10.23: Variational Calculation on the Two-dimensional Hydrogen Atom

Normalized trial wave function:

$$\psi(\alpha, r) = \sqrt{\frac{2}{\pi}}\alpha e^{-\alpha r}$$

$$\int_0^\infty \psi(\alpha, r)^2 2\pi r dr \ assume,\ \alpha > 0 \rightarrow 1$$

Calculate electron kinetic energy:

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

Calculate electron-nucleus potential energy:

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

Calculate total electronic energy for the 2D H atom:

α = 1 α = Minimize (E, α) α = 2 E(α) = -2

Demonstrate that the virial theorem is satisfied:

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