

How about the ground state wave function?

Remember:

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

$$R_{nl}(r) = \frac{1}{r} \rho^{l+1} e^{-\rho} v(\rho) \quad u(\rho) = \rho^{l+1} e^{-\rho} v(\rho) \quad \rho \equiv \kappa r$$

$n=1$ is the lowest energy (the most negative).
Since $n = j_{\max} + l + 1$, then $l=0, j_{\max}=0$. Then

$$\psi_{100}(r, \theta, \phi) = R_{10}(r) Y_0^0(\theta, \phi)$$

with $R_{10}(r) = \frac{c_0}{a} e^{-r/a}$ because
the polynomial has only a
constant c_0 .

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

We then **normalize**, which means we fix the value of c_0 :

$$\int_0^{\infty} |R_{10}|^2 r^2 dr = \frac{|c_0|^2}{a^2} \int_0^{\infty} e^{-2r/a} r^2 dr = |c_0|^2 \frac{a}{4} = 1$$

The very final result (celestial music ...) is:

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

which, amazingly, is remarkably **simple**.

Consider now the **excited states**, starting with $n=2$:

$$E_2 = \frac{-13.6 \text{ eV}}{4}$$

$$= -3.4 \text{ eV}$$

Because $n = j_{\max} + l + 1$, then $n=2$ allows for $l=0, j_{\max}=1$ or $l=1 (m=-1, 0, +1), j_{\max}=0$. This will be the 2s and three 2p's orbitals. **Degeneracy 4** (in general, degeneracy is n^2).

(1) If $l=0, j_{\max}=1$, then $c_{j_{\max}+1}=c_2=0$.

Use $c_1 = [2(j+l+1-n)/(j+1)(j+2l+2)] c_0$ with $n=2, j=0$ (because c_0 means $j=0$) and $l=0$, and you get $c_1 = -c_0$ so the polynomial becomes $\nu(\rho)=c_0(1-\rho)$ with c_0 again used to normalize.

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

$$R_{20}(r) = \frac{c_0}{2a} \left(1 - \frac{r}{2a}\right) e^{-r/2a}$$

The factors 2 arise from $\rho = (1/an)r$ with $n=2$.

(2) If $l=1, j_{\max}=0$, you get $c_{j_{\max}+1}=c_1=0$ so the polynomial is only c_0 as it happens in the ground state.

Use the general formula $R_{nl}(r) = \frac{1}{r} \rho^{l+1} e^{-\rho} v(\rho)$ with $l=1$ and $n=2$.

$$R_{21}(r) = \frac{c_0}{4a^2} r e^{-r/2a}$$

$$\rho = (1/2a)r \\ \text{with } n=2$$

The front factor comes from $\rho^2/r = (r/2a)^2/r$.

The spherical harmonics are:

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

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

In general, the polynomials $v(\rho)$ are called **associated Laguerre polynomials**

$$v(\rho) = L_{n-l-1}^{2l+1}(2\rho) \quad \rho = (1/na) r$$

and there are tables with these polynomials.

Putting all together, for arbitrary (n,l,m) the normalized wave functions are:

$$\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-r/na} \left(\frac{2r}{na}\right)^l \left[L_{n-l-1}^{2l+1}(2r/na) \right] Y_l^m(\theta, \phi)$$

$$R_{nl}(r)$$

$$R_{10} = 2a^{-3/2} \exp(-r/a)$$

$$R_{20} = \frac{1}{\sqrt{2}} a^{-3/2} \left(1 - \frac{1}{2} \frac{r}{a}\right) \exp(-r/2a)$$

$$R_{21} = \frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} \exp(-r/2a)$$

$$R_{30} = \frac{2}{\sqrt{27}} a^{-3/2} \left(1 - \frac{2}{3} \frac{r}{a} + \frac{2}{27} \left(\frac{r}{a}\right)^2\right) \exp(-r/3a)$$

$$R_{31} = \frac{8}{27\sqrt{6}} a^{-3/2} \left(1 - \frac{1}{6} \frac{r}{a}\right) \left(\frac{r}{a}\right) \exp(-r/3a)$$

$$R_{32} = \frac{4}{81\sqrt{30}} a^{-3/2} \left(\frac{r}{a}\right)^2 \exp(-r/3a)$$

$$R_{40} = \frac{1}{4} a^{-3/2} \left(1 - \frac{3}{4} \frac{r}{a} + \frac{1}{8} \left(\frac{r}{a}\right)^2 - \frac{1}{192} \left(\frac{r}{a}\right)^3\right) \exp(-r/4a)$$

$$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}} a^{-3/2} \left(1 - \frac{1}{4} \frac{r}{a} + \frac{1}{80} \left(\frac{r}{a}\right)^2\right) \frac{r}{a} \exp(-r/4a)$$

$$R_{42} = \frac{1}{64\sqrt{5}} a^{-3/2} \left(1 - \frac{1}{12} \frac{r}{a}\right) \left(\frac{r}{a}\right)^2 \exp(-r/4a)$$

$$R_{43} = \frac{1}{768\sqrt{35}} a^{-3/2} \left(\frac{r}{a}\right)^3 \exp(-r/4a)$$

