

Function stored in memory:

$F(\Psi(x), x \in [0, x_e]; \Psi'(x), x \in [0, x_e]; a, b$ for $\Psi(x) = xAi((\frac{2m\sigma}{\hbar^2})^{\frac{1}{3}}(x - \frac{E}{\sigma}))$, $x \in [x_e, \infty)$
 $F()$, $x \in [0, x_e]$ is tabulated at points to be determined. Adaptive shooting methods are at the very least useful for determining good tabulation/mesh points.

Relaxation method:

$$\begin{aligned} \frac{dy}{dx} &= g(x, y) \Rightarrow dy - dx \times g(x, y) = 0 \\ y_k - y_{k-1} - (x_k - x_{k-1})g(\frac{1}{2}(x_k + x_{k-1}), \frac{1}{2}(y_k + y_{k-1})) &= 0 \\ \vec{E}_k(\vec{y}_k, \vec{y}_{k-1}) &\equiv \vec{y}_k - \vec{y}_{k-1} - (x_k - x_{k-1})\vec{g}(\frac{1}{2}(x_k + x_{k-1}), \frac{1}{2}(\vec{y}_k + \vec{y}_{k-1})) = 0 \quad k = 1, 2, \dots, M-1 \\ \vec{E}_k(\vec{y}_k + \Delta\vec{y}_k, \vec{y}_{k-1} + \Delta\vec{y}_{k-1}) &\approx \vec{E}_k(\vec{y}_k, \vec{y}_{k-1}) + \sum_n \frac{\partial E_k}{\partial y_{n,k-1}} \Delta y_{n,k-1} + \sum_n \frac{\partial E_k}{\partial y_{n,k}} \Delta y_{n,k} \\ \vec{E}_0 &= \vec{B}(x_0, y_0) = 0 \\ \vec{E}_M &= \vec{C}(x_{k-1}, y_{k-1}) = 0 \\ -\frac{\hbar^2}{2m} \frac{d^2\Psi}{dr^2} - \frac{\hbar^2}{2mr} \frac{d\Psi}{dr} + (V(r) - E)\Psi &= 0 \\ \frac{d^2\Psi}{dr^2} + \frac{2}{r} \frac{d\Psi}{dr} + \frac{2m(E-V(r))}{\hbar^2} \Psi &= 0 \\ y_0 = \Psi &\Rightarrow y'_0 = y_1 = g_0 \\ y_1 = \Psi' &\Rightarrow y'_1 = \frac{2m(-ry_2 - \frac{4\alpha}{3} + \sigma r^2)y_0 - 2\hbar^2 y_1}{\hbar^2 r} = g_1 \\ y_2 = E &\Rightarrow y'_2 = 0 = g_3 \end{aligned}$$

Interior Points:

$$\begin{aligned} \bar{x} &= \frac{x_k + x_{k-1}}{2}, \quad \bar{y} = \frac{\vec{y}_k + \vec{y}_{k-1}}{2}, \quad h = x_k - x_{k-1} \\ E_{0,k} &= y_{0,k} - y_{0,k-1} - h\bar{y}_1 \\ E_{1,k} &= y_{1,k} - y_{1,k-1} - \frac{h}{\hbar^2 \bar{x}} (2m(-\bar{x}\bar{y}_2 - \frac{4\alpha}{3} + \sigma \bar{x}^2)\bar{y}_0 - 2\hbar^2 \bar{y}_1) \\ E_{2,k} &= y_{2,k} - y_{2,k-1} \end{aligned}$$

kth connection block:

$$\begin{bmatrix} \frac{\partial E_{0,k}}{\partial y_{0,k-1}} & \frac{\partial E_{0,k}}{\partial E_{1,k}} & \frac{\partial E_{0,k}}{\partial y_{1,k-1}} & \frac{\partial E_{0,k}}{\partial E_{1,k}} & \frac{\partial E_{0,k}}{\partial y_{2,k-1}} & \frac{\partial E_{0,k}}{\partial E_{1,k}} & \frac{\partial E_{0,k}}{\partial y_{2,k}} \\ \frac{\partial y_{0,k-1}}{\partial E_{1,k}} & \frac{\partial y_{1,k-1}}{\partial E_{2,k}} & \frac{\partial y_{2,k-1}}{\partial E_{2,k}} & \frac{\partial y_{0,k}}{\partial E_{2,k}} & \frac{\partial y_{1,k}}{\partial E_{2,k}} & \frac{\partial y_{2,k}}{\partial E_{2,k}} & \frac{\partial y_{2,k}}{\partial y_{1,k}} \\ -1 & -\frac{h}{2} & 0 & 1 & -\frac{h}{2} & 0 & 0 \\ -\frac{hm}{\hbar^2 \bar{x}} (-\bar{x}\bar{y}_2 - \frac{4\alpha}{3} + \sigma \bar{x}^2) & -1 + \frac{h}{\bar{x}} & \frac{hm\bar{y}_0}{\hbar^2} & -\frac{hm}{\hbar^2 \bar{x}} (-\bar{x}\bar{y}_2 - \frac{4\alpha}{3} + \sigma \bar{x}^2) & 1 + \frac{h}{\bar{x}} & \frac{hm\bar{y}_0}{\hbar^2} & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 & 1 \end{bmatrix}$$

