

Let's try a model for the Hydrogen Atom

Assume you have a charge distribution given by:  
a point charge  $q$  at  $r=0$  and

$$\rho_0 e^{-\frac{r^2}{a^2}}$$

for  $r > a$ .

The overall charge is zero, so you'll need to fix this. We require:

$$+q + 4\pi \int_{r=a}^{\infty} \rho_0 e^{-\frac{r^2}{a^2}} (r^2 dr) = 0$$

We require:

$$\rho_0 = -\frac{q}{4\pi \int_{r=a}^{\infty} e^{-\frac{r^2}{a^2}} r^2 dr} \Rightarrow \rho_0 = -\frac{q}{4\pi a^3 \int_{\eta=1}^{\infty} e^{-\eta^2} \eta^2 d\eta}$$

This is an integral which can be done in terms of the error function.

At our favorite site, enter:

$$x^2 \text{Exp}[-x^2]$$

The result is:

$$-\frac{1}{2} x e^{-x^2} + \frac{1}{4} \sqrt{\pi} \text{Erf}[x]$$

For our integral, the result is:

$$-\frac{1}{2} \eta e^{-\eta^2} + \frac{1}{4} \sqrt{\pi} \text{Erf}[\eta] \Big|_1^{\infty} = \frac{\sqrt{\pi}}{4} + \frac{e^{-1}}{2} - \frac{\sqrt{\pi}}{4} \text{Erf}[1]$$

The error function of (1) is on the order of  $\frac{1}{2}$ . Look at:

<http://mathworld.wolfram.com/Erf.html>

Now we can find the potential from this:

$$V(\vec{r}_p) = \int_{r=a}^{r=\infty} \int_{\theta=0}^{\theta=\pi} k\rho_0 \frac{e^{-\frac{r^2}{a^2}}}{|\vec{r}-z_p\hat{z}|} r^2 dr + \frac{kq}{r_p}$$

I think it's pretty clear now what to do ... we had:

$$V(\vec{r}_p) = 2\pi \int_{r=a}^{r=\infty} \int_{\theta=0}^{\theta=\pi} k\rho_0 \frac{e^{-\frac{r^2}{a^2}}}{\sqrt{x^2+y^2+(z_p-z)^2}} r^2 \sin(\theta) dr d\theta + \frac{kq}{r_p}$$

$$V_1(\vec{r}_p) = 2\pi \int_{r=a}^{r=\infty} \int_{\theta=0}^{\theta=\pi} k\rho_0 \frac{e^{-\frac{r^2}{a^2}}}{\sqrt{x^2+y^2+(z_p-z)^2}} r^2 \sin(\theta) dr d\theta$$

$$V_1(\vec{r}_p) = 2\pi \int_{r=a}^{r=\infty} \int_{\theta=0}^{\theta=\pi} k\rho_0 \frac{e^{-\frac{r^2}{a^2}}}{\sqrt{x^2+y^2+z^2-2zz_p+z_p^2}} r^2 \sin(\theta) dr d\theta$$

$$V_1(\vec{r}_p) = k\rho_0 2\pi \int_{r=a}^{r=\infty} \int_{\theta=0}^{\theta=\pi} \frac{e^{-\frac{r^2}{a^2}}}{\sqrt{r^2-2rz_p \cos(\theta)+z_p^2}} r^2 \sin(\theta) dr d\theta$$

let

$$x = 2rz_p \cos(\theta) : dx = -2rz_p \sin(\theta) d\theta : \theta = 0 \Rightarrow x = 2rz_p : \theta = \pi \Rightarrow x = -2rz_p$$

$$V_1(\vec{r}_p) = -\frac{k\rho_0\pi}{z_p} \int_{r=a}^{r=\infty} \int_{x=2rz_p}^{x=-2rz_p} \frac{e^{-\frac{r^2}{a^2}}}{\sqrt{r^2-x+z_p^2}} r dr dx$$

at our favorite site, enter:  $(b-x)^{-1/2}$

then,

$$V_1(\vec{r}_p) = 2 \frac{k\rho_0\pi}{z_p} \int_{r=a}^{r=\infty} e^{-\frac{r^2}{a^2}} \sqrt{r^2-x+z_p^2} \Big|_{x=2rz_p}^{x=-2rz_p} r dr$$

$$V_1(\vec{r}_p) = 2 \frac{k\rho_0\pi}{z_p} \int_{r=a}^{r=\infty} e^{-\frac{r^2}{a^2}} \left[ \sqrt{r^2+2rz_p+z_p^2} - \sqrt{r^2-2rz_p+z_p^2} \right] r dr$$

$$V_1(\vec{r}_p) = 2 \frac{k\rho_0\pi}{z_p} \int_{r=a}^{r=\infty} e^{-\frac{r^2}{a^2}} \left[ (r+z_p) - \begin{cases} (r-z_p) & \text{if } r > z_p \\ (z_p-r) & \text{if } r < z_p \end{cases} \right] r dr$$

$$V_1(\vec{r}_p) = 2 \frac{k\rho_0\pi}{z_p} \int_{r=a}^{r=\infty} e^{-\frac{r^2}{a^2}} \left[ (r+z_p) - \begin{cases} (r-z_p) & \text{if } r > z_p \\ (z_p-r) & \text{if } r < z_p \end{cases} \right] r dr$$

This integral has got to be broken into 2 parts then, since in the interval both conditions are true.

