3D isotropic simple harmonics in the Cartesian co-ordinates and spherical co-ordinates

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We discuss the quantum mechanics of the 3D isotropic simple harmonics using the Cartesian co-ordinates and spherical co-ordinates

1. Representation in the Cartesian co-ordinates

The Hamitonian of the 3D isotropic simple harmonics is described by

$$\begin{aligned}\hat{H} &= \frac{1}{2m}(\hat{p}_x{}^2 + \hat{p}_y{}^2 + \hat{p}_z{}^2) + \frac{1}{2}m\omega_0{}^2(\hat{x}^2 + \hat{y}^2 + \hat{z}^2) \\ &= \hat{H}_x + \hat{H}_y + \hat{H}_z\end{aligned}$$

with

$$\hat{H}_x = \frac{1}{2m}\hat{p}_x{}^2 + \frac{1}{2}m\omega_0{}^2\hat{x}^2,$$

$$\hat{H}_y = \frac{1}{2m}\hat{p}_y{}^2 + \frac{1}{2}m\omega_0{}^2\hat{y}^2,$$

$$\hat{H}_z = \frac{1}{2m}\hat{p}_z{}^2 + \frac{1}{2}m\omega_0{}^2\hat{z}^2,$$

where

$$[\hat{H}, \hat{H}_x] = [\hat{H}, \hat{H}_y] = [\hat{H}, \hat{H}_z] = 0$$

The eigenvectors of the Hamiltonian $\hat{H}$ are also eigenvectors of $\hat{H}_x$, $\hat{H}_y$, and $\hat{H}_z$.

$$\hat{H}_x|n_x\rangle = (n_x + \frac{1}{2})\hbar\omega_0|n_x\rangle,$$

$$\hat{H}_y|n_y\rangle = (n_y + \frac{1}{2})\hbar\omega_0|n_y\rangle,$$

$$\hat{H}_z|n_z\rangle = (n_z + \frac{1}{2})\hbar\omega_0|n_z\rangle,$$

where $n_x, n_y, n_z = 0, 1, 2, 3, \ldots\ldots$.
We have

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

and

$$\hat{H}|n_x, n_y, n_z\rangle = (n_x + n_y + n_z + \frac{3}{2})\hbar\omega_0|n_x, n_y, n_z\rangle.$$

With n_x fixed, we have

$$n_y + n_z = n - n_x$$

So there are $(n - n_x + 1)$ possibilities such that

$$\{n_y, n_z\} = \{0, n - n_x\}, \{1, n - n_x - 1\}, \ldots, \{n - n_x, 0\}$$

so the degeneracy g_n can be evaluated as

$$g_n = \sum_{n_x=0}^{n}(n - n_x + 1) = \frac{1}{2}(n+1)(n+2).$$

$E = \frac{3}{2}\hbar\omega_0$ (degeneracy; $g_0 = 1$)

$$|000\rangle.$$

$E = \frac{5}{2}\hbar\omega_0$ (degeneracy; $g_1 = 3$)

$$|100\rangle,\ |010\rangle,\ |001\rangle.$$

$E = \frac{7}{2}\hbar\omega_0$ (degeneracy; $g_2 = 6$)

$$|200\rangle,\ |020\rangle,\ |002\rangle,$$
$$|110\rangle,\ |011\rangle,\ |101\rangle.$$

$E = \frac{9}{2}\hbar\omega_0$ (degeneracy; $g_3 = 10$)

$$|300\rangle,\ |030\rangle,\ |003\rangle,$$
$$|210\rangle,\ |201\rangle,\ |120\rangle,\ |021\rangle,\ |102\rangle,\ |012\rangle,$$
$$|111\rangle.$$

Let us introduce three pairs of creation and annihilation operators.

$$\hat{a}_x = \frac{\beta}{\sqrt{2}}(\hat{x} + \frac{i}{m\omega_0}\hat{p}_x), \qquad \hat{a}_x^+ = \frac{\beta}{\sqrt{2}}(\hat{x} - \frac{i}{m\omega_0}\hat{p}_x),$$

$$\hat{a}_y = \frac{\beta}{\sqrt{2}}(\hat{y} + \frac{i}{m\omega_0}\hat{p}_y), \qquad \hat{a}_y^+ = \frac{\beta}{\sqrt{2}}(\hat{y} - \frac{i}{m\omega_0}\hat{p}_y),$$

$$\hat{a}_z = \frac{\beta}{\sqrt{2}}(\hat{z} + \frac{i}{m\omega_0}\hat{p}_z), \qquad \hat{a}_y^+ = \frac{\beta}{\sqrt{2}}(\hat{z} - \frac{i}{m\omega_0}\hat{p}_z),$$

$$[\hat{a}_x, \hat{a}_x^+] = [\hat{a}_y, \hat{a}_y^+] = [\hat{a}_z, \hat{a}_z^+] = \hat{1},$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}.$$

The eigenvectors $|n_x, n_y, n_z\rangle$ are denoted by

$$|n_x, n_y, n_z\rangle = \frac{(\hat{a}_x^+)^{n_x}(\hat{a}_y^+)^{n_y}(\hat{a}_z^+)^{n_z}}{\sqrt{n_x!n_y!n_z!}}|000\rangle.$$

2. Expression of the Angular momentum in terms of operators $\hat{a}_R$ and $\hat{a}_L$

Here we note that

$$\hat{a}_R^+ = -\frac{1}{\sqrt{2}}(\hat{a}_x^+ + i\hat{a}_y^+), \qquad \hat{a}_L^+ = \frac{1}{\sqrt{2}}(\hat{a}_x^+ - i\hat{a}_y^+),$$

or

$$\hat{a}_R = -\frac{1}{\sqrt{2}}(\hat{a}_x - i\hat{a}_y), \qquad \hat{a}_L = \frac{1}{\sqrt{2}}(\hat{a}_x + i\hat{a}_y).$$

We also have

$$\hat{a}_x = \frac{1}{\sqrt{2}}(\hat{a}_L - \hat{a}_R), \qquad \hat{a}_y = -\frac{i}{\sqrt{2}}(\hat{a}_L + \hat{a}_R),$$

$$\hat{a}_x^+ = \frac{1}{\sqrt{2}}(\hat{a}_L^+ - \hat{a}_R^+) \qquad \hat{a}_y^+ = \frac{i}{\sqrt{2}}(\hat{a}_L^+ + \hat{a}_R^+).$$

The commutation relations:

$$[\hat{a}_R, \hat{a}_R^+] = \frac{1}{2}[\hat{a}_x - i\hat{a}_y, \hat{a}_x^+ + i\hat{a}_y^+] = \hat{1},$$

$$[\hat{a}_L, \hat{a}_L^+] = \frac{1}{2}[\hat{a}_x + i\hat{a}_y, \hat{a}_x^+ - i\hat{a}_y^+] = \hat{1},$$

$$[\hat{a}_R, \hat{a}_L] = -\frac{1}{2}[\hat{a}_x - i\hat{a}_y, \hat{a}_x + i\hat{a}_y] = 0,$$

$$[\hat{a}_R, \hat{a}_L{}^+] = -\frac{1}{2}[\hat{a}_x - i\hat{a}_y, \hat{a}_x^+ - i\hat{a}_y^+] = 0,$$

$$[\hat{a}_L, \hat{a}_R{}^+] = -\frac{1}{2}[\hat{a}_x + i\hat{a}_y, \hat{a}_x^+ + i\hat{a}_y^+] = 0.$$

The Hamiltonain can be rewritten by

$$\hat{H} = \hbar\omega(\hat{a}_x^+\hat{a}_x + \hat{a}_y^+\hat{a}_y + \hat{a}_z^+\hat{a}_z + \frac{3}{2}\hat{1})$$
$$= \hbar\omega(\hat{a}_R^+\hat{a}_R + \hat{a}_L^+\hat{a}_L + \hat{a}_z^+\hat{a}_z + \frac{3}{2}\hat{1})$$
$$= \hbar\omega(\hat{N}_R + \hat{N}_L + \hat{N}_z + \frac{3}{2}\hat{1})$$

where

$$\hat{N}_R = \hat{a}_R^+\hat{a}_R, \qquad \hat{N}_L = \hat{a}_L^+\hat{a}_L.$$

The augular momentum can be expressed by

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = i\hbar(\hat{a}_x\hat{a}_y{}^+ - \hat{a}_x{}^+\hat{a}_y),$$

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = i\hbar(\hat{a}_y\hat{a}_z{}^+ - \hat{a}_y{}^+\hat{a}_z),$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z = i\hbar(\hat{a}_z\hat{a}_x{}^+ - \hat{a}_z{}^+\hat{a}_x).$$

Using

$$\hat{L}_z = i\hbar(\hat{a}_x\hat{a}_y^+ - \hat{a}_x^+\hat{a}_y)$$
$$= \frac{\hbar}{2}(\hat{a}_R^+\hat{a}_R + \hat{a}_R\hat{a}_R^+ - \hat{a}_L^+\hat{a}_L - \hat{a}_L\hat{a}_L^+)$$
$$= \hbar(\hat{a}_R^+\hat{a}_R - \hat{a}_L^+\hat{a}_L)$$
$$= \hbar(\hat{N}_R - \hat{N}_L)$$

