

Hydrogen atom

$$\phi \propto e^{-\alpha r}$$

$$k = \frac{1}{4\pi\epsilon_0}$$

$$H = \frac{\hbar^2}{2m} \nabla^2 - \frac{ke^2}{r}$$

$$\begin{aligned} \nabla^2 &= \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d\phi}{dr} \right) = \frac{1}{r^2} \left[2r \frac{d\phi}{dr} + r^2 \frac{d^2\phi}{dr^2} \right] \\ &= \left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right] \end{aligned}$$

$$\nabla^2 \phi = \frac{d^2\phi}{dr^2} + \frac{2}{r} \frac{d\phi}{dr}$$

$$\langle H \rangle = \int \phi^* \left[-\frac{\hbar^2}{2m} \nabla^2 - \frac{ke^2}{r} \right] \phi \, d\tau$$

$$\int_0^{\infty} r^n e^{-\alpha r} = \frac{n!}{\alpha^{n+1}}$$

$$\int_0^{\alpha} r^2 e^{-\alpha r} = \frac{2!}{\alpha^{2+1}}$$

$$\phi \propto e^{-\alpha r}$$

$$\langle \phi | \frac{d^2}{dr^2} | \phi \rangle = \int_0^{\infty} e^{-\alpha r} \frac{d^2}{dr^2} (e^{-\alpha r}) 4\pi r^2 dr$$

$$= \int_0^{\infty} e^{-\alpha r} \alpha^2 e^{-\alpha r} 4\pi r^2 dr$$

$$= 4\pi \alpha^2 \int_0^{\infty} r^2 e^{-2\alpha r} dr$$

$$= 4\pi \alpha^2 \times \left[\frac{2!}{(2\alpha)^3} \right] = \frac{\pi}{\alpha}$$

α

$$\begin{aligned}
 \langle \phi | \frac{2}{r} \frac{d}{dr} | \phi \rangle &= 4\pi \int_0^{\infty} e^{-\alpha r} \frac{2}{r} \frac{\partial}{\partial r} (e^{-\alpha r}) r^2 dr \\
 &= -8\pi \int_0^{\infty} r e^{-2\alpha r} dr \\
 &= -8\pi \alpha \left[\frac{1}{(2\alpha)^2} \right] = \frac{-8\pi}{4\alpha} = -\frac{2\pi}{\alpha}
 \end{aligned}$$

$$\begin{aligned}
 \langle \phi | \frac{k e^2}{r} | \phi \rangle &= 4\pi k e^2 \int_0^{\infty} \frac{1}{r} r^2 e^{-2\alpha r} dr \\
 &= 4\pi k e^2 \left[\frac{1!}{(2\alpha)^2} \right] \\
 &= \frac{\pi k e^2}{\alpha^2}
 \end{aligned}$$

$$\langle \phi | \phi \rangle = 4\pi \int_0^{\infty} r^2 e^{-2\alpha r} dr = \frac{2!}{2^3 \alpha^3} = \frac{1}{\alpha^3}$$

$$\langle H \rangle = \frac{\int \psi^* \hat{H} \psi d\tau}{\int \psi^* \psi d\tau} = \frac{-\hbar^2}{2M} \left[\frac{\pi}{\alpha} - \frac{2\pi}{\alpha} \right] \frac{-\pi k e^2}{\alpha^2}$$

$(2\alpha)^3 \quad \alpha^3$

π/α^3

$$\langle H \rangle = \frac{\hbar^2 \alpha^2}{2M} - k e^2 \alpha \quad \leftarrow$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = \frac{\hbar^2 \alpha}{M} - k e^2 = 0$$

$$\alpha = \frac{M k e^2}{\hbar^2}$$

$$\langle H \rangle = \frac{\hbar^2}{2M} \left(\frac{M k e^2}{\hbar^2} \right)^2 - \frac{M k e^2}{\hbar^2} k e^2$$

$$\langle H \rangle = \frac{-\mu k e^4}{2\hbar^2}$$