3.18 The Schrödinger Equation for the Isotropic 3D Harmonic Oscillator

After the solution of the 3D Schrödinger equation for the Coulomb potential, the next, equally important, if not more so, potential to tackle in 3D is that of the isotropic harmonic oscillator.

As before, we start with the Hamiltonian for a single particle in spherical coordinates:

$$H = \frac{\hbar^2}{2m} \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) \right) - \frac{\hbar^2}{2m} + \frac{1}{2} m \omega^2 r^2$$

and solve the corresponding eigenvalue problem

$$H \Psi = E \Psi$$

with solutions of the form

$$\langle r, \theta, \phi | \Psi \rangle = Y_{\ell \ell \ell \ell}(r, \theta, \phi) = R_{\ell \ell}(r) \ Y_{\ell \ell}(\theta, \phi)$$

The angular solutions remain unchanged and are still given by the spherical harmonics. We then want to concentrate on solving the radial equation for this problem:

$$\left[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) + \frac{2m}{\hbar^2} \left( E - \frac{1}{2} m \omega^2 r^2 - \frac{\hbar^2 \ell (\ell + 1)}{2m r^2} \right) \right] R_{\ell \ell}(r) = 0$$

We substitute $$R(r) = U(r)/r$$ and find again, as before

$$\frac{d^2 U}{dr^2} + \frac{2m}{\hbar^2} \left( E - \frac{1}{2} m \omega^2 r^2 - \frac{\hbar^2 \ell (\ell + 1)}{2m r^2} \right) U = 0 \quad (3.18.1)$$

Let us first examine the limiting cases for $$r$$:

For $$r \rightarrow 0$$

$$\frac{d^2 U}{dr^2} - \frac{\hbar^2 \ell (\ell + 1)}{r^2} \approx - \frac{1}{r^2}$$

negligible compared to $$\frac{1}{r^2}$$

$$U \propto r^{l+1}$$

$$\ell = \frac{\sqrt{2mE}}{\hbar}$$
For \( r \to \infty \), we have
\[
\frac{d^2U}{dr^2} = \left( \frac{m^2}{\hbar^2} \omega^2 r^2 - \alpha^2 \right) U
\]
which is just the 1D case, with solution of the form
\[
U(r) \propto A e^{-\alpha r^2} u(r)
\]
where \( u(r) \) is some polynomial in \( r \).

Let's try \( u(r) = 1 \), then
\[
U(r) = A e^{-\alpha r^2}
\]
and
\[
\frac{dU(r)}{dr} = -2\alpha r A e^{-\alpha r^2}
\]

\[
\frac{d^2U}{dr^2} = -2\alpha A e^{-\alpha r^2} + 4\alpha^2 r^2 A e^{-\alpha r^2}
\]

\[
= (4\alpha^2 r^2 - 2\alpha) U
\]

So, we make the identification

\[
4\alpha^2 = \frac{m^2 \omega^2}{\hbar^2} \quad \Rightarrow \quad \alpha = \frac{m \omega}{2\hbar}
\]

and
\[
2\alpha = \frac{m \omega}{\hbar} = \hbar^2 = 2\frac{\sqrt{E}}{\hbar^2} \quad \Rightarrow \quad E = \frac{1}{2} \hbar \omega
\]
Next, let's try \( u(r) = r \)

So, we have

\[
U(r) = A e^{-\alpha r^2}
\]

\[
\frac{dU}{dr} = A e^{-\alpha r^2} - 2\alpha r^2 A e^{-\alpha r^2}
\]

\[
\frac{d^2U}{dr^2} = -2\alpha A e^{-\alpha r^2} - 4\alpha r A e^{-\alpha r^2} + 4\alpha^2 r^3 A e^{-\alpha r^2}
\]

\[
= (4\alpha^2 r^2 - 6\alpha) r A e^{-\alpha r^2}
\]

\[
= (4\alpha^2 r^2 - 6\alpha) U
\]

As before,

\[
y\alpha^2 = \frac{m^2}{\hbar^2} \omega^2 \quad \Rightarrow \quad \alpha = \frac{m\omega}{2\hbar}
\]

but now,

\[
6\alpha = \frac{6m\omega}{2\hbar} = \hbar^2 = \frac{2mE}{\hbar^2} \Rightarrow \frac{3}{2} \hbar \omega
\]

\[
= (1 + \frac{1}{3}) \hbar \omega
\]

So, from all this, we postulate that \( U(r) \) can be written as

\[
U(r) = r^{\lambda + 1} e^{-\frac{m\omega}{2\hbar} r^2} U(r)
\]
If we use the following substitution, then eqn. 3.18.1 reduces to

\[ \rho = \sqrt{\frac{m \omega}{h}} \nu \]

\[
\frac{d}{dr} = \frac{dp}{dr} \frac{d}{dp} = \sqrt{\frac{m \omega}{h}} \frac{d}{dp}
\]

\[
\frac{d^2}{dr^2} = \frac{m \omega}{h} \frac{d}{dp}
\]