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y$$
$$= i\hbar(\hat{a}_y\hat{a}_z^+ - \hat{a}_y^+\hat{a}_z) - \hbar(\hat{a}_z\hat{a}_x^+ - \hat{a}_z{}^+\hat{a}_x)$$
$$= \hbar\hat{a}_z^+(\hat{a}_x + i\hat{a}_y) - \hbar\hat{a}_z(\hat{a}_x^+ + i\hat{a}_y^+)$$
$$= \sqrt{2}\hbar(\hat{a}_z^+\hat{a}_L + \hat{a}_z\hat{a}_R^+)$$

$$\hat{L}_- = \hat{L}_x - i\hat{L}_y$$
$$= i\hbar(\hat{a}_y\hat{a}_z^+ - \hat{a}_y^+\hat{a}_z) + \hbar(\hat{a}_z\hat{a}_x^+ - \hat{a}_z{}^+\hat{a}_x)$$
$$= -\hbar\hat{a}_z^+(\hat{a}_x - i\hat{a}_y) + \hbar\hat{a}_z(\hat{a}_x^+ - i\hat{a}_y^+)$$
$$= \sqrt{2}\hbar(\hat{a}_z^+\hat{a}_R + \hat{a}_z\hat{a}_L^+)$$

3. Simultaneous eigenkets of $\hat{H}$ and $\hat{L}_z$

$|N_R, N_L, N_z\rangle$ is an eigenvector of $\hat{H}$ and $\hat{L}_z$ with the eigenvalues

$$(N_R + N_L + N_z + \frac{3}{2})\hbar\omega_0 = (n + \frac{3}{2})\hbar\omega_0 \qquad \text{(eigenvalue of } \hat{H}\text{)}$$

and

$$(N_R - N_L)\hbar = m\hbar \qquad \text{(eigenvalue of } \hat{L}_z\text{)}$$

or

$$n = N_R + N_L + N_z, \qquad m = N_R - N_L.$$

The wave function of the simple harmonics for the one dimension

For $|n = 0\rangle$ state;

$$\varphi_0(x) = \pi^{-1/4}(\frac{m\omega_0}{\hbar})^{1/4} e^{-\frac{m\omega_0 x^2}{2\hbar}}.$$

For $|n = 1\rangle$ state;

$$\varphi_1(x) = \pi^{-1/4}(\frac{m\omega_0}{\hbar})^{1/4} \frac{1}{\sqrt{2^1 1!}}(2\sqrt{\frac{m\omega_0}{\hbar}}x)e^{-\frac{m\omega_0 x^2}{2\hbar}}.$$

For $|n = 2\rangle$ state;

$$\varphi_2(x) = \pi^{-1/4}(\frac{m\omega_0}{\hbar})^{1/4}\frac{1}{\sqrt{2^2 2!}}[4\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 x^2 - 2)e^{-\frac{m\omega_0 x^2}{2\hbar}}.$$

The wave function in the $|xyz\rangle$ representation is defined by

$$\langle xyz|n_x n_y n_z\rangle = \varphi_{n_x}(x)\varphi_{n_y}(y)\varphi_{n_z}(z).$$

(i) The ground state with the energy $\frac{3}{2}\hbar\omega_0$

$$\langle xyz|n_x = 0, n_y = 0, n_z = 0\rangle = \pi^{-3/4}(\frac{m\omega_0}{\hbar})^{3/4}e^{-\frac{m\omega_0}{2\hbar}r^2}.$$

The ground state is in a s state since the wavefunction is independent of θ and ϕ.

(ii) The first excited state with the energy $\frac{5}{2}\hbar\omega_0$,

$$\langle xyz|n_x = 1, n_y = 0, n_z = 0\rangle = \pi^{-3/4}(\frac{m\omega_0}{\hbar})^{3/4}\frac{1}{\sqrt{2^1 1!}}(2\sqrt{\frac{m\omega_0}{\hbar}})xe^{-\frac{m\omega_0 r^2}{2\hbar}}$$

$$\approx re^{-\frac{m\omega_0 r^2}{2\hbar}}(Y_1^1 + Y_1^{-1})$$

$$\langle xyz|n_x = 0, n_y = 1, n_z = 0\rangle = \pi^{-3/4}(\frac{m\omega_0}{\hbar})^{3/4}\frac{1}{\sqrt{2^1 1!}}(2\sqrt{\frac{m\omega_0}{\hbar}})ye^{-\frac{m\omega_0 r^2}{2\hbar}}$$

$$\approx re^{-\frac{m\omega_0 r^2}{2\hbar}}(Y_1^1 - Y_1^{-1})$$

$$\langle xyz|n_x = 0, n_y = 0, n_z = 1\rangle = \pi^{-3/4}(\frac{m\omega_0}{\hbar})^{3/4}\frac{1}{\sqrt{2^1 1!}}(2\sqrt{\frac{m\omega_0}{\hbar}})ze^{-\frac{m\omega_0 r^2}{2\hbar}}$$

$$\approx re^{-\frac{m\omega_0 r^2}{2\hbar}}Y_1^0$$

Then we get

$$\langle xyz|n_x = 1, n_y = 0, n_z = 0\rangle + \langle xyz|n_x = 0, n_y = 1, n_z = 0\rangle \approx re^{-\frac{m\omega_0 r^2}{2\hbar}}Y_1^1,$$

for $\left|l=1,m=1\right\rangle$,

$$\left\langle xyz\middle|n_x=0,n_y=0,n_z=1\right\rangle \approx re^{-\frac{m\omega_0 r^2}{2\hbar}}Y_1^0,$$

for $\left|l=1,m=0\right\rangle$,

$$\left\langle xyz\middle|n_x=1,n_y=0,n_z=0\right\rangle - \left\langle xyz\middle|n_x=0,n_y=1,n_z=0\right\rangle \approx re^{-\frac{m\omega_0 r^2}{2\hbar}}Y_1^{-1},$$

for $\left|l=1,m=-1\right\rangle$,

where

$$Y_1^1+Y_1^{-1}=-i\sqrt{\frac{3}{2\pi}}\sin\theta\sin\phi=-i\sqrt{\frac{3}{2\pi}}\frac{x}{r},$$

$$Y_1^1-Y_1^{-1}=-\sqrt{\frac{3}{2\pi}}\sin\theta\cos\phi=-\sqrt{\frac{3}{2\pi}}\frac{y}{r},$$

$$Y_1^0=\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta=\frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{z}{r},$$

or

$$Y_1^1=-\frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{i\phi}\sin\theta=-\frac{1}{2}\sqrt{\frac{3}{2\pi}}\frac{(x+iy)}{r},$$

$$Y_1^0=\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta=\frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{z}{r},$$

$$Y_1^1=\frac{1}{2}\sqrt{\frac{3}{2\pi}}e^{-i\phi}\sin\theta=\frac{1}{2}\sqrt{\frac{3}{2\pi}}\frac{(x-iy)}{r}.$$

For the first excited states, we find that the angular factors contain Y_1^m (m = 1, 0, -1,) and Y_0^0 (l = 0, m = 0). The six degenerate states can be re-expressed in terms of the three states with l = 1.

(iii) The second excited states

$$\left\langle xyz \middle| n_x = 2, n_y = 0, n_z = 0 \right\rangle = \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} [4\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 x^2 - 2) e^{-\frac{m\omega_0 r^2}{2\hbar}},$$

$$\left\langle xyz \middle| n_x = 0, n_y = 2, n_z = 0 \right\rangle = \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} [4\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 y^2 - 2) e^{-\frac{m\omega_0 r^2}{2\hbar}},$$

$$\left\langle xyz \middle| n_x = 0, n_y = 0, n_z = 2 \right\rangle = \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} [4\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 z^2 - 2) e^{-\frac{m\omega_0 r^2}{2\hbar}},$$

$$\left\langle xyz \middle| n_x = 1, n_y = 1, n_z = 0 \right\rangle = \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \left(\frac{1}{\sqrt{2^1 1!}}\right)^2 \left(2\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 xye^{-\frac{m\omega_0 r^2}{2\hbar}}$$

$$= \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} 4\sqrt{2}\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 xye^{-\frac{m\omega_0 r^2}{2\hbar}}$$

$$\left\langle xyz \middle| n_x = 0, n_y = 1, n_z = 1 \right\rangle = \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \left(\frac{1}{\sqrt{2^1 1!}}\right)^2 \left(2\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 yze^{-\frac{m\omega_0 r^2}{2\hbar}}$$

$$= \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} 4\sqrt{2}\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 yze^{-\frac{m\omega_0 r^2}{2\hbar}}$$

$$\left\langle xyz \middle| n_x = 1, n_y = 0, n_z = 1 \right\rangle = \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \left(\frac{1}{\sqrt{2^1 1!}}\right)^2 \left(2\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 zxe^{-\frac{m\omega_0 r^2}{2\hbar}}$$

$$= \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} 4\sqrt{2}\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 zxe^{-\frac{m\omega_0 r^2}{2\hbar}}$$

