin}[\theta]^2 \\ 2\text{Cos}[\theta]\text{Sin}[\theta]^3 & (1+2\text{Cos}[2\theta])\text{Sin}[\theta]^2 & \frac{1}{2}\sqrt{\frac{3}{2}}\text{Sin}[4\theta] & \frac{1}{2}(\text{Cos}[2\theta]+\text{Cos}[4\theta]) & -2\text{Cos}[\theta]^3\text{Sin}[\theta] \\ \text{Sin}[\theta]^4 & 2\text{Cos}[\theta]\text{Sin}[\theta]^3 & \sqrt{6}\text{Cos}[\theta]^2\text{Sin}[\theta]^2 & 2\text{Cos}[\theta]^3\text{Sin}[\theta] & \text{Cos}[\theta]^4 \end{pmatrix}$$

III. Algebraic Approach to Transformation Matrices.

First recall that the raising/lowering operators $a_x^{\pm}$ act as follows, $a_x^- \mid n\rangle = \sqrt{n} \mid n-1\rangle$ and $a_x^+ \mid n\rangle = \sqrt{n+1} \mid n\rangle$. Another key fact is that $a_x^+ = (a_x^-)^*$. We could therefore construct any state $\mid n_x\rangle = \frac{(a_x^+)^{n_x}}{\sqrt{n_x!}} \mid 0\rangle$ or in the case of the two

dimensional state, $\mid n_x n_y\rangle = \frac{(a_x^+)^{n_x}}{\sqrt{n_x!}} \frac{(a_y^+)^{n_y}}{\sqrt{n_y!}} \mid 00\rangle$. We can also write each rotated state as $\mid \nu_x \nu_y \theta\rangle = \frac{(a_{x'}^+)^{\nu_x}}{\sqrt{\nu_x!}} \frac{(a_{y'}^+)^{\nu_y}}{\sqrt{\nu_y!}} \mid 00\theta\rangle$. Therefore the coefficients that were calculated before can be written as

$$\langle n_x n \mid \nu_x \nu_y \theta\rangle = \left(\langle 00 \mid \frac{(a_x^-)^{n_x}}{\sqrt{n_x!}} \frac{(a_y^-)^{n_y}}{\sqrt{n_y!}} \right) \left(\frac{(a_{x'}^+)^{\nu_x}}{\sqrt{\nu_x!}} \frac{\left(a_{y'}^+\right)^{\nu_y}}{\sqrt{\nu_y!}} \mid 00\theta\rangle \right) \tag{14}$$

The x' and y' referred to above come from the rotated states because $\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} T_{11}x + T_{12}y \\ T_{21}x + T_{22}y \end{pmatrix}$, where the square matrix is the rotation matrix. Since x' is comprised of both the x and y components of the previous state, let us assert that

$$a_{x'}^+ = T_{11} a_x^+ + T_{12} a_y^+ \tag{15}$$

and similarly that

$$a_{y'}^+ = T_{21} a_x^+ + T_{22} a_y^+ \tag{16}$$

Now, by making use of the definition of a binomial expansion; $(a+b)^r = \sum_{k=0}^{r} a^k b^{r-k} \frac{r!}{k!(r-k)!}$, we can substitute (15) and (16) into equation (14) and write it as a double sum.

$$\langle n_x n \mid \nu_x \nu_y \theta\rangle = \frac{1}{\sqrt{n_x! n_y! \nu_x! \nu_y!}} \sum_{j=0}^{\nu_x} \sum_{k=0}^{\nu_y} \frac{\nu_x!}{j!(\nu_x - j)!} \frac{\nu_y!}{k!(\nu_y - k)!} \text{ (continued below)}$$

$$\left(\langle 00 \mid \left(a_x^-\right)^{n_x} \left(a_y^-\right)^{n_y} \left(T_{11} a_x^+\right)^j \left(T_{12} a_y^+\right)^{\nu_x - j} \left(T_{21} a_x^+\right)^k \left(T_{22} a_y^+\right)^{\nu_y - k} \mid 00\rangle \right)$$

We can now bring the powers of the matrix elements outside the bracket because they are not operated on by the raising and lowering operators. Let us rewrite the second line of the above sum as

$$T_{11}^j T_{12}^{\nu_x - j} T_{21}^k T_{22}^{\nu_y - k} \langle 00 \mid \left(a_x^-\right)^{n_x} \left(a_y^-\right)^{n_y} \left(a_x^+\right)^j \left(a_y^+\right)^{\nu_x - j} \left(a_x^+\right)^k \left(a_y^+\right)^{\nu_y - k} \mid 00\rangle$$

