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Atomic Units

$$\psi(r, \vartheta, \varphi) = N_0 e^{-Zr/a_0}$$

Z=1 for Hydrogen atom

$a_0 = \hbar^2/m_e e^2 = 0.529 \text{ \AA} = 0.053 \text{ nm}$ is the Bohr radius

For $Z \neq 1$, $\bar{R} = a_0/Z$

$$E = -Ze^2/2\bar{R} = -Z^2 e^2/2a_0 = -m_e Z^2 e^4/2\hbar^2 = -Z^2 h_0/2$$

where $h_0 = e^2/a_0 = m_e e^4/\hbar^2 = \text{Hartree} = 27.2116 \text{ eV}$
 $= 627.51 \text{ kcal/mol} = 2625.5 \text{ kJ/mol}$

Atomic units:

$m_e = 1$, $e = 1$, $\hbar = 1$ leads to

unit of length = a_0 and unit of energy = h_0

In atomic units: $\text{KE} = \langle \nabla \Phi \cdot \nabla \Phi \rangle / 2$ (leave off \hbar^2/m_e)

$\text{PE} = \langle \Phi | -1/r | \Phi \rangle / 2$ (leave off e^2)

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