Thus we have

(i) $\left| l = 2, m = 2 \right\rangle$

$$\langle xyz | n_x = 2, n_y = 0, n_z = 0\rangle - \langle xyz | n_x = 0, n_y = 2, n_z = 0\rangle$$
$$+\sqrt{2}i\langle xyz | n_x = 1, n_y = 1, n_z = 0\rangle$$
$$= \pi^{-3/4}(\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} 4\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 (x^2 - y^2 + 2ixy)e^{-\frac{m\omega_0 r^2}{2\hbar}}$$
$$\propto Y_2^2$$

(ii) $|l = 2, m = 1\rangle$

$$\langle xyz | n_x = 1, n_y = 0, n_z = 1\rangle + i\langle xyz | n_x = 0, n_y = 1, n_z = 1\rangle$$
$$= \pi^{-3/4}(\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} 4\sqrt{2}\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 (zx + iyz)e^{-\frac{m\omega_0 r^2}{2\hbar}}$$
$$\propto Y_2^1$$

(iii) $|l = 2, m = 0\rangle$

$$2\langle xyz | n_x = 0, n_y = 0, n_z = 2\rangle - \langle xyz | n_x = 2, n_y = 0, n_z = 0\rangle$$
$$-\langle xyz | n_x = 0, n_y = 2, n_z = 0\rangle$$
$$= \pi^{-3/4}(\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} 4\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 (2z^2 - x^2 - y^2)e^{-\frac{m\omega_0 r^2}{2\hbar}}$$
$$\propto Y_2^0$$

(iv) $|l = 2, m = -1\rangle$

$$\langle xyz | n_x = 1, n_y = 0, n_z = 1\rangle - i\langle xyz | n_x = 0, n_y = 1, n_z = 1\rangle$$
$$= \pi^{-3/4}(\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} 4\sqrt{2}\left(\sqrt{\frac{m\omega_0}{\hbar}}\right)^2 (zx - iyz)e^{-\frac{m\omega_0 r^2}{2\hbar}}$$
$$\propto Y_2^{-1}$$

(v) $|l = 2, m = -2\rangle$

$$
\begin{aligned}
&\left\langle xyz \middle| n_x = 2, n_y = 0, n_z = 0 \right\rangle - \left\langle xyz \middle| n_x = 0, n_y = 2, n_z = 0 \right\rangle \\
&- \sqrt{2} i \left\langle xyz \middle| n_x = 1, n_y = 1, n_z = 0 \right\rangle \\
&= \pi^{-3/4} (\frac{m\omega_0}{\hbar})^{3/4} \frac{1}{\sqrt{2^2 2!}} 4 \left(\sqrt{\frac{m\omega_0}{\hbar}} \right)^2 (x^2 - y^2 - 2ixy) e^{-\frac{m\omega_0 r^2}{2\hbar}} \\
&\propto Y_2^{-2}
\end{aligned}
$$

Note that

$$
Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}} e^{2i\phi} \sin^2\theta = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \frac{(x+iy)^2}{r^2} = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \frac{x^2 - y^2 + 2ixy}{r^2},
$$

$$
Y_2^1 = -\frac{1}{2}\sqrt{\frac{15}{2\pi}} e^{i\phi} \sin\theta\cos\theta = -\frac{1}{2}\sqrt{\frac{15}{2\pi}} \frac{z(x+iy)}{r^2},
$$

$$
Y_2^0 = \frac{1}{4}\sqrt{\frac{5}{\pi}} (3\cos^2\theta - 1) = \frac{1}{4}\sqrt{\frac{5}{\pi}} \frac{3z^2 - (x^2 + y^2 + z^2)}{r^2} = \frac{1}{4}\sqrt{\frac{5}{\pi}} \frac{2z^2 - (x^2 + y^2)}{r^2},
$$

$$
Y_2^{-1} = \frac{1}{2}\sqrt{\frac{15}{2\pi}} e^{-i\phi} \sin\theta\cos\theta = \frac{1}{2}\sqrt{\frac{15}{2\pi}} \frac{z(x-iy)}{r^2},
$$

$$
Y_2^{-2} = \frac{1}{4}\sqrt{\frac{15}{2\pi}} e^{-2i\phi} \sin^2\theta = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \frac{(x-iy)^2}{r^2} = \frac{1}{4}\sqrt{\frac{15}{2\pi}} \frac{x^2 - y^2 - 2ixy}{r^2},
$$

and

$$
Y_2^2 + Y_2^{-2} == \frac{1}{2}\sqrt{\frac{15}{2\pi}} \frac{x^2 - y^2}{r^2},
$$

$$
Y_2^2 - Y_2^{-2} = i\sqrt{\frac{15}{2\pi}} \frac{xy}{r^2},
$$

$$
Y_2^1 + Y_2^{-1} = -i\sqrt{\frac{15}{2\pi}} \frac{yz}{r^2},
$$

$$Y_2^1 - Y_2^{-1} = -\sqrt{\frac{15}{2\pi}}\frac{zx}{r^2}.$$

For the second excited states, we find that the angular factors contain Y_2^m (m = 2, 1, 0, -1, -2) and Y_0^0. The six degenerate states can be re-expressed in terms of the five states with l = 2 and one state with l = 0.

4. Representation in the spherical co-ordinates

$$\langle \mathbf{r}|\frac{\hat{\mathbf{p}}^2}{2\mu}|\psi\rangle + \langle \mathbf{r}|V(|\hat{\mathbf{r}}|)|\psi\rangle = E\langle \mathbf{r}|\psi\rangle,$$

or

$$-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial}{\partial r}(\frac{\partial}{\partial r}r\langle \mathbf{r}|\psi\rangle) + \frac{1}{2\mu r^2}\langle \mathbf{r}|\hat{\boldsymbol{L}}^2|\psi\rangle + V(r)\langle \mathbf{r}|\psi\rangle = E\langle \mathbf{r}|\psi\rangle,$$

or

$$[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial}{\partial r}(\frac{\partial}{\partial r}r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)]\langle \mathbf{r}|\psi\rangle = E\langle \mathbf{r}|\psi\rangle,$$

where

$$V(r) = \frac{1}{2}\mu\omega_0^{\,2}r^2$$

Here we assume that

$$\langle \mathbf{r}|\psi\rangle = \psi(\mathbf{r}) = R_{E,l}(r)Y_l^m(\theta,\phi)$$

(separation variable) with

$$\langle \boldsymbol{n}|l,m\rangle = Y_l^m(\theta,\phi).$$

$R_{E,l}(r)$ depends only on E and l, but not on m.

$$[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial}{\partial r}(\frac{\partial}{\partial r}r)+\frac{\hbar^2 l(l+1)}{2\mu r^2}+\frac{1}{2}\mu\omega_0{}^2r^2]R_{E,l}(r)=ER_{E,l}(r)$$

We assume that

$$R_{E,l}(r)=\frac{u(r)}{r},$$

$$u''(r)-[\frac{l(l+1)}{r^2}+\frac{2\mu(-E+V(r)}{\hbar^2}]u(r)=0,$$

or

$$u''(r)-\frac{l(l+1)}{r^2}u-\frac{\mu^2\omega^2}{\hbar^2}r^2u(r)=-\frac{2\mu E}{\hbar^2}u(r).$$

We now introduce a new variable

$$\rho=\sqrt{\frac{\mu\omega_0}{\hbar}}r, \qquad \lambda=\frac{2E}{\hbar\omega_0}.$$

Then we get the differential equation

$$u''(\rho)-\frac{l(l+1)}{\rho^2}u(\rho)-\rho^2u(\rho)=-\lambda u(\rho).$$

In the limit of $\rho\to 0$, u is assumed to have the power form $u(\rho)\approx\rho^s$. The substitution of this form into the above differential equation gives rise to

$$\rho^{s-2}[s(s-1)-l(l+1)]-\rho^{s+2}=-\lambda\rho^s,$$

or

$$\rho^{s-2}[s(s-1)-l(l+1)]=0.$$

So we get $s=l+1$.