We can now let the raising operators act on the ket resulting in

$$T_{11}^j T_{12}^{\nu_x - j} T_{21}^k T_{22}^{\nu_y - k} \sqrt{(j+k)!(\nu_x + \nu_y - j - k)!} \langle 00 \mid \left(a_x^-\right)^{n_x} \left(a_y^-\right)^{n_y} \mid (j+k)(\nu_x + \nu_y - j - k)\rangle$$

We know that in order for the sum to be non-zero, we need the number of raising operators to be equal to the number of lowering operators for each independent variable x and y. Therefore we see that the sum will only be non-zero when $n_x = j + k$ and when $n_y = (\nu_x - j) + (\nu_y - k)$ or in other words when $n_y = \nu_x + \nu_y - j - k$. By substituting in $n_x - k = j$, we have $n_y = \nu_x + \nu_y - (n_x - k) - k \rightarrow n_x + n_y = \nu_y + \nu_x$. This condition is obviously necessary as before since each state can only be comprised of other states with the same energy due to the symmetries of the quantum harmonic oscillator. By now supplying the conditions that $n_x = (j + k)$ and therefore that $j + k - n_x = 0$, which is required to get a non-zero sum and that $n_y = \nu_x + \nu_y - j - k$ which leads to $0 = \nu_x + \nu_y - j - k - n_y$, we can use the lowering operators. Then the previous brackets become

$$\sqrt{(j+k) \cdot (j+k-1) \cdot \ldots \cdot (j+k-n_x)} \sqrt{(\nu_x + \nu_y - j - k) \cdot (\nu_x + \nu_y - j - k - 1) \cdot \ldots \cdot (\nu_x + \nu_y - j - k - n_y)}$$

$$\text{(times the above line)} \langle 00 \mid (j + k - n_x)(\nu_x + \nu_y - j - k - n_y)\rangle$$

This inner product is only non-zero when $j + k - n_x = 0$ and $\nu_x + \nu_y - j - k - n_y = 0$ so it simplifies as follows,

$$\sqrt{\frac{(j+k)!(\nu_x + \nu_y - j - k)!}{(j + k - n_x)!(\nu_x + \nu_y - j - k - n_y)!}} \langle 00 \mid 00\rangle = \sqrt{(j+k)!(\nu_x + \nu_y - j - k)!}$$

Here we used the fact that $10 \cdot 9 \cdot 8 \cdot 7 = \frac{10!}{(10-4)!}$ the same trick used in proving the binomial coefficients. We can then combine the factor from the raising operators with the one from the lowering operators to obtain

$$\sqrt{(j+k)!(\nu_x + \nu_y - j - k)!} \sqrt{(j+k)!(\nu_x + \nu_y - j - k)!} = (j+k)!(\nu_x + \nu_y - j - k)!$$

Finally, we will substitute these results, and the fact that that we can bring the $\nu_x! \nu_y!$ outside the sum, into our original double sum giving us

$$\sqrt{\frac{\nu_x! \nu_y!}{n_x! n_y!}} \sum_{j=0}^{\nu_x} \sum_{k=0}^{\nu_y} \frac{1}{j!(\nu_x - j)! k! (\nu_y - k)!} T_{11}^j T_{12}^{\nu_x - j} T_{21}^k T_{22}^{\nu_y - k} (j+k)!(\nu_x + \nu_y - j - k)!$$

We can now substitute in $j = n_x - k$ to eliminate one of the sums.

$$\sqrt{\frac{\nu_x!\nu_y!}{n_x!n_y!}}\sum_{k=0}^{\nu_y}\frac{1}{(n_x-k)!(\nu_x-n_x+k)!k!(\nu_y-k)!}T_{11}^{n_x-k}T_{12}^{\nu_x-n_x+k}T_{21}^{k}T_{22}^{\nu_y-k}(n_x-k+k)!(\nu_x+\nu_y-n_x-+k-k)!$$

For the another simplification, we can note for one last time that $n_y = \nu_x + \nu_y - n_x$

$$\sqrt{\frac{\nu_x!\nu_y!}{n_x!n_y!}}\sum_{k=0}^{\nu_y}\frac{1}{(n_x-k)!(\nu_x-n_x+k)!k!(\nu_y-k)!}T_{11}^{n_x-k}T_{12}^{\nu_x-n_x+k}T_{21}^{k}T_{22}^{\nu_y-k}(n_x)!(n_y)!$$