So,

\[
\frac{m \omega}{h} \frac{d^2 U}{dp^2} + \left( \frac{2mE}{h^2} - \frac{m^2 \omega^2}{h^2} - \frac{m \omega \rho^2}{h^2} - \frac{m^2 \omega^2}{h^2} \frac{b^2 \ell (\ell + 1)}{2m} \right) U = 0
\]

\[
\frac{d^2 U}{dp^2} + \left( \frac{2E}{h \omega} - \rho^2 - \frac{\ell (\ell + 1)}{\rho^2} \right) U = 0
\]

\[
\frac{d^2 U}{dp^2} + \left( \lambda - \rho^2 - \frac{\ell (\ell + 1)}{\rho^2} \right) U = 0 \quad \lambda = \frac{2E}{h \omega}
\]

we then use \( U(p) = \rho \ell + 1 e^{-\frac{\rho^2}{2}} \) as the solution. So we find

\[
\frac{dU}{dp} = (\ell + 1) \rho^2 e^{-\frac{\rho^2}{2}} U(p) - \rho e^2 e^{-\frac{\rho^2}{2}} U(p) + \rho e^2 e^{-\frac{\rho^2}{2}} U(p)
\]
and
\[
\frac{d^2u}{d\rho^2} = \ell(\ell+1)\rho^{\ell-1}e^{-\frac{\rho^2}{2}}u(\rho) - (\ell+1)\rho^{\ell+1}e^{-\frac{\rho^2}{2}}u(\rho) + \\
(\ell+1)\rho^le^{-\frac{\rho^2}{2}}u'(\rho) - (\ell+2)\rho^{\ell+1}e^{-\frac{\rho^2}{2}}u'(\rho) + \\
\rho^{\ell+3}e^{-\frac{\rho^2}{2}}u(\rho) - \rho^{\ell+2}e^{-\frac{\rho^2}{2}}u''(\rho) + \\
(\ell+1)\rho^le^{-\frac{\rho^2}{2}}u''(\rho) - \rho^{\ell+2}e^{-\frac{\rho^2}{2}}u''(\rho) + \rho^{\ell+1}e^{-\frac{\rho^2}{2}}u'(\rho)
\]
\[
= \rho^{\ell+1}e^{-\frac{\rho^2}{2}}u''(\rho) + \left(\frac{2(\ell+1)}{\rho} - 2\ell\right)\rho^{\ell+1}e^{-\frac{\rho^2}{2}}u'(\rho) + \\
\left(\frac{\ell(\ell+1)}{\rho^2} - (\ell+1) - (\ell+2) + \rho^2\right)\rho^{\ell+1}e^{-\frac{\rho^2}{2}}u(\rho)
\]

So, together with the rest of the radial equation, we have
\[
u''(\rho) + \left(\frac{2(\ell+1)}{\rho} - 2\ell\right)\nu'(\rho) + (\lambda - 2\ell - 3)\nu(\rho) = 0
\]

Now, use
\[
u(\rho) = \sum_{k=0}^{\infty} a_k \rho^k
\]
Then,
\[
u'(\rho) = \sum_{k=0}^{\infty} k a_k \rho^{k-1}
\]
\[
u''(\rho) = \sum_{k=0}^{\infty} k(k-1)a_k \rho^{k-2}
\]
So, we get
\[ \sum_{k=0}^{\infty} k(k-1) a_k \rho^{k-2} + \left( \frac{2(\ell+1)}{\rho} - 2\rho \right) \sum_{k=0}^{\infty} k a_k \rho^{k-1} + (\lambda - 2\ell - 3) \sum_{k=0}^{\infty} a_k \rho^k = 0 \]

Or,
\[ \sum_{k=0}^{\infty} k(k-1) a_k \rho^{k-2} + (2\ell+2) \sum_{k=0}^{\infty} k a_k \rho^{k-2} - 2 \sum_{k=0}^{\infty} k a_k \rho^k + (\lambda - 2\ell - 3) \sum_{k=0}^{\infty} a_k \rho^k = 0 \]

Now, in the first two terms we make the following replacement: \( k \rightarrow k+2 \)

Then,
\[ \sum_{k=-2}^{\infty} (k+1)(k+2) a_{k+2} \rho^k + (2\ell+2) \sum_{k=-2}^{\infty} (k+2) a_{k+2} \rho^k + (\lambda - 2\ell - 3 - 2k) \sum_{k=0}^{\infty} a_k \rho^k = 0 \]

