## Variational solution to H-atom

The Schrödinger equation (in atomic units) for the hydrogen atom is

$$\left(-\frac{1}{2}\nabla^2 - \frac{1}{r}\right)\Psi(r) = E\Psi(r),$$

where

$$\nabla^2 f(r) = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)f(r).$$

For this problem the exact wavefunction is $\Psi(r) = \sqrt{\zeta^3/\pi}\exp(-\zeta r)$, where the optimal $\zeta$ which minimizes the ground state energy of H atom turns out to be 1. The corresponding ground state energy of H atom is $E = \int_0^\infty dr\, 4\pi r^2\, \Psi^\dagger(r)\hat{H}\Psi(r) = -0.5$ hartree.

1. Use a trial function $\widetilde{\Psi}(r) = (2\alpha/\pi)^{3/4}\exp(-\alpha r^2)$ and minimize the energy expectation value. Report the optimal value of $\alpha$ along with $\widetilde{E}$. Since the trial function varies non-linearly with respect to the variational parameter $\alpha$, this problem is a non-linear variational problem.

2. Estimate $\alpha_{\mathrm{opt}}$ by maximizing the overlap integral, $S$, between the trial function $\widetilde{\Psi}(r)$ and the exact wavefunction, $\Psi(r) = \sqrt{1/\pi}\exp(-r)$

$$S(\alpha) = \int_0^\infty dr\, 4\pi r^2\, (2\alpha/\pi)^{3/4}\exp(-\alpha r^2)\cdot\sqrt{1/\pi}\exp(-r).$$

   Report this $\alpha_{\mathrm{opt}}$ along with $\widetilde{E}$ computed using the corresponding trial function. NOTE: When using $\alpha_{\mathrm{opt}}$ this trial function made with one Gaussian approximates best the hydrogen wavefunction (which is also known as the Slater-type orbital, STO). For this reason, $\widetilde{\Psi}(r) = (2\alpha_{\mathrm{opt}}/\pi)^{3/4}\exp(-\alpha_{\mathrm{opt}}r^2)$ is known as STO-1G basis function (where 1G stands for one-Gaussian) for H atom.