In the limit of $\rho\to\infty$, the differential equation can be approximated as

$$u''(\rho) - \rho^2 u(\rho) = 0 .$$

We assume that $u(\rho) \approx \exp(-\rho^2/2)$.

$$u''(\rho) - \rho^2 u(\rho) = (\rho^2 - 1)u(\rho) - \rho^2 u(\rho) = -u(\rho) ,$$

This is almost the same as the original differential equation; $u''(\rho) - \rho^2 u(\rho) = 0$. These suggests that our solution $u(\rho)$ can be expressed by the form

$$u(\rho) = \rho^{l+1} e^{-\rho^2/2} f(\rho) .$$

Then we have the differential equation for $f(\rho)$ as

$$\rho f''(\rho) + 2(l + 1 - \rho^2) f'(\rho) + (\lambda - 2l - 3)\rho f(\rho) = 0 .$$

We solve this problem by using the series expansion

$$f(\rho) = \sum_{k=0}^{\infty} C(k)\rho^k .$$

Using the Mathematica, we get

$$2(1+l)C(1) = 0 ,$$

$$(-3 - 2l + \lambda)C(0) + 2(3 + 2l)C(2) = 0 ,$$

$$(-5 - 2l + \lambda)C(1) + 6(2 + l)C(3) = 0 ,$$

$$(-7 - 2l + \lambda)C(2) + 4(5 + 2l)C(4) = 0 .$$

Then we have

$$C(1) = C(3) = C(5) = ... = 0 .$$

In other words, $f(\rho)$ is an even function of ρ. So we assume that

$$f(\rho) = \sum_{k=0}^{\infty} C(2k)\rho^{2k} \ ,$$

Then we have

$$\sum_{k=1} (2k)(2k-1)C(2k)\rho^{2k-1} + 2(l+1-\rho^2)\sum_{k=1}(2k)C(2k)\rho^{2k-1}$$
$$+(\lambda - 2l - 3)\sum_{k=0} C(2k))\rho^{2k+1} = 0$$

or

$$\sum_{k=1} 2k[2k-1+2(l+1)]C(2k)\rho^{2k-1}$$
$$-\sum_{k=1} C(2k)(4k)\rho^{2k+1} + (\lambda - 2l - 3)\sum_{k=0} C(2k))\rho^{2k+1} = 0$$

Using the relation

$$\sum_{k=1} 2k[2k-1+2(l+1)]C(2k)\rho^{2k-1} = \sum_{k=0} (2k+2)[2k+1+2(l+1)]C(2k+1)\rho^{2k+1}$$

(conventional mathematical procedure)

$$\sum_{k=1} C(2k)(4k)\rho^{2k+1} = \sum_{k=0} C(2k)(4k)\rho^{2k+1}$$ (no change with the addition of k = 0 term)

this can be rewritten as

$$\sum_{k=0} \{2(k+1)(2k+2l+3)C(2k+2) - (4k+2l+3-\lambda)C(2k)\}\rho^{2k+1} 0$$

From this we get the recursion relation,

$$C(2k+2) = \frac{(4k+2l+3-\lambda)}{2(k+1)(2k+3+2l)} C(2k) ,$$

When

$$3 + 4n_r + 2l = \lambda \qquad (n_r = 0, 1, 2, 3, ...),$$

the co-efficient $C(2+2n_r)$ should be equal to zero, corresponding to the termination of the power series. Then, from the recursion relation, we have

$$C(2+2n_r) = C(4+2n_r) = ... = 0 .$$

So the energy quantization condition is that

$$3 + 4n_r + 2l = \lambda = \frac{2E}{\hbar\omega_0} ,$$

or

$$E(n_r, l) = (\frac{3}{2} + 2n_r + l)\hbar\omega_0 .$$

We define the principal quantum number n as

$$E_n = (n + \frac{3}{2})\hbar\omega_0 ,$$

with $n = 2n_r + l$.

n	l	n_r	Degeneracy
0	0	0	1
1	1	0	3
2	0	1	1
2	2	0	5
3	1	1	3
3	3	0	7
4	0	2	1
4	2	1	5
4	4	0	9
5	1	2	3

5	3	1	7
5	5	0	11
6	0	3	1
6	2	2	5
6	4	1	9
6	6	0	13

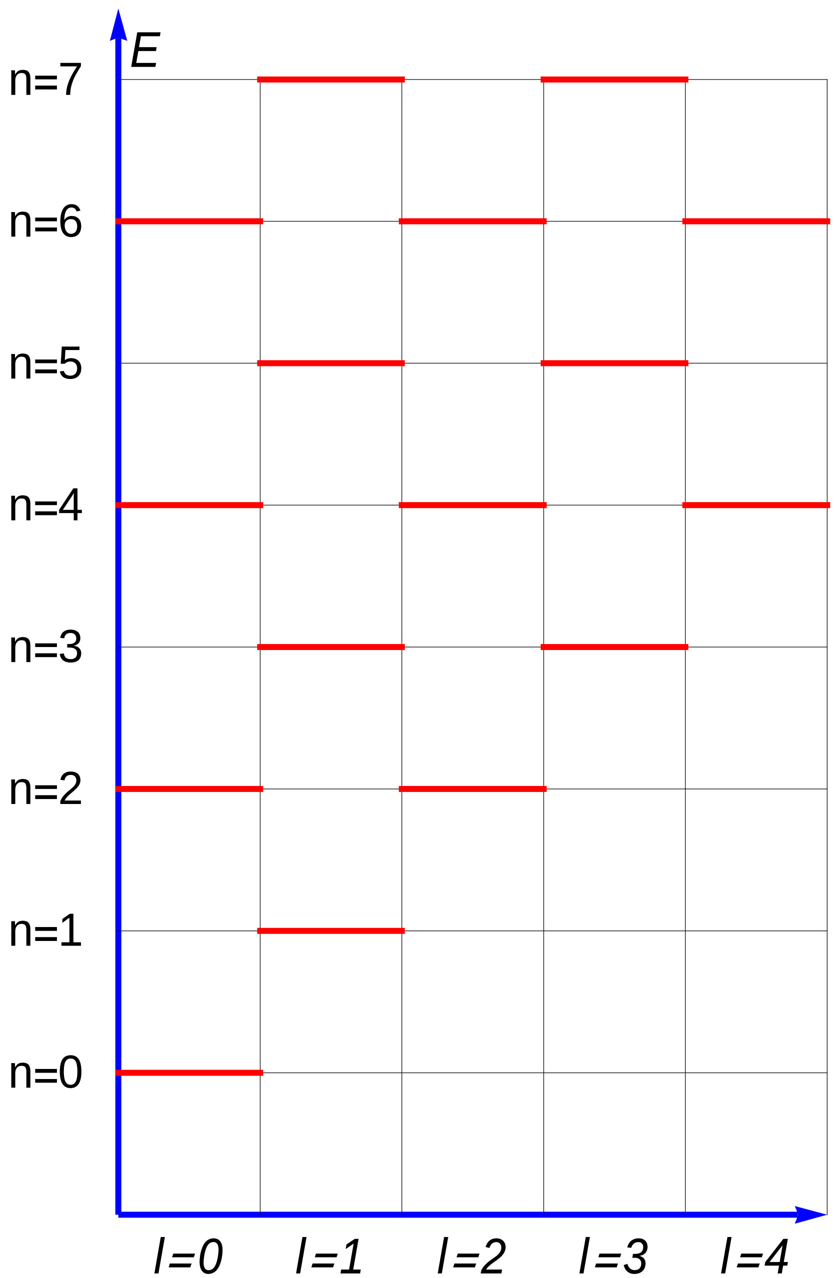


Fig. The energy levels $E_n = (n+\frac{3}{2})\hbar\omega$ of the 3D isotropic simple harmonics, showing the degeneracy. The degeneracy is 1 (n = 0), 3 (n = 1), 6 (=1 + 5) (n = 2), 10 (=3 +7) (n = 3), 15 (1 + 5 + 9) (n = 4), 21 (n = 5), 28 (n = 6).

5. Hypergeometric function

We use the Mathematica to solve the differential equation given by

$$\rho f''(\rho) + 2(l+1-\rho^2) f'(\rho) + 2(n-l)\rho f(\rho) = 0$$

The solution is given by

$$f(\rho) = \text{Hypergeometric1F1}[\frac{l-n}{2}, \frac{3}{2}+l, \rho^2]$$

This function is dependent on n and l, where n_r is given by

$$n = 2n_r + l$$

n	l	n_r	$f(\rho)$
0	0	0	1
1	1	0	1
2	0	1	$1-\frac{2\rho^2}{3}$
2	2	0	1
3	1	1	$1-\frac{2\rho^2}{5}$
3	3	0	1
4	0	2	$1-\frac{4\rho^2}{3}+\frac{4\rho^4}{15}$
4	2	1	$1-\frac{2\rho^2}{7}$
4	4	0	1

5	1	2	$1-\frac{4\rho^2}{5}+\frac{4\rho^4}{35}$
5	3	1	$1-\frac{2\rho^2}{9}$
5	5	0	1
6	0	3	$1-2\rho^2+\frac{4\rho^4}{5}-\frac{8\rho^6}{105}$
6	2	2	$1-\frac{4\rho^2}{7}+\frac{4\rho^4}{63}$
6	4	1	$1-\frac{2\rho^2}{11}$
6	6	0	1

