Solving Schoedinger Equation for H2

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\,\psi(\vec{r}) = E\,\psi(\vec{r}) \qquad V(\vec{r}) = -\frac{e^2}{4\pi\varepsilon_0}\frac{\hat{r}}{|\vec{r}|}$$

$$(*)\quad -\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2} r\psi(r)\right) - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\,\psi(r) = E\,\psi(r)$$

Unità Atomiche

$e \to 1 \qquad m \to 1 \qquad \hbar \to 1 \qquad a_0 \to$ Bohr Radius

$$E_h \triangleq \frac{e^2}{4\pi\varepsilon_0}\frac{1}{a_0} \Rightarrow V = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} = -E_h a_0 \frac{1}{r}$$

E_h → "Hartree energy"

$$\Rightarrow \underbrace{\frac{V}{E_h}}_{V^*} = -\frac{1}{\underbrace{r/a_0}_{r^*}} \Rightarrow V^* = -\frac{1}{r^*} \rightsquigarrow V = -\frac{1}{r}$$

così il potenziale è espresso in unità atomiche

lasciamo stare l'asterisco per comodità

$$(*)\quad \boxed{-\frac{1}{2}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2} r\psi\right) - \frac{\psi}{r} = E\psi}$$

Schroedinger's equation in atomic units

now let's solve the equation

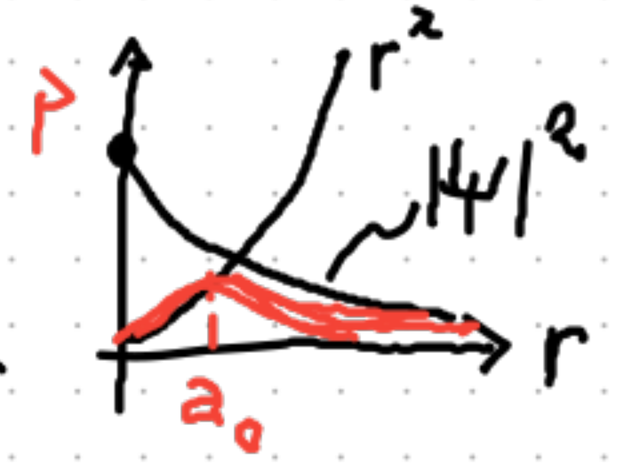
$$*\quad -\frac{1}{2}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi)\right) - \frac{\psi}{r} = E\psi$$

$$-\frac{1}{2r}\partial$$

$$*\quad -\frac{1}{2}\left(-\frac{1}{r}\left(-2\psi + \psi r\right)\right) - \frac{\psi}{r} = E\psi$$

$$E = -\frac{1}{r} + \frac{1}{2} - \frac{1}{r} \Rightarrow \boxed{E = \frac{1}{2}}$$

$$\int_0^\infty |\psi|^2 d^3r \longrightarrow \psi = \frac{1}{\sqrt{\pi}}e^{-r}$$



$$|\psi|^2 \propto e^{-2r}$$

$$P\,dr = 4\pi r^2 dr\,|\psi|^2$$