The final "touch" requires putting all together

$$\boxed{Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)}$$

where $\boxed{\Theta(\theta) = A P_l^m(\cos\theta)}$ and $\boxed{\Phi(\phi) = e^{im\phi}}$

with the "quantization" condition:

$$\boxed{l = 0,\ 1,\ 2, \ldots ; \quad m = -l,\ -l+1,\ \ldots,\ -1,\ 0,\ 1,\ \ldots,\ l-1,\ l}$$

We also need to normalize using $d^3\mathbf{r} = r^2 \sin\theta \, dr \, d\theta \, d\phi$

$$\int |\psi|^2 r^2 \sin\theta \, dr \, d\theta \, d\phi = \underbrace{\int |R|^2 r^2 \, dr}_{=1} \underbrace{\int |Y|^2 \sin\theta \, d\theta \, d\phi}_{=1} = 1$$

For the angular component this means:

$$\int_0^{2\pi}\int_0^{\pi} |Y|^2 \sin\theta \, d\theta \, d\phi = 1$$

By this procedure the famous **spherical harmonics** arise:

1 "s"

$$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$$

3 "p"

pz

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$

px, py

$$Y_1^{\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$$

5 "d"

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$$

$$Y_2^{\pm 1} = \mp\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{\pm i\phi}$$

$$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$$

7 "f"

$$Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$$

$$Y_3^{\pm 1} = \mp\left(\frac{21}{64\pi}\right)^{1/2} \sin\theta\,(5\cos^2\theta - 1) e^{\pm i\phi}$$

$$Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta\cos\theta e^{\pm 2i\phi}$$

$$Y_3^{\pm 3} = \mp\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta e^{\pm 3i\phi}$$

In a compact form:

$$\boxed{Y_l^m(\theta, \phi) = \epsilon \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}}\, e^{im\phi}\, P_l^m(\cos\theta)}$$

with $\epsilon = (-1)^m$ for $m \geq 0$ and $\epsilon = 1$ for $m \leq 0$

and the orthonormality condition

$$\boxed{\int_0^{2\pi} \int_0^{\pi} [Y_l^m(\theta, \phi)]^* [Y_{l'}^{m'}(\theta, \phi)] \sin\theta \, d\theta \, d\phi = \delta_{ll'} \delta_{mm'}}$$

"l" is the azimuthal quantum number (or angular momentum)
"m" is the magnetic quantum number (or z-axis projection of the angular momentum)

4.1.3: The Radial Equation

For the angular component we are DONE. But the radial portion depends on V(r).

Reminder:

$$\boxed{\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}[V(r)-E]R=l(l+1)R}$$

Before proceeding another redefinition! $\boxed{u(r) = r\,R(r)}$

$$dR/dr = d[u(r)/r]/dr = (1/r)du/dr - u/r^2$$

$$\boxed{d/dr[\, r^2 dR/dr] = r\, d^2u(r)/dr^2}$$

It is indeed a simplification!

The new radial equation becomes … (make sure you **do the math** to prove that this is correct; you have to multiply all by -ħ²/2mr)

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

Mathematically identical to a 1D problem (if u -> ψ) with an effective potential that includes a centrifugal term:

$$\boxed{V_{\text{eff}} = V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}}$$

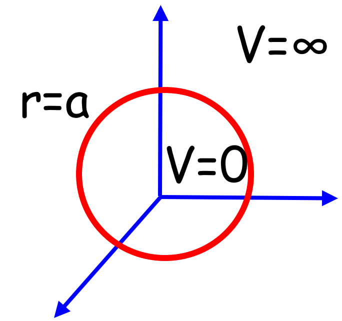
Normalization becomes

$$\boxed{\int_0^\infty |u|^2\, dr = 1}$$

[u(r) = r R(r)]

Example 4.1: infinite spherical well

$$V(r) = \begin{cases} 0, & \text{if } r \leq a. \\ \infty, & \text{if } r > a \end{cases}$$



(in HW9 you will solve the infinite cubic well)

Steps very similar to 1D. Same k etc., but with a centrifugal component

$$\frac{d^2u}{dr^2} = \left[\underbrace{\frac{l(l+1)}{r^2}}_{\text{Math diff between 1D and 3D radial}} - k^2\right]u \qquad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

If $l=0$, then it is the exact **same** Sch. Eq. of the 1D infinite square well! We know the general solution:

$$\frac{d^2u}{dr^2} = -k^2 u \;\Rightarrow\; u(r) = A\sin(kr) + B\cos(kr)$$

But the boundary conditions are different. On one hand, $u(r=a)=0$ as before. But $u(r=0)$ is just one point.

