Exercise Hydrogen

1 Gradient of Rosenbrock function

1. Find the extremum of the Rosenbrock function

$$f(x, y) = (1 - x)^2 + 100(y - x^2)^2, \qquad (1)$$

   by finding the root of it's gradient (that is, the point where the gradient is zero). You have to calculate the gradient analytically.

2. Print out the number of iterations it took the algorithm to converge.

3. Print out the points where the algorithm calculated the values of the gradient.

4. (Optional) Make a contour plot of the Rosenbrock function (1) together with the path the alogorithm used to converge to the extremum.

2 Bound states of hydrogen atom with shooting method for boundary value problems

2.1 Introduction

The s-wave radial Schrdinger equation for the Hydrogen atom reads (in units "Bohr radius" and "Hartree"),

$$-\frac{1}{2}f'' - \frac{1}{r}f = \epsilon f \ , \qquad (2)$$

where $f(r)$ is the radial wave-function, ϵ is the energy, and primes denote the derivative over r.

The bound s-state wave-function satisfies this equation and the two boundary conditions,

$$\begin{aligned} f(r \to 0) &= r - r^2 \ , (\text{provethis}) \qquad (3) \\ f(r \to \infty) &= 0. \qquad (4) \end{aligned}$$

These two boundary conditions can only be satisfied for certain discrete (negative) values of the energy.

Since one cannot integrate numerically to ∞ one substitutes ∞ with a reasonably large number, $r_{\max}$, such that it is much larger than the typical size of the hydrogen atom but still managable for the numerical inregrator (say, $r_{\max} = 10$ Bohr radii),

$$f(r_{\max}) = 0. \qquad (5)$$

Let $F_\epsilon(r)$ be the solution (to be found numericall via `gsl_odeiv` to our differential equation with energy ϵ and initial condition $F_\epsilon(r \to 0) = r - r^2$.

Generally, for a random negative ϵ, this solution will not satisfy the boundary condition at $r_{\max}$. It will only be satisfied when ϵ is equal one of the bound state energies of the system.

Now define an auxiliary function

$$M(\epsilon) \equiv F_\epsilon(r_{\max}) \ . \qquad (6)$$

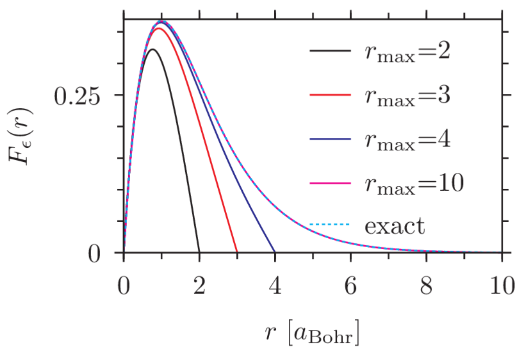
The shooting method is then equivalent to finding the (negative) root of the equation

$$M(\epsilon) = 0. \qquad (7)$$

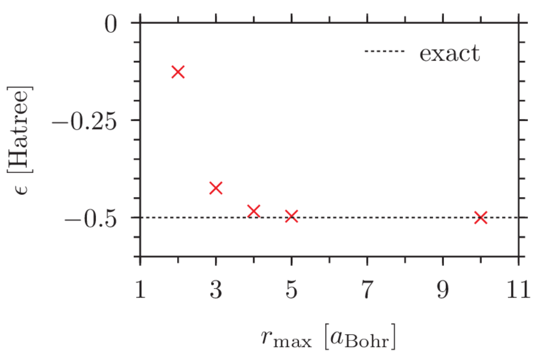
2.2 Exercises

1. Find the lowest root, ϵ_0, of the equation $M(\epsilon) = 0$ for, say, $r_{max} = 8$. Plot the resulting function and compare with the exact result (which is $\epsilon_0 = -\frac{1}{2}$, $f_0(r) = re^{-r}$ – check this by inserting ϵ_0 and $f_0(r)$ into the Schredinger equation above).

Hydrogen s-wave shooting to $F_\epsilon(r_{\max}) = 0$



Obtained energy as function of $r_{\max}$



2. (Optional) Investigate the convergence of the solution towards the exact result as function of r_{max}.

3. (Optional) Try also to use a more precise boundary condition for bound states (which have $\epsilon < 0$),

$$f(r \to \infty) = re^{-kr} , \tag{8}$$

where $k = \sqrt{-2\epsilon}$. This should allow you to use a smaller r_{max}.