1 Introduction

In this assignment, we are aiming to solve the radial part of the Schrödinger equation

$$\left(-\frac{1}{2\mu}\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{2\mu r^2}+V(r)\right)u_{n_r\ell}(r)=E_{n_r\ell}u_{n_r\ell}(r) \tag{1}$$

numerically for an arbtrary confining potential $V(r)$. In particular, we would like to obtain the bound state wavefunctions and the energy eigenvalues $E_{n_r\ell}$.

Since

$$u_{n_r\ell}(r)=rR_{n_r\ell}(r) \tag{2}$$

the boundary conditions for bound state solutions are

$$\begin{aligned}\lim_{r\to 0}u_{n_r\ell}(r)&=0\\ \lim_{r\to\infty}u_{n_r\ell}(r)&=0\end{aligned} \tag{3}$$

We will assume that as $r\to 0$, the potential $V(r)$ is no more singular than $1/r$. In this assignment, we will solve this problem in two different ways.

2 The Shooting Method

To put Eq.(1) on a computer, it is convenient to scale the variables so that we deal with only dimensionless variables. If we know an approximate size of the energy eigenvalues, $E_a>0$, then the best way to scale the radial coordinate r is

$$x=kr \tag{4}$$

where $k=\sqrt{2\mu E_a}$. The resulting equation is

$$\left(-\frac{d^2}{dx^2}+\frac{\ell(\ell+1)}{x^2}+\tilde{V}(x)+\tilde{E}_{n_r\ell}\right)\tilde{u}_{n_r\ell}(x)=0 \tag{5}$$

where $\tilde{u}_{n_r\ell}(x)=u_{n_r\ell}(x/k)$, $\tilde{V}(x)=V(x/k)/E_a$ and $\tilde{E}_{n_r\ell}=|E_{n_r\ell}|/E_a$. Here we used the fact that for a bound state, $E_{n_r\ell}=-|E_{n_r\ell}|$. The boundary conditions for bound state solutions are

$$\begin{aligned}\lim_{x\to 0}\tilde{u}_{n_r\ell}(x)&=0\\ \lim_{x\to\infty}\tilde{u}_{n_r\ell}(x)&=0\end{aligned} \tag{6}$$

The strategy to solve for a bound state is as follows. This relies on the fact that the wavefunction and its derivative must be continuous everywhere.

1. Choose a value for $\tilde{E}_{n_r\ell}$.
2. Solve the differential equation forward from $x = 0$. Call this solution $\tilde{u}_I(x)$. The boundary condition is $\tilde{u}_I(0) = 0$.
3. Solve the differential equation backward from $x = x_{\max}$. Call this solution $\tilde{u}_{II}(x)$. The boundary condition is $\tilde{u}_{II}(x_{\max}) = \epsilon$ where $x_{\max}$ is sufficiently large and ϵ is sufficiently small.
4. At some chosen point x_b, compare $u'_I(x_b)/u_I(x_b)$ and $u'_{II}(x_b)/u_{II}(x_b)$. If they are not the same, choose a different $\tilde{E}_{n_r,\ell}$ and go back to 2 and repeat the process until convergence is achieved within a set tolerance.

Idea is simple. Implementation not so simple. Let's discuss them one by one in more detail.

Determining E_a
First, let's see how we can determine a typical energy scale E_a. For this, of course, one needs to know how the effective potential

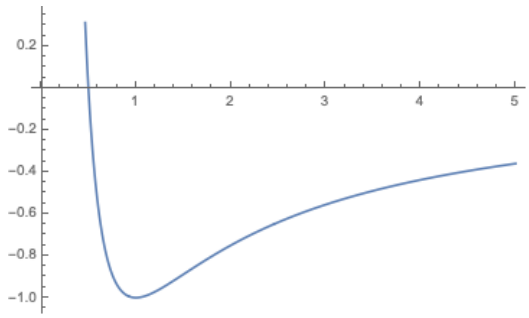
$$V_{\text{eff},\ell}(r) = \frac{\ell(\ell+1)}{2\mu r^2} + V(r) \tag{7}$$

behaves.

To be concrete, let's take a Coulomb-like potential $V(r) = -\alpha/r$. One may think that at this point we should distinguish whether ℓ is zero or not. But that is not the case. This is because there is the Kinetic energy term in the Hamiltonian, $\hat{H}_K = -(1/2\mu)d^2/dr^2$. The result of operating this operator on a smooth wavefunction is roughly the same size as multiplying the centrifugal potential term to the wavefunction. Hence, to get the rough estimate of the energy scale, it is sufficient to set $\ell(\ell+1) = 1$ so that the function we would like to consider is

$$V_{\text{eff}}(r) = \frac{1}{2\mu r^2} + V(r) \tag{8}$$

This roughly has the following shape (arbitrary unit)



If this was a classical mechanics problem, we know how to get the classical ground state energy: We take the value of $V_{\text{eff}}(r)$ at the minimum. To get that we solve

$$V'_{\text{eff}}(r) = -\frac{1}{\mu r^3} + \frac{\alpha}{r^2} = 0 \tag{9}$$

which gives

$$r_{\text{min}} = \frac{1}{\mu\alpha} \tag{10}$$

and

$$V_{\text{eff}}(r_{\text{min}}) = \frac{1}{\mu}\frac{\mu^2\alpha^2}{2} - \alpha\mu\alpha = -\frac{\mu\alpha^2}{2} \tag{11}$$

This should be a good estimate. For example, if we are really solving the Hydrogen atom problem, the ground state energy is known to be

$$E_{\text{hydrogen}} = -\frac{\mu\alpha_{\text{EM}}^2}{2} \tag{12}$$

The nuclear potentials we will consider are the Hulthen potential

$$V_{\text{Hulthen}}(r) = -V_0\frac{e^{-r/a}}{1-e^{-r/a}} \tag{13}$$

which behaves like $-1/r$ near $r = 0$, and the Woods-Saxon potential

$$V_{\text{WS}}(r) = -\frac{V_0}{1+e^{(r-R)/a}} \tag{14}$$

which is regular at $r = 0$. Analytic solutions for the minimum for these potentials are, unfortunately, not available. Therefore, we will need a numerical method to find the minimum of a function. Or in general, we need a numerical method or two to solve $f(x) = 0$.