A simple numerical solution of the Schrödinger Equation

Spreadsheets provide a nice way to solve the dimensionless S.E. in radial coord:

$$\left\{-\frac{d^2}{d\rho^2}+\frac{\ell(\ell+1)}{\rho^2}+\mathrm{sgn}(s)\,\rho^s\right\}U_{\varepsilon\ell}(\rho)=\varepsilon\, U_{\varepsilon\ell}(\rho)$$

relation to "dimensioned": $r = a\times\rho$ $\quad a=\left(\frac{\hbar^2}{2\mu|V_0|}\right)^{1/s+2}$

$\varepsilon = E/E_0$, $E_0 = |V_0|\left(\frac{\hbar^2}{2\mu|V_0|}\right)^{\frac{s}{s+2}}$, $V(r)=V_0 r^s$ $\quad \mu=$ mass

Start off with $\ell = 0$

Then, rearranging above,

$$U''_{\varepsilon 0}(\rho) = -(\varepsilon - \mathrm{sgn}(s)\rho^s)\,U_{\varepsilon 0}(\rho)$$

change notation: $\psi(\rho)\equiv U_{\varepsilon 0}(\rho)$

then $\psi''(\rho) = -(\varepsilon - \mathrm{sgn}(s)\rho^s)\,\psi(\rho)$ $\quad (*)$

which is a straightforward second-order differential equation. Given ψ and ψ' at some point, it is straightforward to integrate the above equation, WHEN ε IS KNOWN.

The simple numerical technique I present entails guessing an ε, then integrating ψ using $(*)$ to large ρ. When ψ nicely goes to zero at large ρ, then ε is appropriate for a bound state.

Why does ψ going to 0 as $\rho \to \infty$ mean that ε is appropriate for a bound state? If ψ does not go to 0, it will diverge as $\propto e^{+k\rho}$ and all the probability will be infinitely far away. There is no chance of finding the particle in the potential.

Let's pick $\rho = 0$ as the point from which we begin to integrate.

as $\rho \to 0$, $\psi(\rho) \to \rho^{\ell+1}$; with $\ell = 0$, $\psi(\rho) \to$

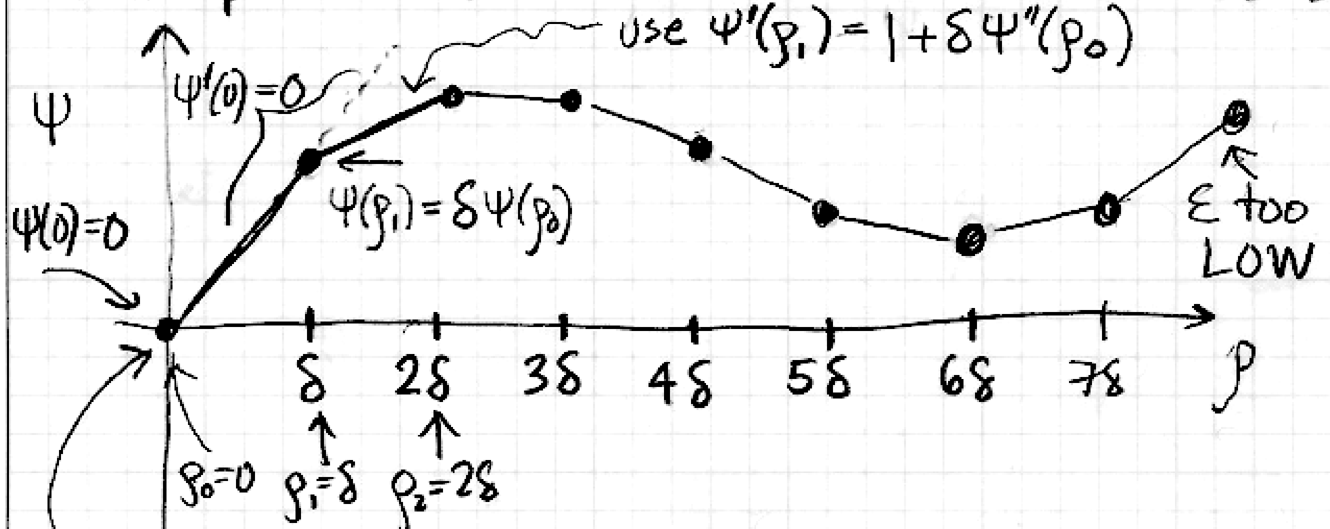
$\psi'(\rho) \to \underline{1}$ ... really a <u>constant</u>, since normalization can be adjusted