Approximate solution as r goes to infinity:

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial R}{\partial r}) + V(r)R &= ER \\ V(r) &= -\frac{4\alpha}{3r} + \sigma r \approx V(r \rightarrow \infty) = \sigma r \\ -\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} (rR) + \sigma rR &= ER \\ -\frac{\hbar^2}{2m} \frac{\partial^2 u}{\partial r^2} + (\sigma r - E)u &= 0 \\ \sigma r - E &= (r - a)g \Rightarrow g = \sigma, \quad a = \frac{E}{\sigma} \\ z(r) &= (\frac{2m\sigma}{\hbar^2})^{\frac{1}{3}} (r - \frac{E}{\sigma}) \\ \frac{\partial^2 u}{\partial z^2} - zu &= 0 \Rightarrow u = Ai(z) = Ai((\frac{2m\sigma}{\hbar^2})^{\frac{1}{3}} (r - \frac{E}{\sigma})) \\ R(r \rightarrow \infty) &\approx \frac{re^{-\frac{2}{3}z^{\frac{3}{2}}}}{2\sqrt{\pi}z^{\frac{1}{4}}} \end{aligned}$$

Boundary conditions:

$$\frac{2m(-ry_2 - \frac{4\alpha}{3} + \sigma r^2)y_0 - \hbar^3 y_1}{\hbar^2 r} = \text{finite} \Rightarrow 2m(-ry_2 - \frac{4\alpha}{3} + \sigma r^2)y_0 - 2\hbar^2 y_1 = 0$$

$$x = 0 \Rightarrow 2m(-ry_2 - \frac{4\alpha}{3} + \sigma r^2)y_0 - \hbar^2 y_1 = 0$$

$$x = x_{Max} \Rightarrow y_0 = r Ai(z(r))$$

$$x = x_{Max} \Rightarrow y_1 = (r Ai(z(r)))' = Ai(z(r)) + r Ai'(z(r))z'$$

$$z(r) = (\frac{2m\sigma}{\hbar^2})^{\frac{1}{3}}(r - \frac{E}{\sigma}) \Rightarrow z'(r) = (\frac{2m\sigma}{\hbar^2})^{\frac{1}{3}}$$

$$Ai(z) \approx \frac{e^{-\frac{2}{3}z^{\frac{3}{2}}}}{2\sqrt{\pi}z^{\frac{1}{4}}}$$

$$Ai'(z) \approx \frac{z^{\frac{1}{4}}}{2\sqrt{\pi}}(1 - \frac{1}{4z^{\frac{3}{2}}})e^{-\frac{2}{3}z^{\frac{3}{2}}}$$

1st condition block:

$$E_{0,0} = 2m(-ry_2 - \frac{4\alpha}{3} + \sigma r^2)y_0 - 2\hbar^2 y_1 = 0$$

$$\begin{bmatrix} \frac{\partial E_{0,0}}{\partial y_{0,0}} & \frac{\partial E_{0,0}}{\partial y_{1,0}} & \frac{\partial E_{0,0}}{\partial y_{2,0}} \\ 2m(-x_0 y_{2,0} - \frac{4\alpha}{3} + \sigma x_0^2) & -2\hbar^2 & m x_0 y_{0,0} \\ -\frac{8m\alpha}{3} & -2\hbar^2 & 0 \end{bmatrix}$$

2nd condition block:

$$E_{0,M-1} = y_{0,M-1} - x_{M-1} Ai(z(x_{M-1}, y_2))$$

$$E_{1,M-1} = y_{1,M-1} - Ai(z(x_{M-1}, y_2)) - x_{M-1} Ai'(z(x_{M-1}, y_2))z'$$

$$\begin{bmatrix} \frac{\partial E_{0,M-1}}{\partial y_{0,M-1}} & \frac{\partial E_{0,M-1}}{\partial y_{1,M-1}} & \frac{\partial E_{0,M-1}}{\partial y_{2,M-1}} \\ \frac{\partial E_{1,M-1}}{\partial y_{0,M-1}} & \frac{\partial E_{1,M-1}}{\partial y_{1,M-1}} & \frac{\partial E_{1,M-1}}{\partial y_{2,M-1}} \\ 1 & 0 & -x_{M-1} \frac{\partial Ai(z(x_{M-1}, y_2))}{\partial y_2} \\ 0 & 1 & -\frac{\partial Ai(z(x_{M-1}, y_2))}{\partial y_2} - x_{M-1} \frac{\partial Ai'(z(x_{M-1}, y_2))z'}{\partial y_2} \end{bmatrix}$$

