We derive the spectrum for the 3D quantum harmonic oscillator.

Sakurai, Modern QM, p.211

We consider the radial Schrödinger equation, which can be derived using separation of variables in spherical coordinates:

$$-\frac{\hbar^2}{2m}u'' + \left(V(r) + \frac{\hbar^2}{2mr^2}l(l+1)\right)u = Eu$$

The Hamiltonian for the simple harmonic oscillator is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 r^2 .$$

We introduce dimensionless variables

$$E = \frac{1}{2}\hbar\omega\lambda \,, \quad r = \left[\frac{\hbar}{m\omega}\right]^{1/2}\rho \implies$$

$$\frac{d^2}{dr^2} = \frac{m\omega}{\hbar}\frac{d^2}{d\rho^2} \implies$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left(V(r) + \frac{\hbar^2}{2mr^2}l(l+1)\right)u(r) = Eu(r) \longrightarrow$$

$$-\frac{\hbar^{\cancel{2}}}{\cancel{2}\cancel{m}}\cdot\frac{\cancel{m}\omega}{\cancel{\hbar}}\frac{d^2u}{d\rho^2} + \left[2V(\rho) + \frac{\hbar^{\cancel{2}}}{\cancel{2}\cancel{m}}\frac{\cancel{m}\omega}{\cancel{\hbar}\rho^2}l(l+1)\right]u(\rho) = \frac{1}{\cancel{2}}\hbar\omega\lambda u(\rho)$$

$$\Rightarrow -\cancel{\hbar\omega}\, u''(\rho) + \left(\cancel{m\omega}^2 \frac{\cancel{\hbar}}{\cancel{m\omega}} \rho^2 + \frac{\hbar\omega\, l(l+1)}{\rho^2}\right) u(\rho) = \cancel{\hbar\omega}\, \lambda u(\rho)$$

$$\Rightarrow u''(\rho) + (\lambda - \rho^2) u(\rho) - \frac{l(l+1)}{\rho^2} u(\rho) = 0.$$

We will solve this by separately treating the behavior as $\rho \to 0$, $\rho \to \infty$, and connecting these two regimes using a series expansion.

Case 1: $\rho \to 0$

For $\rho \ll 1$, the differential equation can be approximated by

$$u''(\rho) \approx \frac{l(l+1)}{\rho^2} u(\rho)$$

which we can observe is solved by ρ^{l+1}.*

* ρ^{-l} is also a solution, but we can throw it away, at least in part because it is not normalizable.

Case 2: $\rho \to \infty$.

For $\rho \gg 1$, the equation can be approximated by

$$u''(\rho) \approx \rho^2 u(\rho)$$

which has the solutions $u(\rho) = e^{\pm \rho^2/2}$. So as to have a normalizable wavefunction, we choose the decaying solution.

Thus, our full radial wavefunction is $u(\rho)=\rho^{\ell+1}e^{-\rho^2/2}f(\rho)$. We plug into the radial Schrödinger equation:

$$u''(\rho)=\frac{d}{d\rho}\left[(\ell+1)\rho^{\ell}e^{-\rho^2/2}f(\rho)-\rho^{\ell+2}e^{-\rho^2/2}f(\rho)+\rho^{\ell+1}e^{-\rho^2/2}f'(\rho)\right]$$

$$=\ell(\ell+1)\rho^{\ell-1}e^{-\rho^2/2}f(\rho)-(\ell+1)\rho^{\ell+1}e^{-\rho^2/2}f(\rho)+(\ell+1)\rho^{\ell}e^{-\rho^2/2}f'(\rho)$$

$$-(\ell+2)\rho^{\ell+1}e^{-\rho^2/2}f(\rho)+\rho^{\ell+3}e^{-\rho^2/2}f(\rho)-\rho^{\ell+2}e^{-\rho^2/2}f'(\rho)+$$

$$(\ell+1)\rho^{\ell}e^{-\rho^2/2}f'(\rho)-\rho^{\ell+2}e^{-\rho^2/2}f'(\rho)+\rho^{\ell+1}e^{-\rho^2/2}f''(\rho)=$$

$$e^{-\rho^2/2}\rho^{\ell+1}\Big(f''(\rho)+f'(\rho)\left[\frac{(\ell+1)}{\rho}-\rho+\frac{(\ell+1)}{\rho}-\rho\right]$$

$$+f(\rho)\left[\frac{\ell(\ell+1)}{\rho^2}-(\ell+1)-(\ell+2)+\rho^2\right]\Big)=$$

$$e^{-\rho^2/2}\rho^{\ell+1}\left(f''(\rho)+2f'(\rho)\left(\frac{\ell+1}{\rho}-\rho\right)+f(\rho)\left(\frac{\ell(\ell+1)}{\rho^2}+\rho^2-2\ell-3\right)\right).$$

The full radial Schrödinger equation then reads

$$e^{-\rho^2/2}\rho^{\ell+1}\left(f''(\rho)+2f'(\rho)\left(\frac{\ell+1}{\rho}-\rho\right)+f(\rho)\left(\frac{\ell(\ell+1)}{\rho^2}+\rho^2-2\ell-3\right)\right)+$$

$$(\lambda-\rho^2)\rho^{\ell+1}e^{-\rho^2/2}f(\rho)-\frac{\ell(\ell+1)}{\rho^2}\rho^{\ell+1}e^{-\rho^2/2}f(\rho)=0 \iff$$

$$f''(\rho)+2f'(\rho)\left(\frac{\ell+1}{\rho}-\rho\right)+f(\rho)(\lambda-2\ell-3)=0.$$

We propose a power series solution for $f(\rho)$!

$$f(\rho)=\sum_n a_n\rho^n \implies$$

$$\sum_{n=0}^{\infty} n(n-1)a_n\rho^{n-2}+2na_n\rho^{n-1}\left(\frac{\ell+1}{\rho}-\rho\right)+a_n\rho^n(\lambda-2\ell-3)=$$

$$\sum_{n=0}^{\infty} n(n-1)a_n\rho^{n-2}+2na_n\rho^{n-2}(\ell+1)-2na_n\rho^n+a_n\rho^n(\lambda-2\ell-3)=$$

$$\frac{2a_1}{\rho}(\ell+1)+\sum_{n=0}^{\infty}(n+2)(n+1)a_{n+2}\rho^n+2(n+2)a_{n+2}\rho^n(\ell+1)-2na_n\rho^n+$$

$$a_n\rho^n(\lambda-2\ell-3)=\frac{2a_1}{\rho}(\ell+1)+$$

$$\sum_{n=0}^{\infty}\rho^n\left[(n+2)(n+1)a_{n+2}+2(n+2)(\ell+1)a_{n+2}+a_n(\lambda-2\ell-3-2n)\right]=0.$$

We set this to zero by powers of ρ: $a_1 = 0$. Also,

$$(n+2)(n+1+2(\ell+1))a_{n+2} + a_n(\lambda - 2\ell - 3 - 2n) = 0 \iff$$

$$a_{n+2} = \frac{2n+2\ell+3-\lambda}{(n+2)(n+2\ell+3)} a_n .$$

Since $a_1 = 0$, we conclude that $a_{2n+1} = 0$ for all n. We are left with even vales of n. To ensure that $f(\rho)$ remains finite at large ρ and large n, the series must terminate, implying that

$$2n+2\ell+3-\lambda = 0 \Rightarrow \lambda = 2n+2\ell+3 \Longrightarrow$$

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

$$= \hbar\omega(n+\ell+3/2) \equiv \boxed{\hbar\omega(N+3/2)}$$

Where we recognize that $n+\ell$ is the principal quantum number.