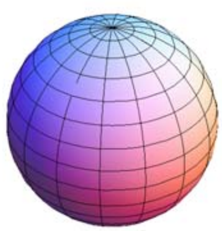
APPENDIX

Spherical harmonics

(i) $\langle n | l=0, m=0 >$

l=0 m=0 $Y^0_{l=0}(\theta,\phi)$

0 0 $\frac{1}{2\sqrt{\pi}}$



l = 0, m = 0

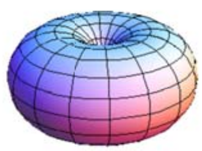
(ii) $\langle n | l=1, m >$ (m = -1, 0, 1)

l=1 m $Y^m_{l=1}(\theta,\phi)$

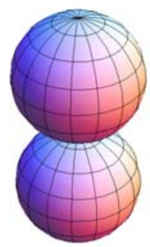
$1 \quad -1 \quad \frac{1}{2} e^{-i\phi} \sqrt{\frac{3}{2\pi}} \, \mathrm{Sin}[\theta]$

$1 \quad 0 \quad \frac{1}{2} \sqrt{\frac{3}{\pi}} \, \mathrm{Cos}[\theta]$

$1 \quad 1 \quad -\frac{1}{2} e^{i\phi} \sqrt{\frac{3}{2\pi}} \, \mathrm{Sin}[\theta]$



$l = 1, m = \pm 1$



$l = 1, m = 0$

(iii) $\langle n | l = 2, m >$ $(m = -2, -1, 0, 1, 2)$

l=2 m $Y_{l=2}^{m}(\theta, \phi)$

$2 \quad -2 \quad \frac{1}{4} e^{-2i\phi} \sqrt{\frac{15}{2\pi}} \, \mathrm{Sin}[\theta]^2$

$2 \quad -1 \quad \frac{1}{2} e^{-i\phi} \sqrt{\frac{15}{2\pi}} \, \mathrm{Cos}[\theta] \, \mathrm{Sin}[\theta]$

$2 \quad 0 \quad \frac{1}{8} \sqrt{\frac{5}{\pi}} \, (1 + 3\,\mathrm{Cos}[2\theta])$

$2 \quad 1 \quad -\frac{1}{2} e^{i\phi} \sqrt{\frac{15}{2\pi}} \, \mathrm{Cos}[\theta] \, \mathrm{Sin}[\theta]$

$2 \quad 2 \quad \frac{1}{4} e^{2i\phi} \sqrt{\frac{15}{2\pi}} \, \mathrm{Sin}[\theta]^2$

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A. Messiah, *Quantum Mechanics*, vol.I and vol.II (North-Holland, 1961).

Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë, *Quantum Mechanics volume I and volume II* (John Wiley & Sons, New York, 1977).

APPENDIX SphericalPlot3D of the probability

The probability is defined by

$$P = |\langle \xi | n_x \rangle|^2 |\langle \eta | n_y \rangle|^2 |\langle \varsigma | n_z \rangle|^2 ,$$

where

$$\xi = \beta x , \qquad \eta = \beta y , \qquad \varsigma = \beta z ,$$

where

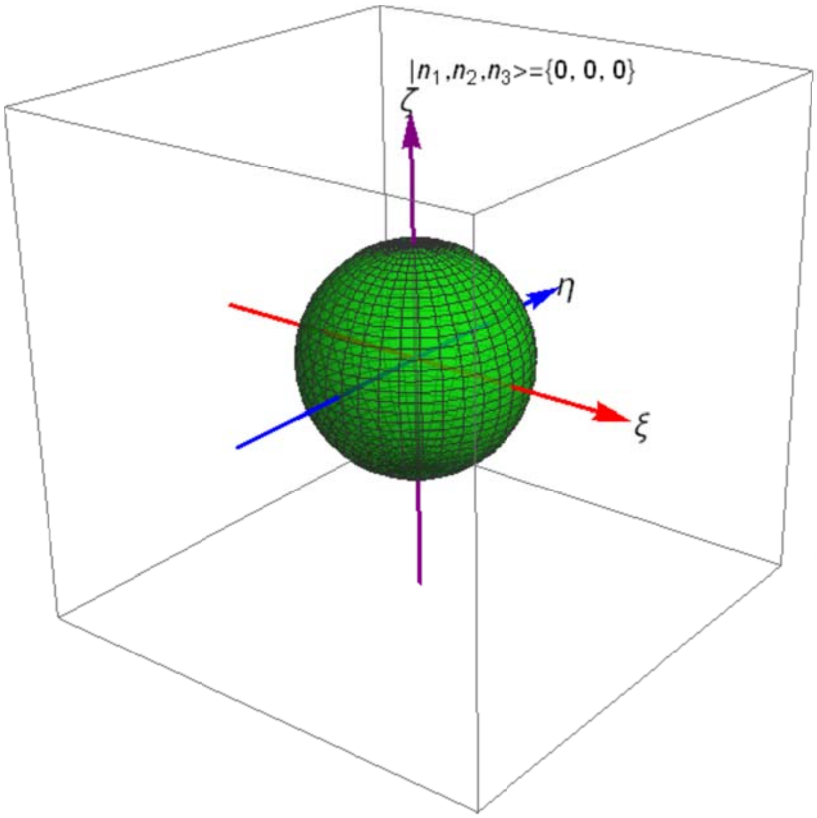
$$\beta = \sqrt{\frac{m\omega_0}{\hbar}} .$$

We change the co-ordinates of the system from the Cartesian to the spherical by the relation,

$$x = r \sin\theta \cos\phi , \qquad y = r \sin\theta \sin\phi , \qquad z = r\cos\theta .$$

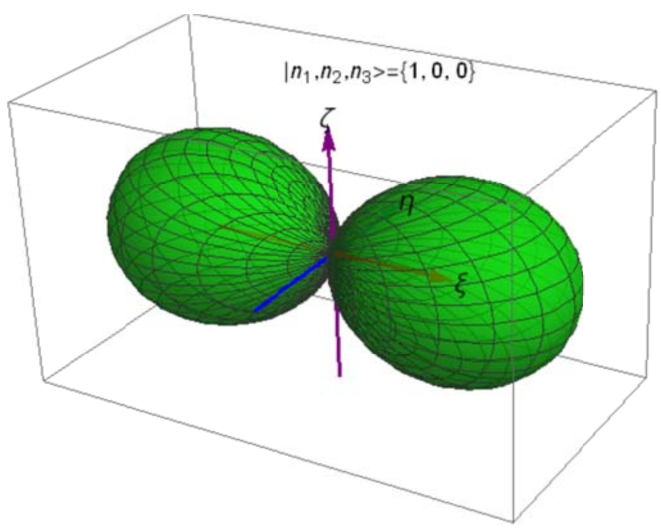
For convenience we assume that $\beta r = 1$. Using the Mathematica, we make a S.phericalPlot3D of the probability P as a function of θ and ϕ, where $0 \le \theta < \pi$ and $0 \le \phi < 2\pi$.

(a) $E = \frac{3}{2}\hbar\omega_0$. $|n_x, n_y, n_z\rangle = |0,0,0\rangle$

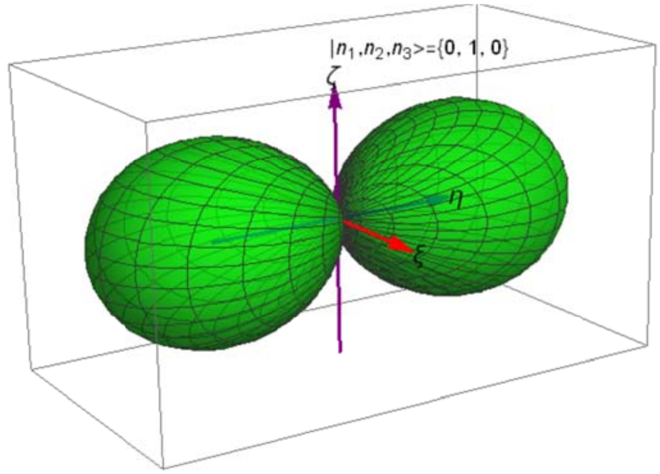


(b) $E=\frac{5}{2}\hbar\omega_0$. $\left|n_x,n_y,n_z\right\rangle=\left|1,0,0\right\rangle$, $\left|0,1,0\right\rangle$, $\left|0,0,1\right\rangle$

