1) Hidrojen atomu için $n=2$ durumunda tüm olası m ve ℓ'leri belirleyiniz. Her durumun dalga fonksiyonu $\psi_{n\ell m}$'yi oluşturunuz ve enerjilerini hesaplayınız.

$n: 1, 2, \dots \infty$

$\ell: 0, 1, \dots n-1$

$m: -\ell, -\ell+1, \dots, \ell-1, \ell$

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\, Y_\ell^m(\theta,\phi), \quad E_n = -\frac{13.6}{n^2}\, eV$$

$$n=2 \Rightarrow \ell = 0, 1$$

$\ell=0 \rightarrow m=0$; $\ell=1 \rightarrow m=-1,0,1$

n	ℓ	m	$\psi_{n\ell m}$
$n=2$	$\ell=0$	$m=0$	ψ_{200}
	$\ell=1$	$m=-1$	ψ_{21-1}
		$m=0$	ψ_{210}
		$m=1$	ψ_{211}

- $$\psi_{200} = R_{20} Y_0^0 = \frac{1}{\sqrt{2a^3}}\left(1-\frac{r}{2a}\right)e^{-r/2a}\frac{1}{\sqrt{4\pi}} \rightarrow E_2 = \frac{-13.6}{4} eV$$

- $$\psi_{21-1} = R_{21} Y_1^{-1} = \frac{1}{\sqrt{24a^3}}\frac{r}{a}e^{-r/2a}\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi} \rightarrow E_2 = \frac{-13.6}{4} eV$$

- $$\psi_{210} = R_{21} Y_1^0 = \frac{1}{\sqrt{24a^3}}\frac{r}{a}e^{-r/2a}\sqrt{\frac{3}{4\pi}}\cos\theta \rightarrow E_2 = \frac{-13.6}{4} eV$$

- $$\psi_{211} = R_{21} Y_1^1 = \frac{1}{\sqrt{24a^3}}\frac{r}{a}e^{-r/2a}\left(-\sqrt{\frac{3}{8\pi}}\right)\sin\theta\, e^{+i\phi} \rightarrow E_2 = \frac{-13.6}{4} eV$$

$$a = \frac{4\pi\varepsilon_0 \hbar^2}{me^2} = 0,529\times10^{-10} m \quad \text{Bohr yarıçapı}$$

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2} = -\frac{13.6}{n^2} eV$$

$$\int_V \psi^*_{n'\ell'm'}\psi_{n\ell m}\, dV = \delta_{nn'}\delta_{\ell\ell'}\delta_{mm'}$$

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2) Hidrojen atomunun taban durumundaki bir elektron için $\langle r\rangle$ ve $\langle r^2\rangle$'yi bulunuz ve r'deki belirsizlik Δr'yi hesaplayınız. Yanıtlarınızı Bohr yarıçapı cinsinden veriniz.

Taban durumda; $n=1,\ l=0,\ m=0$

$$\psi_{nlm} \rightarrow \psi_{100} = R_{10} Y_0^0 = \frac{2}{\sqrt{a^3}} e^{-r/a} \underbrace{\frac{1}{\sqrt{4\pi}}}_{Y_0^0}$$

$$\bullet\ \langle r\rangle_{100} = \int \psi_{100}^* \, r \, \psi_{100} \, dV = \frac{4}{a^3}\frac{1}{4\pi}\int_V e^{-2r/a} \, r \, r^2 \sin\theta \, dr \, d\theta \, d\phi$$

$$\langle r\rangle_{100} = \frac{4}{a^3}\frac{1}{4\pi}\int_0^\infty r^3 e^{-2r/a} dr \underbrace{\int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\phi}_{4\pi} = \frac{4}{a^3}\int_0^\infty r^3 e^{-2r/a} dr$$

$$I = \int_0^\infty r^n e^{-r/b} dr = n!\,(b)^{n+1}$$

$$n=3 \Rightarrow I = 3!\left(\frac{a}{2}\right)^{3+1}$$

$$\langle r\rangle_{100} = \frac{4}{a^3}\, 3!\left(\frac{a}{2}\right)^4 = \frac{\cancel{4}}{a^3}\cdot 3 \cdot \cancel{2} \cdot 1 \, \frac{a^4}{\cancel{2}\cdot\cancel{2}\cdot\cancel{2}\cdot 2} = \frac{3a}{2}$$

