

# Variational Calculation on the Two-Dimensional Hydrogen Atom

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Normalized trial wave function:

$$\Psi(\alpha, r) := \sqrt{\frac{2}{\pi}} \cdot \alpha \cdot e^{-\alpha \cdot r} \quad \int_0^{\infty} \Psi(\alpha, r)^2 \cdot 2 \cdot \pi \cdot r \, dr \text{ assume, } \alpha > 0 \rightarrow 1$$

Calculate electron kinetic energy:

$$T(\alpha) := \int_0^{\infty} \Psi(\alpha, r) \cdot \frac{-1}{2 \cdot r} \cdot \frac{d}{dr} \left( r \cdot \frac{d}{dr} \Psi(\alpha, r) \right) \cdot 2 \cdot \pi \cdot r \, dr \text{ assume, } \alpha > 0 \rightarrow \frac{1}{2} \cdot \alpha^2$$

Calculate electron-nucleus potential energy:

$$V_{\text{NE}}(\alpha, Z) := \int_0^{\infty} \Psi(\alpha, r) \cdot \frac{-Z}{r} \cdot \Psi(\alpha, r) \cdot 2 \cdot \pi \cdot r \, dr \text{ assume, } \alpha > 0 \rightarrow (-2) \cdot \alpha \cdot Z$$

Calculate total electronic energy for the 2D H atom:  $E(\alpha) := T(\alpha) + V_{\text{NE}}(\alpha, 1)$

$$\alpha := 1 \quad \alpha := \text{Minimize}(E, \alpha) \quad \alpha = 2 \quad E(\alpha) = -2$$

Demonstrate that the virial theorem is satisfied:

$$\frac{T(\alpha)}{E(\alpha)} = -1 \quad \frac{T(\alpha)}{V_{\text{NE}}(\alpha, 1)} = -0.5 \quad \frac{V_{\text{NE}}(\alpha, 1)}{E(\alpha)} = 2$$