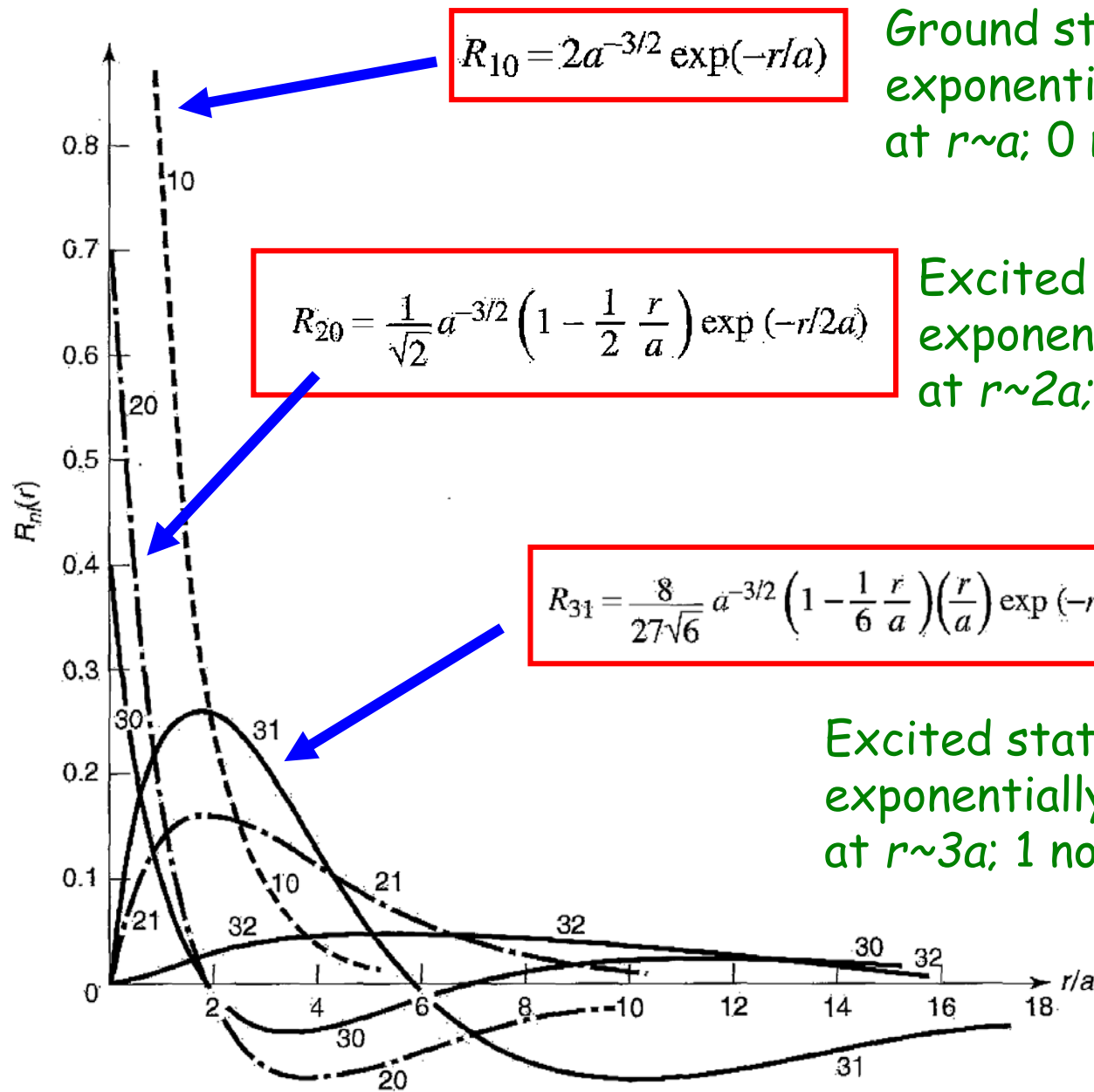
Only $l=0$ are nonzero at the center $r=0$, as in the spherical well.

3 nodes

2 nodes

1 nodes

0 nodes



$$R_{10} = 2a^{-3/2} \exp(-r/a)$$

Ground state $n=1$ $l=0$;
exponentially suppressed
at $r \sim a$; 0 node

$$R_{20} = \frac{1}{\sqrt{2}} a^{-3/2} \left(1 - \frac{1}{2} \frac{r}{a}\right) \exp(-r/2a)$$

Excited state $n=2$ $l=0$;
exponentially suppressed
at $r \sim 2a$; 1 node.

$$R_{31} = \frac{8}{27\sqrt{6}} a^{-3/2} \left(1 - \frac{1}{6} \frac{r}{a}\right) \left(\frac{r}{a}\right) \exp(-r/3a)$$

Excited state $n=3$ $l=1$;
exponentially suppressed
at $r \sim 3a$; 1 node.