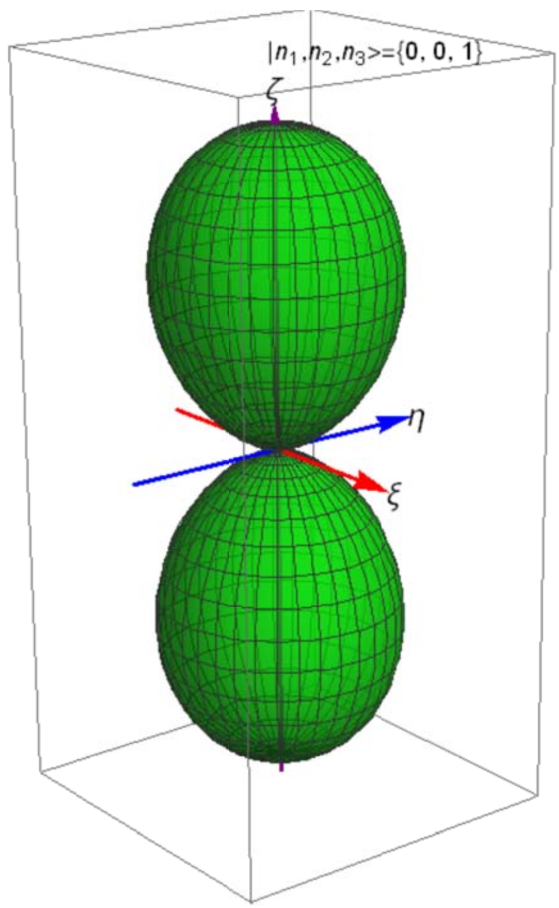
(i) $\left|n_x,n_y,n_z\right\rangle=\left|1,0,0\right\rangle$



(ii) $\left|n_x,n_y,n_z\right\rangle=\left|0,1,0\right\rangle$

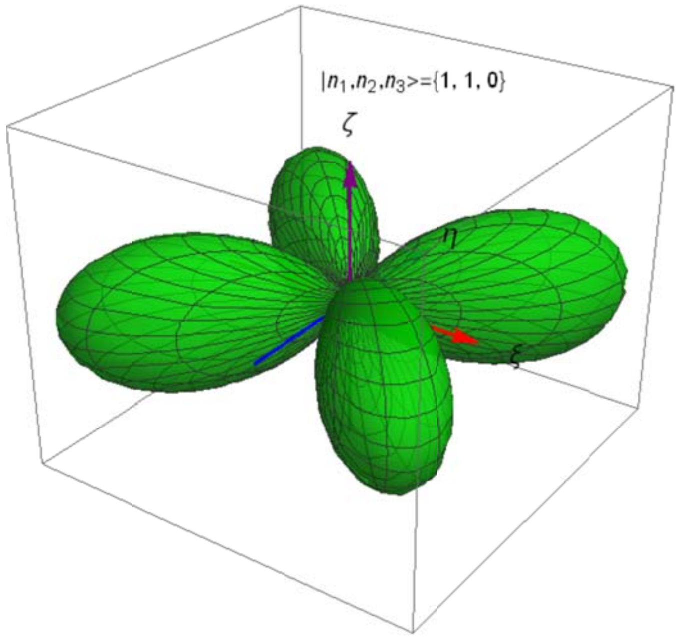


(iii) $\left|n_x, n_y, n_z\right\rangle = \left|0,0,1\right\rangle$

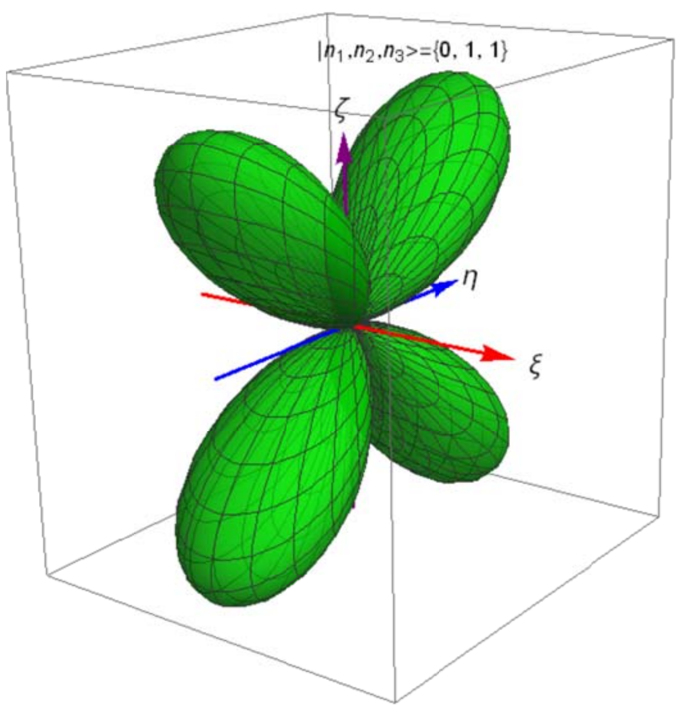


(c) $E = \frac{7}{2}\hbar\omega_0$. $\left|n_x, n_y, n_z\right\rangle = \left|1,1,0\right\rangle$, $\left|0,1,1\right\rangle$, $\left|1,0,1\right\rangle$, $\left|2,0,0\right\rangle$, $\left|0,2,0\right\rangle$, $\left|0,0,2\right\rangle$

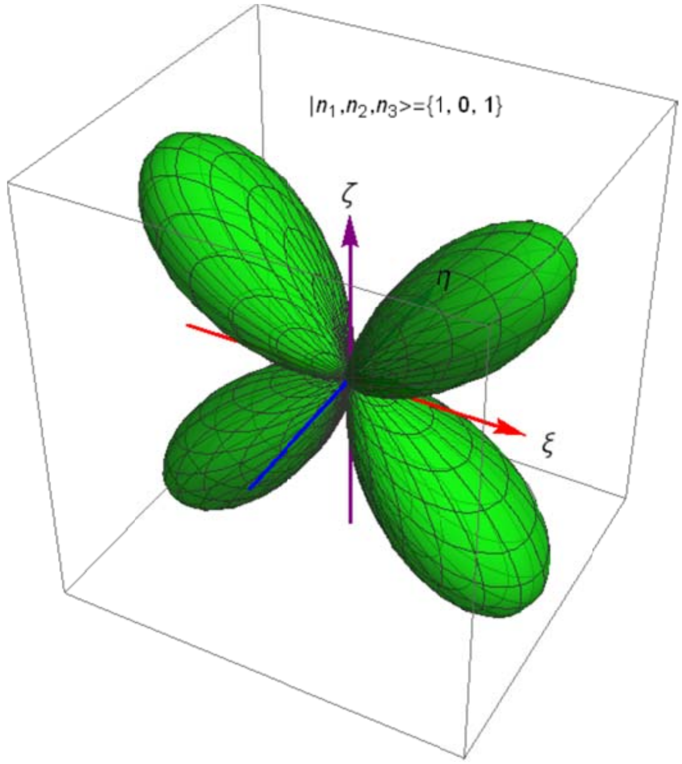
(i) $\left|n_x, n_y, n_z\right\rangle = \left|1,1,0\right\rangle$



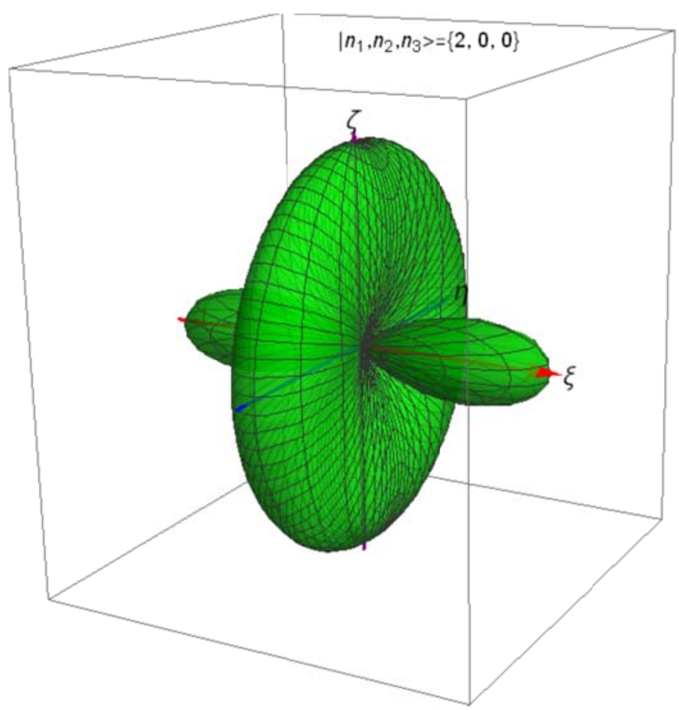
(ii) $\left|n_x, n_y, n_z\right\rangle = \left|0,1,1\right\rangle$



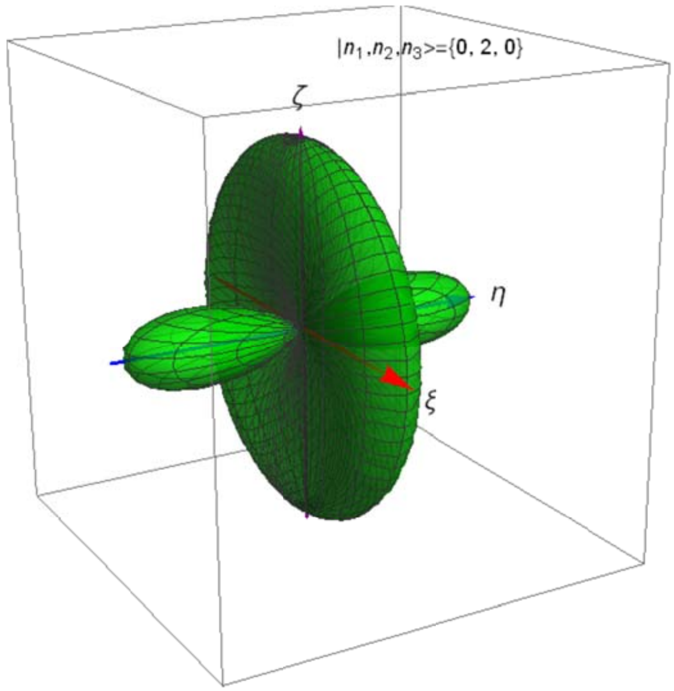
(iii) $\left|n_x, n_y, n_z\right\rangle = \left|1,0,1\right\rangle$