Thus:

$$V_1(\vec{r}_p) = 2 \frac{k\rho_0\pi}{z_p} \int_{r=a}^{r=z_p} e^{-\frac{r^2}{a^2}} \left[ (r + z_p) - (z_p - r) \right] r dr + 2 \frac{k\rho_0\pi}{z_p} \int_{r=z_p}^{r=\infty} e^{-\frac{r^2}{a^2}} \left[ (r + z_p) - (r - z_p) \right] r dr$$

$$V_1(\vec{r}_p) = 4 \frac{k\rho_0\pi}{z_p} \int_{r=a}^{r=z_p} e^{-\frac{r^2}{a^2}} r^2 dr + 4 \frac{k\rho_0\pi}{z_p} \int_{r=z_p}^{r=\infty} e^{-\frac{r^2}{a^2}} z_p r dr$$

These integrals can be simplified somewhat by a scale factor:

$$\eta = \frac{r}{a} \Rightarrow a d\eta = dr : r = z_p \Rightarrow \eta = \frac{z_p}{a} : r = a \Rightarrow \eta = 1 : r = \infty \Rightarrow \eta = \infty$$

$$V_1(\vec{r}_p) = 4 \frac{k\rho_0\pi}{z_p} \int_{\eta=1}^{\eta=\frac{z_p}{a}} e^{-\eta^2} a^3 \eta^2 d\eta + 4 \frac{k\rho_0\pi}{z_p} \int_{\eta=\frac{z_p}{a}}^{\eta=\infty} e^{-\eta^2} z_p a^2 \eta d\eta$$

$$V_1(\vec{r}_p) = 4\pi a^3 \frac{k\rho_0}{z_p} \int_{\eta=1}^{\eta=\frac{z_p}{a}} e^{-\eta^2} \eta^2 d\eta + 4\pi a^2 k\rho_0 \int_{\eta=\frac{z_p}{a}}^{\eta=\infty} e^{-\eta^2} \eta d\eta$$

The second integral is straight-forward:

enter x (E<sup>-x<sup>2</sup></sup>) at our favorite site

$$\int_{\eta=\frac{z_p}{a}}^{\eta=\infty} e^{-\eta^2} \eta d\eta = -\frac{e^{-\eta^2}}{2} \Big|_{\eta=\frac{z_p}{a}}^{\eta=\infty} = -\frac{1}{2} \left[ 0 - e^{-\frac{z_p^2}{a^2}} \right] = \frac{1}{2} e^{-\frac{z_p^2}{a^2}}$$

The first integral is also not all that bad:

$$\int_{\eta=1}^{\eta=\frac{z_p}{a}} e^{-\frac{\eta^2}{a^2}} \eta^2 d\eta = -\eta \frac{e^{-\eta^2}}{2} + \frac{\sqrt{\pi}}{4} \text{Erf}[\eta] \Big|_{\eta=1}^{\eta=\frac{z_p}{a}}$$

$$\int_{\eta=1}^{\eta=\frac{z_p}{a}} e^{-\frac{r^2}{a^2}} \eta^2 d\eta = -\frac{z_p}{a} \frac{e^{-\frac{z_p^2}{a^2}}}{2} + \frac{\sqrt{\pi}}{4} \operatorname{Erf} \left[ \frac{z_p}{a} \right] + \frac{e^{-1}}{2} - \frac{\sqrt{\pi}}{4} \operatorname{Erf} [1]$$

We thus have the potential  $V_1$ :

$$V_1 = 4\pi a^2 k \rho_0 \frac{1}{2} e^{-\frac{z_p^2}{a^2}} + 4\pi a^3 \frac{k \rho_0}{z_p} \left[ -\frac{z_p}{a} \frac{e^{-\frac{z_p^2}{a^2}}}{2} + \frac{\sqrt{\pi}}{4} \operatorname{Erf} \left[ \frac{z_p}{a} \right] + \frac{e^{-1}}{2} - \frac{\sqrt{\pi}}{4} \operatorname{Erf} [1] \right]$$

$$V_1 = 4\pi a^3 \frac{k \rho_0}{z_p} \left[ \frac{\sqrt{\pi}}{4} \left( \operatorname{Erf} \left[ \frac{z_p}{a} \right] - \operatorname{Erf} [1] \right) + \frac{e^{-1}}{2} \right]$$

Finally, let's add onto this the potential of the positive charge located at the origin:

$$V = \frac{kq}{z_p} + 4\pi a^3 \frac{k \rho_0}{z_p} \left[ \frac{\sqrt{\pi}}{4} \left( \operatorname{Erf} \left[ \frac{z_p}{a} \right] - \operatorname{Erf} [1] \right) + \frac{e^{-1}}{2} \right]$$

Let's now realize spherical symmetry to obtain:

$$V(\vec{r}_p) = \frac{kq}{r_p} + 4\pi a^3 \frac{k \rho_0}{r_p} \left[ \frac{\sqrt{\pi}}{4} \left( \operatorname{Erf} \left[ \frac{r_p}{a} \right] - \operatorname{Erf} [1] \right) + \frac{e^{-1}}{2} \right]$$

This form is valid so long as  $r_p > a$ . You'll need to do more calculations if you go inside the radius  $a$ .

Oh ... remember also that

$$\rho_0 = - \frac{q}{4\pi a^3 \int_{\eta=1}^{\infty} e^{-\eta^2} \eta^2 d\eta}$$

If you let  $I_1 \approx \int_{\eta=1}^{\infty} e^{-\eta^2} \eta^2 d\eta$

Then

$$\rho_0 = - \frac{q}{4\pi a^3 I_1}$$

and the potential would appear as:

$$V(\vec{r}_p) = \frac{kq}{r_p} \left[ 1 - \frac{1}{I_1} \left[ \frac{\sqrt{\pi}}{4} \left( \operatorname{Erf} \left[ \frac{r_p}{a} \right] - \operatorname{Erf} [1] \right) + \frac{e^{-1}}{2} \right] \right]$$