3D Symmetric HO in Spherical Coordinates *

We have already solved the problem of a 3D harmonic oscillator by separation of variables in Cartesian coordinates. It is instructive to **solve the same problem in spherical coordinates** and compare the results. The potential is

$$V(r) = \frac{1}{2}\mu\omega^2 r^2.$$

Our radial equation is

$$\begin{aligned}
\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) R_{E\ell}(r) + \frac{2\mu}{\hbar^2}\left(E - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right) R_{E\ell}(r) &= 0 \\
\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{\mu^2\omega^2}{\hbar^2}r^2 R - \frac{\ell(\ell+1)}{r^2}R + \frac{2\mu E}{\hbar^2}R &= 0
\end{aligned}$$

Write the equation in terms of the dimensionless variable

$$\begin{aligned}
y &= \frac{r}{\rho}. \\
\rho &= \sqrt{\frac{\hbar}{\mu\omega}} \\
r &= \rho y \\
\frac{d}{dr} &= \frac{dy}{dr}\frac{d}{dy} = \frac{1}{\rho}\frac{d}{dy} \\
\frac{d^2}{dr^2} &= \frac{1}{\rho^2}\frac{d}{dy^2}
\end{aligned}$$

Plugging these into the radial equation, we get

$$\begin{aligned}
\frac{1}{\rho^2}\frac{d^2R}{dy^2} + \frac{1}{\rho^2}\frac{2}{y}\frac{dR}{dy} - \frac{1}{\rho^4}\rho^2 y^2 R - \frac{1}{\rho^2}\frac{\ell(\ell+1)}{y^2}R + \frac{2\mu E}{\hbar^2}R &= 0 \\
\frac{d^2R}{dy^2} + \frac{2}{y}\frac{dR}{dy} - y^2 R - \frac{\ell(\ell+1)}{y^2}R + \frac{2E}{\hbar\omega}R &= 0.
\end{aligned}$$

Now find the behavior for large y.

$$\frac{d^2R}{dy^2} - y^2R = 0$$
$$R \approx e^{-y^2/2}$$

Also, find the behavior for small y.

$$\frac{d^2R}{dy^2} + \frac{2}{y}\frac{dR}{dy} - \frac{\ell(\ell+1)}{y^2}R = 0$$
$$R \approx y^s$$
$$s(s-1)y^{s-2} + 2sy^{s-2} = \ell(\ell+1)y^{s-2}$$
$$s(s+1) = \ell(\ell+1)$$
$$R \approx y^\ell$$

Explicitly put in this behavior and use a power series expansion to solve the full equation.

$$R = y^\ell \sum_{k=0}^{\infty} a_k y^k e^{-y^2/2} = \sum_{k=0}^{\infty} a_k y^{\ell+k} e^{-y^2/2}$$

We'll need to compute the derivatives.

$$\frac{dR}{dy} = \sum_{k=0}^{\infty} a_k [(\ell+k)y^{\ell+k-1} - y^{\ell+k+1}]e^{-y^2/2}$$

$$\frac{d^2R}{dy^2} = \sum_{k=0}^{\infty} a_k [(\ell+k)(\ell+k-1)y^{\ell+k-2} - (\ell+k)y^{\ell+k}$$

$$-(\ell+k+1)y^{\ell+k} + y^{\ell+k+2}]e^{-y^2/2}$$

$$\frac{d^2R}{dy^2} = \sum_{k=0}^{\infty} a_k [(\ell+k)(\ell+k-1)y^{\ell+k-2}$$

$$-(2\ell+2k+1)y^{\ell+k} + y^{\ell+k+2}]e^{-y^2/2}$$

We can now plug these into the radial equation.

$$\frac{d^2R}{dy^2} + \frac{2}{y}\frac{dR}{dy} - y^2R - \frac{\ell(\ell+1)}{y^2}R + \frac{2E}{\hbar\omega}R = 0$$

Each term will contain the exponential $e^{-y^2/2}$, so we can factor that out. We can also run a single sum over all the terms.

$$\sum_{k=0}^{\infty} a_k \left[(\ell+k)(\ell+k-1)y^{\ell+k-2} - (2\ell+2k+1)y^{\ell+k} + y^{\ell+k+2}\right.$$

$$\left. +2(\ell+k)y^{\ell+k-2} - 2y^{\ell+k} - y^{\ell+k+2} - \ell(\ell+1)y^{\ell+k-2} + \frac{2E}{\hbar\omega}y^{\ell+k}\right] = 0$$

The terms for large y which go like $y^{\ell+k+2}$ and some of the terms for small y which go like $y^{\ell+k-2}$ should cancel if we did our job right.

