

10.23: Variational Calculation on the Two-dimensional Hydrogen Atom

Normalized trial wave function:

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

Calculate electron kinetic energy:

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

Calculate electron-nucleus potential energy:

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

Calculate total electronic energy for the 2D H atom:

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

Demonstrate that the virial theorem is satisfied:

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

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