$$\langle r\rangle_{100} = \frac{3a}{2} \,//$$

$$\bullet\ \langle r^2\rangle = \int \psi_{100}^* \, r^2 \, \psi_{100} \, dV = \frac{4}{a^3}\frac{1}{4\pi}\int e^{-2r/a} \, r^2 r^2 \sin\theta \, d\theta \, d\phi \, dr$$

$$\langle r^2\rangle = \frac{4}{a^3}\frac{1}{4\pi}\int_0^\infty r^4 e^{-2r/a} dr \underbrace{\int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\phi}_{4\pi} = \frac{2}{a^3}\underbrace{\int_0^\infty r^4 e^{-2r/a} dr}_{4!\left(\frac{a}{2}\right)^{4+1}}$$

$$\langle r^2\rangle = \frac{4}{a^3}\, 4!\left(\frac{a}{2}\right)^5 = \frac{\cancel{2}\cdot\cancel{2}}{a^3}\cancel{4}\cdot 3 \cdot \cancel{2} \cdot 1 \, \frac{a^5}{\cancel{2}\cdot\cancel{2}\cdot\cancel{2}\cdot\cancel{2}\cdot\cancel{2}} \Rightarrow \langle r^2\rangle = 3a^2 \,//$$

$$\bullet\ \Delta r = \sigma_r = \sqrt{\langle r^2\rangle - \langle r\rangle^2} = \sqrt{3a^2 - \left(\frac{3a}{2}\right)^2} \Rightarrow \Delta r = a\sqrt{\frac{3}{4}} = \frac{a\sqrt{3}}{2} \,//$$

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3) Hidrojen atomunun taban durumu için $\langle x\rangle$ ve $\langle x^2\rangle$'yi hesaplayınız ve x'deki belirsizliği bulunuz.

$$\psi_{100} = \frac{2}{\sqrt{a^3}} e^{-r/a} \frac{1}{\sqrt{4\pi}}$$

$$\langle x\rangle_{100} = \int \psi_{100}^* \, x \, \psi_{100} \, dV$$

$$\langle x^2\rangle_{100} = \int \psi_{100}^* \, x^2 \, \psi_{100} \, dV$$

$\psi_{100}(r)$
küresel koordinatlarda;
$x = r\sin\theta\cos\phi$
$y = r\sin\theta\sin\phi$
$z = r\cos\theta$
$dV = r^2\sin\theta\, dr\, d\theta\, d\phi$

• $$\langle x\rangle_{100} = \frac{4}{a^3}\frac{1}{4\pi}\int e^{-r/a} \underbrace{r\sin\theta\cos\phi}_{x} \, r^2\sin\theta\, dr\, d\theta\, d\phi$$

$$\langle x\rangle = \frac{1}{\pi a^3}\int_0^\infty r^3 e^{-r/a}\int_0^\pi \sin^2\theta\, d\theta \cancel{\int_0^{2\pi}\cos\phi\, d\phi}^{\,0}$$

$$\int_0^{2\pi}\cos\phi\, d\phi = \sin\phi\Big|_0^{2\pi} = \sin 2\pi - \sin 0 = 0$$

$\langle x\rangle = 0$ //

• $$\langle x^2\rangle_{100} = \frac{1}{a^3\pi}\int e^{-r/a} (r\sin\theta\cos\phi)^2 \, r^2\sin\theta\, dr\, d\theta\, d\phi$$

$$\langle x^2\rangle = \frac{1}{\pi a^3}\underbrace{\int_0^\infty r^4 e^{-2r/a}}_{4!\left(\frac{a}{2}\right)^{4+1}}\underbrace{\int_0^\pi \sin^3\theta}_{\frac{4}{3}}\underbrace{\int_0^{2\pi}\cos^2\phi\, d\phi}_{\pi}$$

$$\int_0^\pi \sin^3\theta\, d\theta = \frac{4}{3} \quad (\text{integral tablosu})$$

$$\int_0^{2\pi}\cos^2\phi\, d\phi = \left(\frac{1+\cos 2\phi}{2}\right)\Big|_0^{2\pi} = \frac{1}{2}(2\pi) = \pi \;//$$

$$\langle x^2\rangle = \frac{1}{\pi a^3}\, 4!\left(\frac{a}{2}\right)^5 \frac{4}{3}\pi = \frac{1}{\cancel{\pi} a^3}\,\cancel{4}.\cancel{3}.\cancel{2}.1\,\frac{a^5}{\cancel{2}.\cancel{2}.\cancel{2}.\cancel{2}.\cancel{2}}\,\frac{\cancel{4}}{\cancel{3}}\cancel{\pi} = a^2$$