$$\sum_{k=0}^{\infty} a_k \left[[(\ell+k)(\ell+k-1) - \ell(\ell+1) + 2(\ell+k)] y^{\ell+k-2} + \left[\frac{2E}{\hbar\omega} - 2 - (2\ell+2k+1) \right] y^{\ell+k} \right] = 0$$

$$\sum_{k=0}^{\infty} a_k \left[[\ell(\ell-1) + k(2\ell+k-1) - \ell(\ell+1) + 2\ell + 2k] y^{\ell+k-2} + \left[\frac{2E}{\hbar\omega} - 2 - (2\ell+2k+1) \right] y^{\ell+k} \right] = 0$$

$$\sum_{k=0}^{\infty} a_k \left[[k(2\ell+k+1)] y^{\ell+k-2} + \left[\frac{2E}{\hbar\omega} - (2\ell+2k+3) \right] y^{\ell+k} \right] = 0$$

Now as usual, the coefficient for each power of y must be zero for this sum to be zero for all y. Before shifting terms, we must examine the first few terms of this sum to learn about conditions on a_0 and a_1. The first term in the sum runs the risk of giving us a power of y which cannot be canceled by the second term if $k < 2$. For $k = 0$, there is no problem because the term is zero. For $k = 1$ the term is $(2\ell+2)y^{\ell-1}$ which cannot be made zero unless

$$a_1 = 0.$$

This indicates that all the odd terms in the sum will be zero, as we will see from the recursion relation.

Now we will do the usual shift of the first term of the sum so that everything has a $y^{\ell+k}$ in it.

$$k \rightarrow k+2$$

$$\sum_{k=0}^{\infty}\left[a_{k+2}(k+2)(2\ell+k+3)y^{\ell+k}+a_k\left[\frac{2E}{\hbar\omega}-(2\ell+2k+3)\right]y^{\ell+k}\right]=0$$

$$a_{k+2}(k+2)(2\ell+k+3)+a_k\left[\frac{2E}{\hbar\omega}-(2\ell+2k+3)\right]=0$$

$$a_{k+2}(k+2)(2\ell+k+3)=-a_k\left[\frac{2E}{\hbar\omega}-(2\ell+2k+3)\right]$$

$$a_{k+2}=-\frac{\frac{2E}{\hbar\omega}-(2\ell+2k+3)}{(k+2)(2\ell+k+3)}a_k$$

For large k,

$$a_{k+2}\approx\frac{2}{k}a_k,$$

Which will cause the wave function to diverge. We must terminate the series for some $k=n_r=0,2,4...$, by requiring

$$\frac{2E}{\hbar\omega}-(2\ell+2n_r+3)=0$$

$$E=\left(n_r+\ell+\frac{3}{2}\right)\hbar\omega$$

These are the same energies as we found in Cartesian coordinates. Lets plug this back into the recursion relation.

$$a_{k+2}=-\frac{(2\ell+2n_r+3)-(2\ell+2k+3)}{(k+2)(2\ell+k+3)}a_k$$

$$a_{k+2}=\frac{2(k-n_r)}{(k+2)(2\ell+k+3)}a_k$$

To rewrite the series in terms of y^2 and let k take on every integer value, we make the substitutions $n_r \rightarrow 2n_r$ and $k \rightarrow 2k$ in the recursion relation for a_{k+1} in terms of a_k.

$a_{k+1} = \frac{(k-n_r)}{(k+1)(\ell+k+3/2)} a_k$
$R_{n_r\ell} = \sum_{k=0}^{\infty} a_k y^{\ell+2k} e^{-y^2/2}$
$E = \left(2n_r + \ell + \frac{3}{2}\right) \hbar\omega$

The table shows the quantum numbers for the states of each energy for our separation in spherical coordinates, and for separation in Cartesian coordinates. Remember that there are $2\ell + 1$ states with different z components of angular momentum for the spherical coordinate states.

E	$n_r\ell$	$n_x n_y n_z$	$N_{Spherical}$	$N_{Cartesian}$
$\frac{3}{2}\hbar\omega$	00	000	1	1
$\frac{5}{2}\hbar\omega$	01	001(3 perm)	3	3
$\frac{7}{2}\hbar\omega$	10, 02	002(3 perm), 011(3 perm)	6	6
$\frac{9}{2}\hbar\omega$	11, 03	003(3 perm), 210(6 perm), 111	10	10
$\frac{11}{2}\hbar\omega$	20, 12, 04	004(3), 310(6), 220(3), 211(3)	15	15

The number of states at each energy matches exactly. The parities of the states also match. Remember that the parity is $(-1)^\ell$ for the angular momentum states and that it is $(-1)^{n_x+n_y+n_z}$ for the Cartesian states. If we were more industrious, we could verify that the wavefunctions in spherical coordinates are just linear combinations of the solutions in Cartesian coordinates.

Next Up Previous Contents

Next: Operators Matrices and Spin **Up:** Quantum Physics 130 **Previous:** Sample Test Problems **Contents**

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