$$\psi''(\rho) \to -(\varepsilon - \mathrm{sgn}(s)\, 0^s)\,\psi(0)$$

< 0 for all s

$\to$ finite when $s \geq -1$

Concept of the numerical solution is:



$\psi''(0) < 0$, can be computed by a <u>guess</u> of ε

Spreadsheet "power.xls" available on the course web page.

At top, you can input:

ε → energy guess

R → "scaled" maximum radius. Set up so $R=1.0$ will usually give good results. To see more of small radius, try $R<1.0$, like $R=0.25$; to go to larger radius, try $R>1.0$ like $R=3.0$.

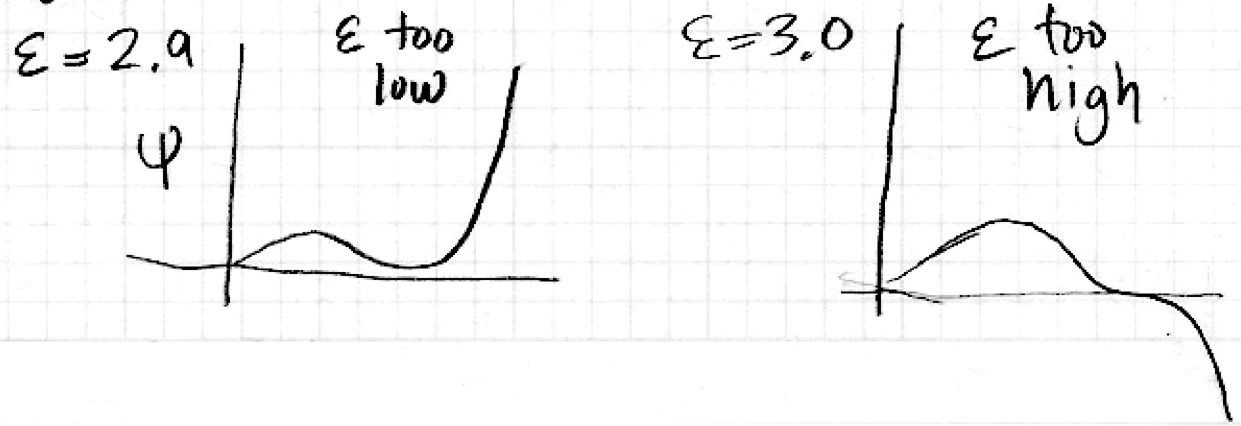
s → power

δ → DON'T enter this in most cases, unless you are exploring on your own; leave alone. The value is there for display.

$\psi(0)$; $\psi'(0)$ → you <u>can</u> input them

Beneath these values is the integration. Two plots are displaced; $\psi(\rho)$ on top; $V(\rho)$ below.

To warm up, try $s=2$ (S.H.O.) and notice:



But you know already the energies for the S.H.O.

$$E = (n+\tfrac{1}{2})\hbar\omega \quad \text{in one dimension}$$

In 3-d, $\psi(0) = 0$, which selects only the <u>odd</u> values of n. Or, $n = 2m+1$

$$E = (2m+\tfrac{3}{2})\hbar\omega \quad m = 0, 1, 2, \ldots$$

From dimensionless SE,

$$E_0 = |V_0| \left(\frac{\hbar^2}{2\mu |V_0|}\right)^{s/s+2} \qquad V(r) = \tfrac{1}{2}kr^2 \quad \text{so } V_0 = \tfrac{1}{2}k$$