$\langle x^2\rangle = a^2$

• $$\Delta x = \sigma_x = \sqrt{\langle x^2\rangle - \cancel{\langle x\rangle}^{2}_{\,0}} = \sqrt{\langle x^2\rangle} = \sqrt{a^2} = a$$

$\Delta x = a$ //

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4) Hidrojen atomunun taban durumu için $\langle V \rangle$'yi hesaplayınız.

$$\psi_{100} = \frac{2}{\sqrt{a^3}} \frac{1}{\sqrt{4\pi}} e^{-r/a} \qquad \langle V \rangle_{100} = \langle \psi_{100} | \left(\frac{-e^2}{4\pi\varepsilon_0} \frac{1}{r} \right) | \psi_{100} \rangle$$

$$\Rightarrow \langle V \rangle = \frac{-e^2}{4\pi\varepsilon} \langle r^{-1} \rangle = \frac{-e^2}{4\pi\varepsilon} \int \frac{4}{a^3} \frac{1}{4\pi} e^{-2r/a} \frac{1}{r} r^2 \sin\theta \, dr \, d\theta \, d\phi$$

$$\langle V \rangle = \left(\frac{-e^2}{4\pi\varepsilon_0} \right) \frac{4}{a^3} \frac{1}{4\pi} \int_0^\infty r e^{-2r/a} dr \underbrace{\int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\phi}_{2 \cdot 2\pi = 4\pi}$$

$$\langle V \rangle = \left(\frac{-e^2}{4\pi\varepsilon} \right) \frac{4}{a^3} \int_0^\infty r e^{-2r/a} dr \qquad I = \int_0^\infty r^n e^{-r/b} dr = n! \, (b)^{n+1}, \quad n=1, \; b = a/2$$

$$I = 1! \left(\frac{a}{2} \right)^{1+1}$$

$$\langle V \rangle = \left(-\frac{e^2}{4\pi\varepsilon} \right) \frac{4}{a^3} \, 1! \left(\frac{a}{2} \right)^2$$

$$\langle V \rangle = -\frac{e^2}{4\pi\varepsilon} \frac{1}{a}, \qquad a = \frac{4\pi\varepsilon\hbar^2}{me^2}$$

$$\langle V \rangle = -\frac{e^2}{4\pi\varepsilon} \frac{me^2}{4\pi\varepsilon\hbar^2} = -\left[\frac{m}{\hbar^2} \left(\frac{e^2}{4\pi\varepsilon} \right)^2 \right] \cdot \frac{2}{2} = -\underbrace{\left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\varepsilon} \right)^2 \right]}_{E_1 = 13.6 eV} \cdot 2$$

$$\langle V \rangle_{100} = -2 \cdot 13{,}6 eV$$

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5) Bir Hidrojen atomunun başlangıç dalga fonksiyonu $n=2, l=1, m=1$ ve $n=2, l=1, m=-1$ kararlı durumlarının lineer kombinasyonudur. Yani;

$$\Psi(r,t=0) = \frac{1}{\sqrt{2}}\left(\psi_{211} + \psi_{21-1}\right)$$

'dir.

a) $\psi(r,t)$'yi kurunuz ve mümkün olduğunca basitleştiriniz.

b) Potansiyel enerjinin beklenen değerini $(\langle V \rangle)$ bulunuz.

a: $$\Psi(r,t) = \sum_n \Psi_{nlm}(r,0)\, e^{-iE_nt/\hbar} = \frac{1}{\sqrt{2}}\left(\psi_{211}\, e^{-iE_2t/\hbar} + \psi_{21-1}\, e^{-iE_2t/\hbar}\right)$$