Finally, by taking the $(n_x)!(n_y)!$ out of the sum, we have

$$\langle n_x n \mid \nu_x\nu_y\theta\rangle = \sqrt{\nu_x!\nu_y!n_x!n_y!}\sum_{k=0}^{\nu_y}\frac{1}{(n_x-k)!(\nu_x-n_x+k)!k!(\nu_y-k)!}T_{11}^{n_x-k}T_{12}^{\nu_x-n_x+k}T_{21}^{k}T_{22}^{\nu_y-k}\delta_{n_x+n_y,\nu_x+\nu_y}$$

Using this, we can generate the transformation matrices that were found using integrals above. Here, $T_{11} = \mathrm{Cos}[\theta]$, $T_{12} = -\mathrm{Sin}[\theta]$, $T_{21} = \mathrm{Sin}[\theta]$, and $T_{22} = \mathrm{Cos}[\theta]$. The fact that the elements of the matrix involve a sum makes sense if you observe the above matrices which are identical to these except they were generated in a different manner.

IV. Discussion

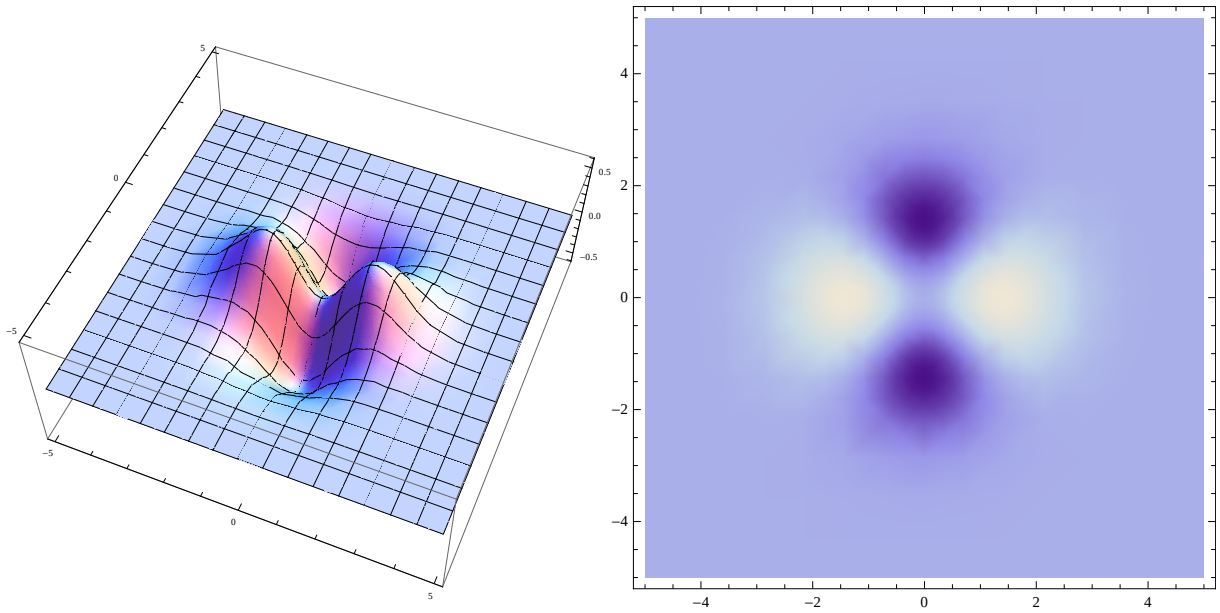
The time scales on which the two methods of matrix generation occurred were quite different. For the integration method, I used the high performance computing cluster at AU called Zorro. The time needed to generate the matrices was from 1.5 seconds to 5291 seconds for matrices of unto a total $N = 10$ (an 11×11) matrix. On the right are the times for matrix generation on my laptop with the max of a 101×101 matrix, which was generated in 82 seconds, faster than the 4×4 matrix using the integrals.

Energy	Time (sec)
0	1.55967
1	6.69498
2	32.0691
3	110.419
4	278.474
5	623.997
6	1062.91
7	1724.45
8	2503
9	3692
10	5291

Energy	Time (sec)
0	0
10	0.202
20	0.951
30	1.825
40	3.51
50	6.833
60	16.505
70	28.252
80	42.963
90	59.951
100	82.946

V. Conclusion

I may have included too much of Quantum Mechanics that was not necessary for understanding my results, but I thought it was better to have too much rather than too little. I spent a lot of my time while researching messing with fun/pretty graphs. Here are some of the more boring ones, but enough to give a picture of what they looked like. Eventually we were searching for eigen vectors/values for these matrices, but Mathematica was taking too long to compute them for the general θ so we need a new way to do this. Here is an eigen state for rotation by π.


5
0
−5
−5
0
5
0.5
0.0
−0.5
4
2
0
−2
−4
−4
−2
0
2
4