Variational 2

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Hydrogen - let's try a gaussian

$e^{-\alpha r^2}$ → adjust α to get the lowest energy (to take derivative)

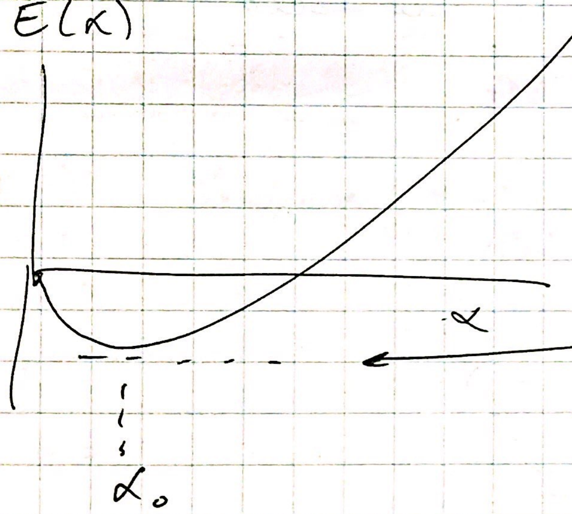
α: variational parameter

$E[\psi] \to E(\alpha)$ functional → function

$$E(\alpha) = \frac{\int d^3r \left(e^{-\alpha r^2}\right)\left(-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{r}\right)e^{-\alpha r^2}}{\int d^3r\, e^{-2\alpha r^2}}$$

$$E(\alpha) = A\alpha - B\sqrt{\alpha}, \quad A = \frac{3\hbar^2}{2\mu} \quad B = 2e^2\sqrt{\frac{2}{\pi}}$$

Can compute the integrals



We want this minimum

$$E(\alpha_0) = A\sqrt{\frac{B}{2A}} - B\sqrt{\sqrt{\frac{B}{2A}}}$$

$$E'(\alpha) = A - \frac{1}{2}B\alpha_0^{-1/2} = 0$$

$$\to \alpha_0 = \sqrt{\frac{B}{2A}} = \sqrt{\frac{1}{2}2e^2\sqrt{\frac{2}{\pi}}\frac{2\mu}{3\hbar^2}} =$$

$$E(\alpha_0) = \underbrace{\frac{-\mu e^4}{2\hbar^2}\frac{8}{3\pi} = -0.85\,Ry}$$

always upper bound

[Compare to -1 Ry → we get an upper bound]

What would a better trial function be?

[$\psi(r) = \sum_i b_i e^{-\alpha_i r^2}$ → "Gaussian Type Orbit"]