Calculator got into the mix between the definition of $Ai(z(x,E))$ and the first lines

$$\frac{\partial Ai(z(x,y_2))}{\partial y_2} = \left(\frac{\hbar^{\frac{1}{6}} 2^{\frac{11}{12}}}{16(\sigma x - y_2)(-y_2 - \sigma x)(m\sigma)^{\frac{1}{3}}/\sigma)^{\frac{1}{4}} \sqrt{\pi}} + \frac{(\sigma x - y_2)(m\sigma)^{\frac{2}{3}} 2^{\frac{5}{12}}}{2\hbar^{\frac{5}{6}} \sigma^2 \sqrt{\pi}(-y_2 - \sigma x)(m\sigma)^{\frac{1}{3}}/\sigma)^{\frac{3}{4}}} \right) e^{-\frac{2\sqrt{2}}{3\hbar}(-y_2 - \sigma x)(m\sigma)^{\frac{1}{3}}/\sigma)^{\frac{3}{2}}}$$

$$\frac{\partial Ai(z(x,y_2))}{\partial y_2} = \left(\frac{\hbar^{\frac{1}{6}} 2^{\frac{11}{12}}}{16(\sigma x - y_2)(x - \frac{y_2}{\sigma})^{\frac{1}{4}}(m\sigma)^{\frac{1}{2}} \sqrt{\pi}} + \frac{(x - \frac{y_2}{\sigma})(m\sigma)^{\frac{2}{3}} 2^{\frac{5}{12}}}{2\hbar^{\frac{5}{6}} \sigma \sqrt{\pi}(x - \frac{y_2}{\sigma})^{\frac{3}{4}}(m\sigma)^{\frac{1}{4}}} \right) e^{-\frac{2\sqrt{2}}{3\hbar}((x - \frac{y_2}{\sigma})(m\sigma)^{\frac{1}{3}})^{\frac{3}{2}}}$$

$$\frac{\partial Ai(z(x,y_2))}{\partial y_2} = \left(\frac{\hbar^{\frac{1}{6}}}{8\sqrt{\pi}(\sigma x - y_2)(x - \frac{y_2}{\sigma})^{\frac{1}{4}}(2m\sigma)^{\frac{1}{2}}} + \frac{(x - \frac{y_2}{\sigma})^{\frac{1}{4}}(2m\sigma)^{\frac{5}{12}}}{2\hbar^{\frac{5}{6}} \sigma \sqrt{\pi}} \right) e^{-\frac{2\sqrt{2}}{3\hbar}(x - \frac{y_2}{\sigma})^{\frac{3}{2}}(m\sigma)^{\frac{1}{2}}}$$

$$\frac{\partial Ai'(z(x,y_2))}{\partial y_2} = \left(-\frac{(m\sigma)^{\frac{1}{3}} 2^{\frac{7}{12}}((m\sigma)^{\frac{1}{3}}(\sigma x - y_2)/\sigma)^{\frac{3}{4}}}{2\hbar^{\frac{7}{6}} \sqrt{\pi} \sigma} - \frac{5\hbar^{\frac{5}{6}} \sigma 2^{\frac{7}{12}}}{64(m\sigma)^{\frac{1}{3}} \sqrt{\pi}(\sigma x - y_2)^2((m\sigma)^{\frac{1}{3}}(\sigma x - y_2)/\sigma)^{\frac{1}{4}}} \right) e^{-\frac{2\sqrt{2}}{3\hbar}(-y_2 - \sigma x)(m\sigma)^{\frac{1}{3}}/\sigma)^{\frac{3}{2}}}$$

$$\frac{\partial Ai'(z(x,y_2))}{\partial y_2} = \left(-\frac{(2m\sigma)^{\frac{1}{3}}((2m\sigma)^{\frac{1}{3}}(x - \frac{y_2}{\sigma}))^{\frac{3}{4}}}{2\hbar^{\frac{2}{3}} \hbar^{\frac{1}{2}} \sqrt{\pi} \sigma} - \frac{5\hbar^{\frac{1}{6}} \hbar^{\frac{2}{3}} \sigma}{32(2m\sigma)^{\frac{1}{3}} \sqrt{\pi}(\sigma x - y_2)^2((2m\sigma)^{\frac{1}{3}}(x - \frac{y_2}{\sigma}))^{\frac{1}{4}}} \right) e^{-\frac{2\sqrt{2}}{3\hbar}(x - \frac{y_2}{\sigma})^{\frac{3}{2}}(m\sigma)^{\frac{1}{2}}}$$