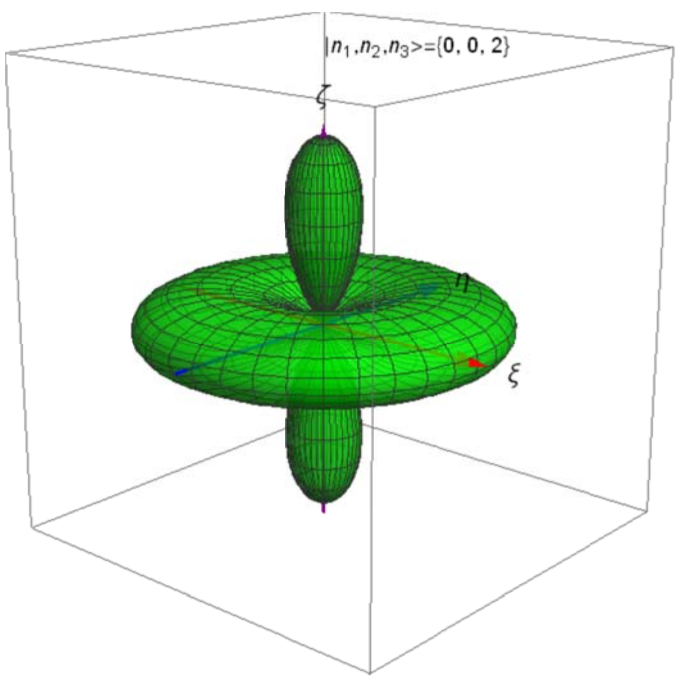
(iv) $\left|n_x, n_y, n_z\right\rangle = \left|2,0,0\right\rangle$



(v) $\left|n_x, n_y, n_z\right\rangle = \left|0,2,0\right\rangle$

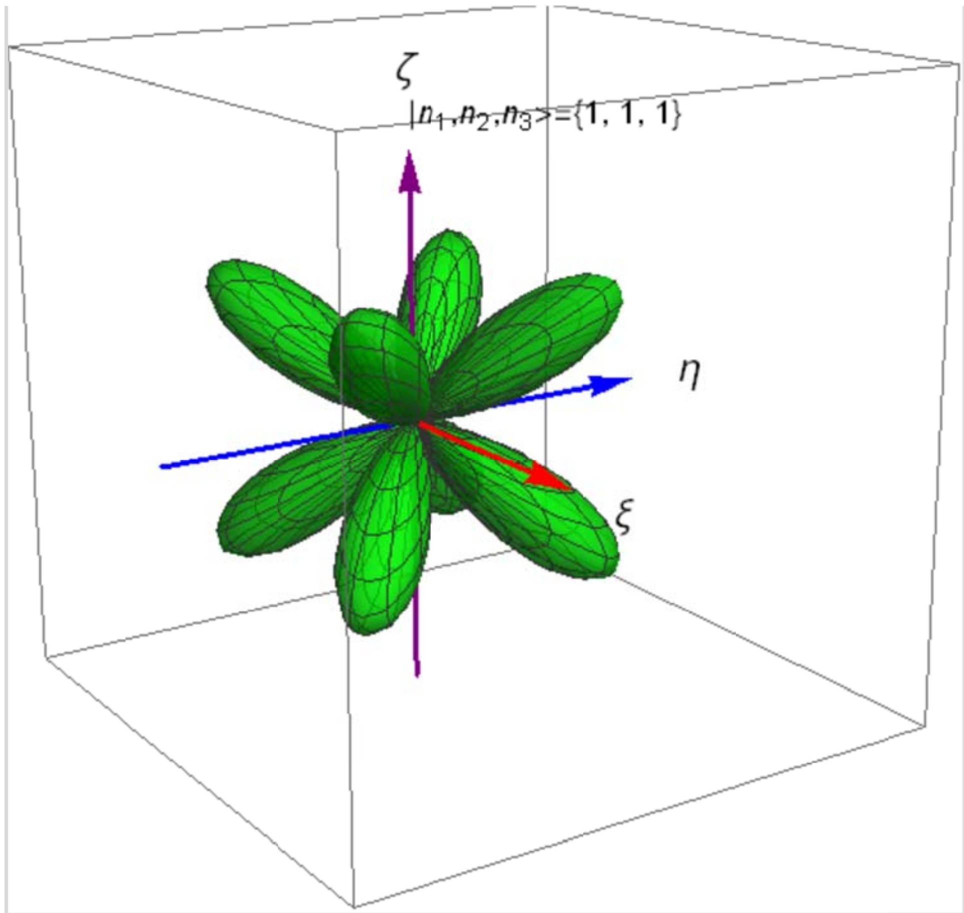


(vi) $\left|n_x, n_y, n_z\right\rangle = \left|0,0,2\right\rangle$

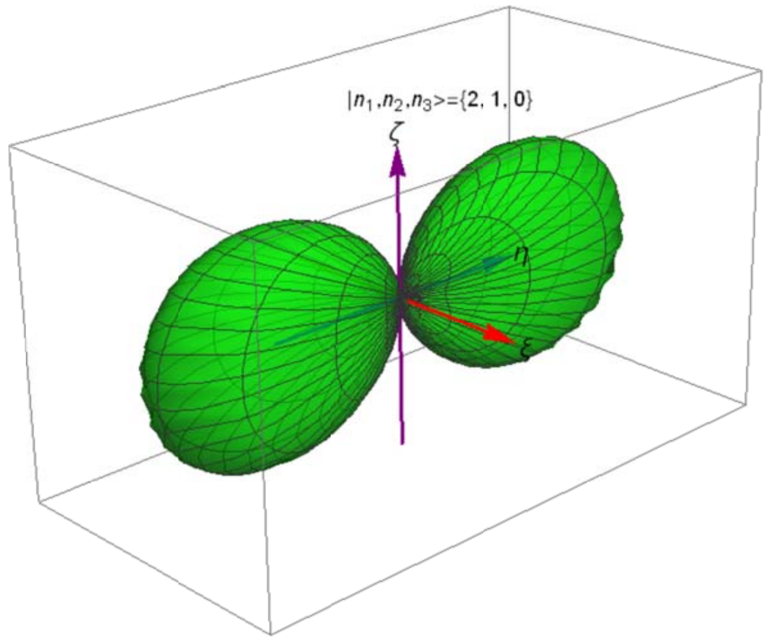


(d) $E = \frac{9}{2}\hbar\omega_0$. $\left|n_x, n_y, n_z\right\rangle = \left|1,1,1\right\rangle$, $\left|2,1,0\right\rangle$, $\left|2,0,1\right\rangle$, $\left|1,2,0\right\rangle$, $\left|0,2,1\right\rangle$, $\left|1,0,2\right\rangle$, $\left|0,1,2\right\rangle$, $\left|3,0,0\right\rangle$, $\left|0,3,0\right\rangle$, $\left|0,0,3\right\rangle$

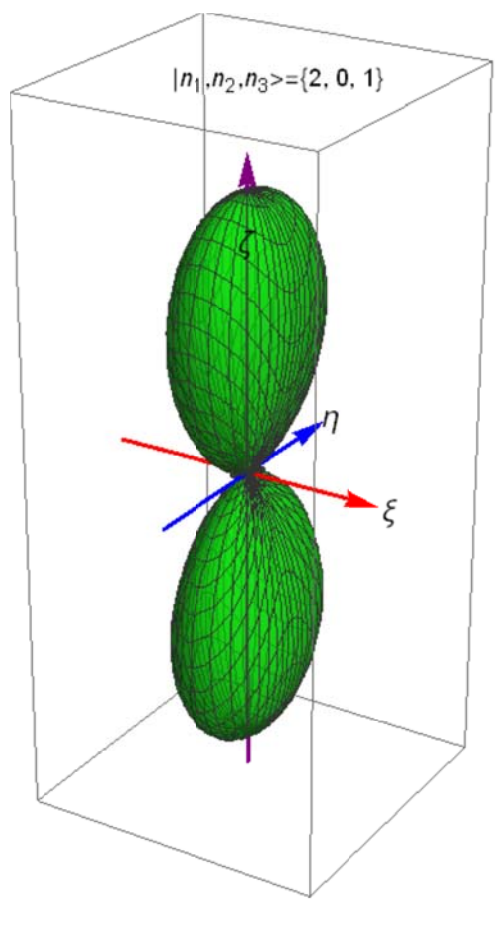
(i) $\left|n_x, n_y, n_z\right\rangle = \left|1,1,1\right\rangle$