However, the true function we need is $R(r) = u(r)/r$.
Thus, we must choose $B=0$ to avoid a divergence at $r=0$
A nonzero "A" is ok because limit $x \to 0$ $\sin(x)/x = 1$.

Then, at "the end of the day" it is all the same as in 1D: $ka=n\pi$, with $n=1,2,3, \ldots$ i.e.

$$\boxed{E_{n0} = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

Now we have to put all together! In general:

$$\boxed{\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\,Y_l^m(\theta,\phi)}$$

$R_{nl}(r) = u_{nl}(r)/r$

$$Y_0^0(\theta,\phi) = 1/\sqrt{4\pi}$$

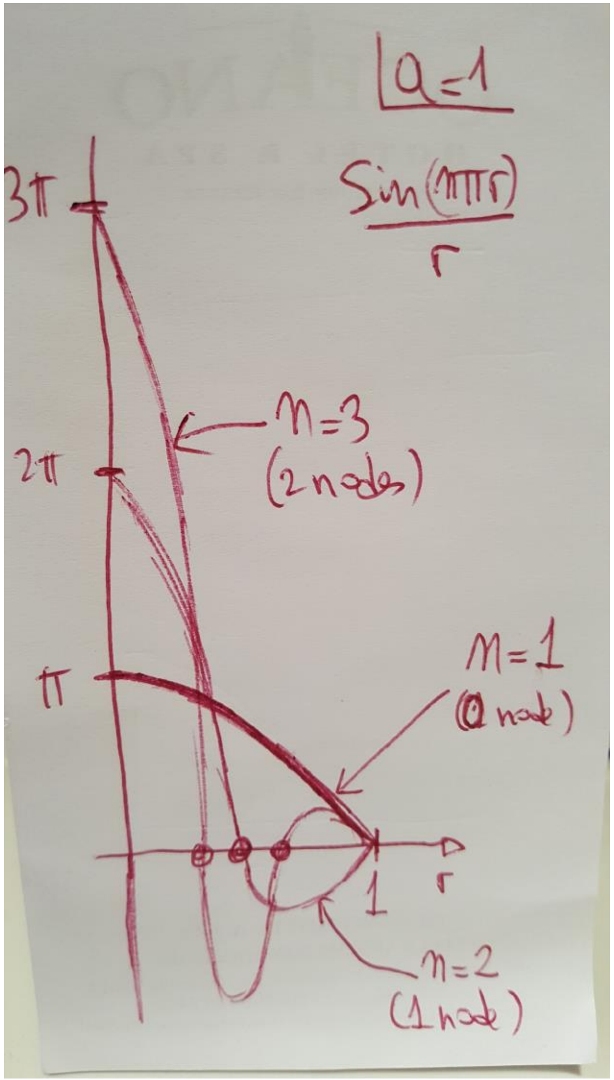
$u(r) = A\sin(kr)$ for l=0 with normalization $A = \sqrt{2/a}$

Then, the final answer for arbitrary n, l=0, m=0 is:

$$\boxed{\psi_{n00} = \frac{1}{\sqrt{2\pi a}}\frac{\sin(n\pi r/a)}{r}}$$

Common error: forgetting this r.

$$\boxed{\psi_{n00} = \frac{1}{\sqrt{2\pi a}} \frac{\sin(n\pi r/a)}{r}}$$



THIS PORTION IS FYI ONLY.

In general, for arbitrary "l" the solution is more complicated because of the centrifugal term.

$$u_{nl}(r) = Ar\, j_l(kr)$$

Spherical Bessel function of order "l" denoted as $j_l(x)$

$$R_{nl}(r) = A j_l(kr)$$

Boundary condition:

$$j_l(ka) = 0$$

$$\boxed{\begin{aligned} j_0 &= \frac{\sin x}{x} \\ j_1 &= \frac{\sin x}{x^2} - \frac{\cos x}{x} \\ j_2 &= \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x \end{aligned}}$$

k no longer "easy"

Do NOT worry about the **Spherical Neumann function** of order "l" denoted as $n_l(x)$. They diverge at r=0.

As x->0, converges to 1.
"s" wave is nonzero at r=0

$$j_0 = \frac{\sin x}{x}$$

As x->0,
converges to 0

$$j_1 = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

$$j_2 = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x$$