$$= \tfrac{1}{2}k \left(\frac{\hbar^2}{2\mu \times \frac{1}{2}k}\right)^{\frac{2}{4}} = \tfrac{1}{2}\hbar\sqrt{\frac{k}{m}}$$

$$E_0 = \tfrac{1}{2}\hbar\omega$$

so,
$$\varepsilon = \frac{E}{E_0} = \frac{(2m+\frac{3}{2})\hbar\omega}{\frac{1}{2}\hbar\omega} = (4m+3)$$

$$\boxed{\begin{aligned}\varepsilon &= (4m+3) \quad m = 0, 1, 2, \ldots \\ &= 3, 7, 11, \ldots\end{aligned}}$$

Some pointers:
- $-2 \leq s \leq -1$ is a bit unstable. (on the spreadsheet)
- changing R <u>does</u> slightly influence results for ε
- $\ell > 0$?? Technique must be adapted... take $\psi(\rho) = \rho^{\ell+1} \times \phi(\rho)$, and get equation for $\underline{\underline{\phi}}$ to integrate.
- could use "arbitrary" potential.

Hydrogenic atom (+Z charge at center)

in dimensionless form:

$$\left\{-\frac{d^2}{d\rho^2}+\frac{l(l+1)}{\rho^2}-\frac{1}{\rho}\right\}U_{\varepsilon l}(\rho)=\varepsilon U_{\varepsilon l}(\rho)$$

$$|V_0|=Ze^2 \qquad a=\frac{\hbar^2}{2\mu Ze^2}=\frac{1}{2Z}a_0 \quad \left(a_0=\frac{\hbar^2}{me^2} = \text{Bohr Radius}\right)$$

$$\rho=\frac{r}{a} \qquad E_0=|V_0|\left(\frac{\hbar^2}{2\mu|V_0|}\right)^{\frac{-1}{1}}=\frac{2\mu}{\hbar^2}|V_0|^2=2Z^2\left(\frac{e^2}{\hbar c}\right)^2\mu c^2$$

The constant $\frac{e^2}{\hbar c}\equiv\alpha$ is known as the fine structure constant, and has the value $\alpha\cong 1/137$. This constant is dimensionless, and characterizes the strength of electromagnetism.

The traditional solution of the hydrogenic atom uses a slightly different length scale

$$\tilde{a}=2a=\frac{\hbar^2}{\mu Ze^2}=\frac{1}{Z}a_0 \qquad \tilde{E}_0=\frac{1}{4}E_0=\frac{1}{2}Z^2\alpha^2\mu c^2$$

$$\tilde{\rho}=\frac{r}{\tilde{a}}=\frac{r}{2a}=\frac{1}{2}\rho \quad \text{so} \quad \rho=2\tilde{\rho}$$

Plugging into the dimensionless Schrödinger equation, with $\rho=\tilde{\rho}/2$

$$\left\{\frac{-d^2}{d(2\tilde{\rho})^2}+\frac{l(l+1)}{(2\tilde{\rho})^2}-\frac{1}{2\tilde{\rho}}\right\}U_{\varepsilon l}(\tilde{\rho})=\left(\frac{E}{E_0}\right)U_{\varepsilon l}(\tilde{\rho})$$

or

$$\left\{-\frac{d^2}{d\tilde{\rho}^2}+\frac{l(l+1)}{\tilde{\rho}^2}-\frac{2}{\tilde{\rho}}\right\}U_{\varepsilon l}(\tilde{\rho})=4\left(\frac{E}{E_0}\right)U_{\varepsilon l}(\tilde{\rho})$$

$$=\frac{E}{\tilde{E}_0}U_{\varepsilon l}(\tilde{\rho})$$

$$\boxed{\left\{-\frac{d^2}{d\tilde{\rho}^2}+\frac{l(l+1)}{\tilde{\rho}^2}-\frac{2}{\tilde{\rho}}\right\}U_{\tilde{\varepsilon} l}(\tilde{\rho})=\tilde{\varepsilon}U_{\tilde{\varepsilon} l}(\tilde{\rho})}$$