$\psi_{211} = R_{21}Y_1^1$ $\qquad$ $\psi_{21-1} = R_{21}Y_1^{-1}$

$$\Psi(r,t) = \frac{1}{\sqrt{2}}\left[R_{21}Y_1^1 + R_{21}Y_1^{-1}\right]e^{-iE_2t/\hbar} \qquad E_2 = -\frac{E_1}{4} = \frac{-13.6\,eV}{2^2}$$

$$\Psi(r,t) = \frac{1}{\sqrt{2}}R_{21}\left[Y_1^1 + Y_1^{-1}\right]e^{-iE_1t/4\hbar} \qquad R_{21} = \frac{1}{\sqrt{24}}\frac{1}{\sqrt{a^3}}\frac{r}{a}e^{-r/2a}$$

$$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$$

$$\Psi(r,t) = \frac{e^{-iE_1t/4\hbar}}{\sqrt{48}}\frac{r}{a^{5/2}}e^{-r/2a}\Bigg[+\sqrt{\frac{3}{8\pi}}\sin\theta\underbrace{\left(e^{-i\phi} - e^{+i\phi}\right)}_{-2i\sin\phi}\Bigg] \qquad \sin\phi = \frac{e^{i\phi}-e^{-i\phi}}{2i}$$

$$\Psi(r,t) = \sqrt{\frac{3}{8\pi}}\frac{1}{\sqrt{48}}\frac{(-2i)}{a^{5/2}}\, r\, e^{-r/2a}\sin\theta\sin\phi\, e^{-iE_1t/4\hbar}$$

$$\Psi(r,t) = -\frac{i}{\sqrt{\pi a}\,4a^2}\, r\, e^{-r/2a}\sin\theta\sin\phi\, e^{-E_1t/4\hbar} \;//$$

b: $$\langle V\rangle_\Psi = \int \Psi^*\left(\frac{-e^2}{4\pi\varepsilon_0}\frac{1}{r}\right)\Psi\, dV$$

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$$\langle V \rangle = \frac{1}{(2\pi a)(16a^4)}\left(\frac{-e^2}{4\pi\varepsilon}\right)\int_V r^2 e^{-r/a} \sin^2\theta \sin^2\phi \, \frac{1}{r}\, r^2 \sin\theta \, dr\, d\theta\, d\phi \; e^{iE_1t/\hbar}\, e^{-iE_1t/\hbar}$$

$$\langle V \rangle = \frac{1}{32\pi a^5}\left(\frac{-e^2}{4\pi\varepsilon}\right)\underbrace{\int_0^\infty r^3 e^{-r/a}\,dr}_{3!\,(a)^4}\;\underbrace{\int_0^\pi \sin^3\theta\, d\theta}_{\frac{4}{3}}\;\underbrace{\int_0^{2\pi}\sin^2\phi\, d\phi}_{\int_0^{2\pi}\frac{1}{2}(1-\cos 2\phi)\,d\phi = \pi}\; e^{i\overbrace{(E_1-E_1)}^{0}t/\hbar}$$

(integral tablosu)

$$\langle V \rangle = \frac{1}{32\pi a^5}\left(\frac{-e^2}{4\pi\varepsilon}\right) 3!\, a^4\, \frac{4}{3}\, \cancel{\pi} = \frac{1}{\cancel{32}_{\,4}\, a^5}\left(\frac{-e^2}{4\pi\varepsilon_0}\right)\cancel{3}\cdot\cancel{2}\cdot 1\; a^4\, \frac{\cancel{4}}{\cancel{3}}$$

$$\langle V \rangle = \frac{1}{4a}\left(\frac{-e^2}{4\pi\varepsilon}\right), \qquad a = \frac{4\pi\varepsilon\hbar^2}{me^2}$$

$$\langle V \rangle = \frac{1}{4}\left(\frac{me^2}{4\pi\varepsilon\hbar^2}\right)\left(\frac{-e^2}{4\pi\varepsilon}\right) = -\frac{1}{2}\left(\underbrace{\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon}\right)^2}_{-E_1}\right) = +\frac{E_1}{2}$$

$$\langle V \rangle_I = \frac{E_1}{2} = -\frac{13{,}6}{2}\,\text{eV} \qquad \langle V \rangle_{II} = 6{,}8\,\text{eV}$$

zamandan bağımsız $\langle V \rangle$

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