$$\frac{\partial Ai'(z(x,y_2))}{\partial y_2} = \left(-\frac{(2m\sigma)^{\frac{1}{3}}((2m\sigma)^{\frac{1}{3}}(x - \frac{y_2}{\sigma}))^{\frac{3}{4}}}{2\hbar^{\frac{2}{3}} \hbar^{\frac{1}{2}} \sqrt{\pi} \sigma} - \frac{5\hbar^{\frac{5}{6}}}{32\sqrt{\pi}(\sigma x - y_2)((2m\sigma)^{\frac{1}{3}}(x - \frac{y_2}{\sigma}))^{\frac{5}{4}}} \right) e^{-\frac{2\sqrt{2}}{3\hbar}(x - \frac{y_2}{\sigma})^{\frac{3}{2}}(m\sigma)^{\frac{1}{2}}}$$

$$a = \frac{2m\sigma}{\hbar^2}, \quad b(x) = x - \frac{y_2}{\sigma}, \quad z = a^{\frac{1}{3}} b$$

$$\frac{\partial Ai(z(x,y_2))}{\partial y_2} = \left(\frac{1}{8\sqrt{\pi}(\sigma x - y_2)z^{\frac{1}{4}}} - \frac{z^{\frac{1}{4}} a^{\frac{1}{3}}}{2\sqrt{\pi} \sigma} \right) e^{-\frac{2}{3}z^{\frac{3}{2}}}$$

$$\frac{\partial Ai'(z(x,y_2))z'}{\partial y_2} = -a^{\frac{1}{3}} \left(\frac{a^{\frac{1}{3}} z^{\frac{3}{4}}}{2\sqrt{\pi} \sigma} + \frac{5}{32\sqrt{\pi}(\sigma x - y_2)z^{\frac{5}{4}}} \right) e^{-\frac{2}{3}z^{\frac{3}{2}}}$$

Relaxation method requires an ansatz. This is my ansatz:

$$\begin{aligned}\Psi(x) &= \Psi_{Hydrogen}(x), \quad x \in [0, x_e] \\ \Psi(x) &= x Ai\left(\left(\frac{2m\sigma}{\hbar^2}\right)^{\frac{1}{3}}\left(x - \frac{E}{\sigma}\right)\right), \quad x \in [x_e, \infty] \\ E &= \int_0^{x_e} \Psi(H\Psi)x^2 dx\end{aligned}$$

The ansatz will be discontinuous in, at least, either the function or derivative of the function at the cutoff. I will choose the function to be continuous at the cutoff by multiplying the function by a coefficient and building it from the cutoff down to zero.

x_e is difficult to reasonably define consistently. If you define it at static location, then E can get big enough that the large radius approximation will no longer apply. $x Ai(z)$ will still apply. The approximation of $Ai(z)$ will not apply. At the moment I have decided that the cutoff will be the greater of point that the coulomb potential will have a slope of .0001 or $z(x)$ is 6. The energy were the change is from the static to dynamic is 15 GeV. The static cutoff is around 16.1 fm. The wavefunction that is smaller than the cutoff will be numerically solved. The wavefunction higher than the cutoff will be approximately correct so long as the potential's approximation is given as correct.

Just so we know what the sign of the energy should be, here is the ground state of hydrogen in the coulomb potential as calculated in my program (no solving involved):

$$\begin{aligned}\Psi(r) &= 2a^{-\frac{3}{2}} e^{-\frac{r}{a}} \\ a &= .26817291008342 \frac{1}{keV} \\ m &= 510.99866622411 keV \\ \alpha_s &= 3/4 * .0072973525540509 \\ \hbar &= 1 \\ \sigma &= 0 \\ \infty &= 100 * a \\ E &= \frac{\int_0^{\infty} x^2 \Psi'(x)^2 - \frac{2mx(\sigma x^2 - \frac{4\alpha_s}{3})}{\hbar^2} \Psi(x)^2}{\int_0^{\infty} \frac{2mx^2}{\hbar^2} \Psi(x)^2} \approx -13.605685 eV\end{aligned}$$

$\langle \Psi | H | \Psi \rangle$ as implemented at the moment is giving me garbage and I have no idea what the cause is. It also happens to require the wavefunction to be normalized.

Current condition:

The relaxation algorithm is telling me that the energy of the ground state is 3.1 GeV, it should fall apart. The above energy calculation is telling me that the wavefunction that results is -.62318467 GeV which is reasonable as it started out at -.48855014 GeV. It is also telling me that the value of the wavefunction at the origin is 1.3e6 and that the wavefunction is normalized. I'm not trusting the normalization or energy outcomes of the algorithm at this time. The shape seems to be otherwise reasonable at this time. gprof is telling me that the program is making calls to functions that I have not called myself.