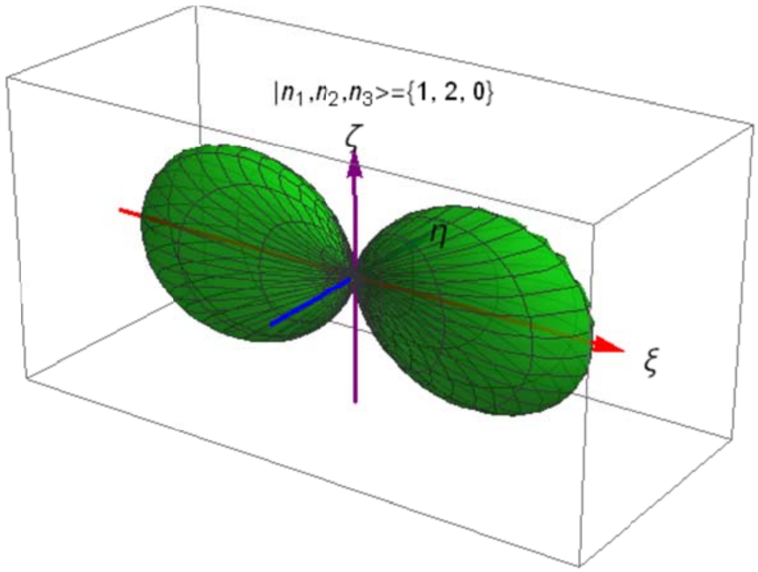
(ii) $\left|n_x, n_y, n_z\right\rangle = \left|2,1,0\right\rangle$



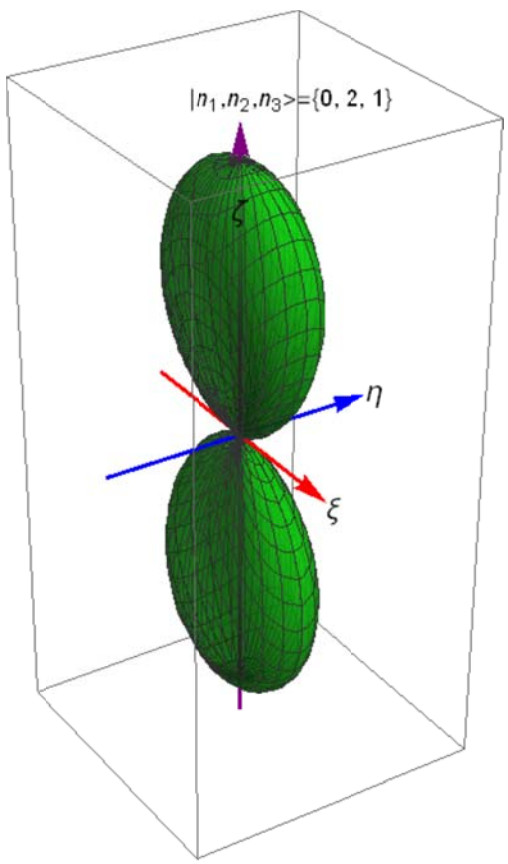
(iii) $\left|n_x, n_y, n_z\right\rangle = \left|2,0,1\right\rangle$



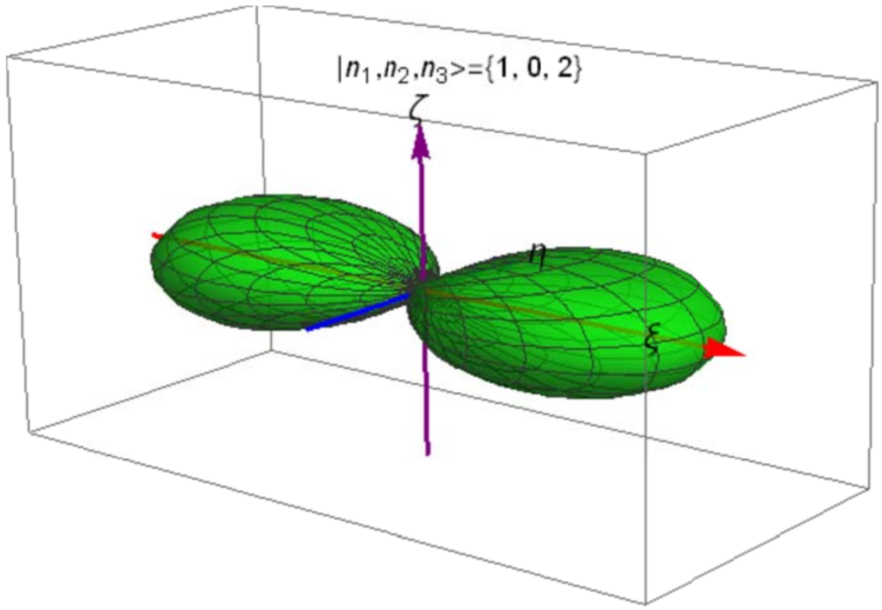
(iv) $\left|n_x, n_y, n_z\right\rangle = \left|1,2,0\right\rangle$



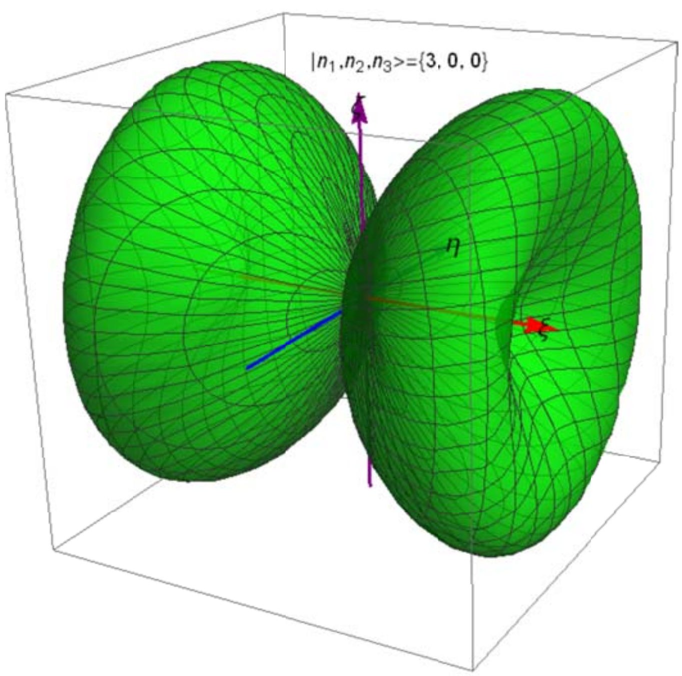
(v) $\left|n_x, n_y, n_z\right\rangle = \left|0,2,1\right\rangle$



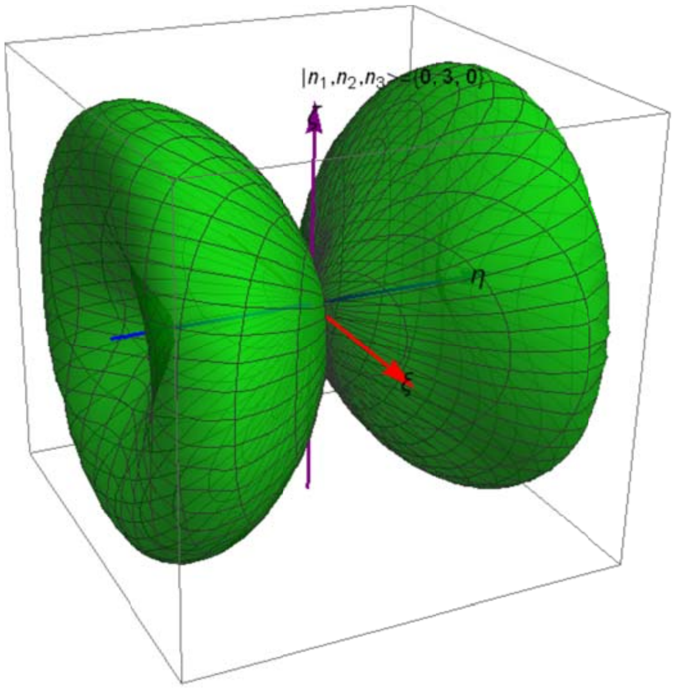
(vi) $\left|n_x, n_y, n_z\right\rangle = \left|1,0,2,\right\rangle$



(iix) $\left|n_x, n_y, n_z\right\rangle = \left|3,0,0\right\rangle$



(ix) $\left|n_x, n_y, n_z\right\rangle = \left|0,3,0\right\rangle$



(x) $\left|n_x, n_y, n_z\right\rangle = \left|0,0,3\right\rangle$