Or,
\[ \sum_{k=0}^{\infty} (k+1)(k+2) a_{k+2} \rho^k + (2\ell+2) \sum_{k=-1}^{\infty} (k+2) a_{k+2} \rho^k + (\lambda - 2\ell - 3 - 2k) \sum_{k=0}^{\infty} a_k \rho^k = 0 \]
The only way for this equation to hold is to have both terms evaluate to zero separately, since there is no way to expand \( \rho^{-1} \) in a power series for all \( \rho \). So we must have

\[
(2\ell + 2) a_{\ell} \rho^{-1} = 0
\]

and

\[
\sum_{k=0}^{\infty} \left[ (k+2)(k+1) a_{k+2} + (2\ell+2)(k+2) a_{k+2} + (\lambda-2\ell-2\mu-3) a_k \right] \rho^k = 0
\]

Since \( \ell \) cannot be half integral and is never negative, the first condition leads to \( a_{\ell} = 0 \). While the second condition leads to the recursion relation

\[
a_{k+2} = \frac{2k+3 + 2\ell - \lambda}{(k+2)(k+1) + (2\ell+2)(k+2)} a_k
\]

Since \( a_{\ell} = 0 \), this leads to the conclusion that all coefficients corresponding to odd values of \( k \) are zero. We therefore have the following result for the radial equation:

\[
U(\rho) = \rho^{2\ell+1} e^{-\rho^2/2} \sum_{k=0}^{\infty} a_{2k} \rho^{2k}
\]

This function diverges for \( r \to \infty \) as \( \exp(\rho^2) \) unless the series is terminated at some point. So for some maximal \( k \), the coefficient \( a_{k+2} \) must be zero. This can be achieved if the following condition is satisfied:

\[
2k + 3 + 2\ell - \lambda = 0
\]
The quantized energy eigenvalues for the 3D isotropic harmonic oscillator are given by:

$$\frac{2E}{\hbar \omega} = 2\hbar + 2\ell + 3$$

$$E = \frac{1}{2} \hbar \omega (2\hbar + 2\ell + 3)$$

$$E_{n\ell} = \hbar \omega (n + \frac{3}{2}) \quad n = \hbar + \ell = 0, 1, 2, 3, \ldots$$

These are the quantized energy eigenvalues for the 3D isotropic harmonic oscillator. The corresponding eigenfunctions are:

$$\psi_{n\ell m}(r, \theta, \phi) = A r^\ell e^{-\frac{m\omega r^2}{2\hbar}} \psi(r) Y_{\ell m}(\theta, \phi)$$

Where the normalization constant $A$ is still to be determined.

Some examples:

**Ground state**, $n = 0$, $\ell = 0$, $\hbar = 0$

$$\psi(r) = 1$$

$$\psi_{000}(r, \theta, \phi) = A_0 e^{-\frac{m\omega r^2}{2\hbar}} \frac{1}{\sqrt{4\pi}}$$

$$= \frac{1}{\sqrt{4\pi}} \frac{2}{\sqrt{\hbar}} \left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}} e^{-\frac{m\omega r^2}{2\hbar}}$$
2) First excited state:

\[ n = 1, \ l = 1, \ m = 0 \quad (m \text{ must be even!}) \]

\[ \Psi_{11m}(v, \theta, \phi) = \sqrt{\frac{8}{3 \sqrt{\pi}}} \left( \frac{m \omega}{\hbar} \right)^{\frac{3}{4}} r e^{-\frac{m \omega^2}{2 \hbar} r^2} \gamma_{1m}(\theta, \phi) \]

3) Second excited state

\[ n = 2, \ l = 0, \ m = 2 \]

or \[ n = 2, \ l = 2, \ m = 0 \]

Case 1)

\[ a_2 = \frac{3 - \lambda}{6} a_0 = -\frac{4}{3} a_0 = -\frac{2}{3} a_0 \]

\[ \Upsilon(p) = a_0 + a_2 p^2 = a_0 + a_2 \frac{m \omega^2}{\hbar} r^2 \]

\[ = a_0 + \left( -\frac{2}{3} a_0 \right) \frac{m \omega^2}{\hbar} r^2 \]

\[ = a_0 \frac{2}{3} \left( \frac{3}{2} - \frac{m \omega^2}{\hbar} r^2 \right) \]

\[ \Psi_{200}(v, \theta, \phi) = \sqrt{\frac{8}{3 \sqrt{\pi}}} \left( \frac{m \omega}{\hbar} \right)^{\frac{3}{4}} \left( \frac{3}{2} - \frac{m \omega^2}{\hbar} r^2 \right)^{\frac{3}{4}} e^{-\frac{m \omega^2}{2 \hbar} r^2} \gamma_{00}(\theta, \phi) \]
The general solution is:

\[ \Psi_{nm}(r, \theta, \phi) = \left( \frac{m \omega}{\pi \hbar^2 (\hbar \Omega)^2} \right)^{3/4} e^{-\frac{m \omega}{2 \hbar^2} r^2} H_n \left( \frac{\sqrt{m \omega}}{\hbar} r \right) \times Y_{nm}(\theta, \phi) \]