BÖLÜM 12

HİDROJEN ATOMU

Potansiyel $V(r) = -\dfrac{Ze^2}{r}$

Radyal Schrödinger denklemi

$$\left(\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr}\right) + \frac{2\mu}{\hbar^2}\left[E + \frac{Ze^2}{r} - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]R = 0$$

$E < 0$ olduğu bağlı durumlara konsantre olacağız ve

$$\rho = \left(\frac{8\mu|E|}{\hbar^2}\right)^{1/2} r$$

değişken değiştirmesini yapacağız.

$$\frac{d}{dr} = \frac{d\rho}{dr}\frac{d}{d\rho} = \left(\frac{8\mu|E|}{\hbar^2}\right)^{1/2}\frac{d}{d\rho}$$

$$\frac{d^2}{dr^2} = \left(\frac{8\mu|E|}{\hbar^2}\right)\frac{d^2}{d\rho^2}$$

$$\Rightarrow \quad \frac{8\mu|E|}{\hbar^2}\left[\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho}\right] + \frac{2\mu E}{\hbar^2}R$$

$$+ \frac{2\mu Ze^2}{\hbar^2\rho}\left(\frac{8\mu|E|}{\hbar^2}\right)^{1/2}R - \frac{\ell(\ell+1)}{\rho^2}\frac{8\mu|E|}{\hbar^2} = 0$$

$$\lambda = \frac{Ze^2}{\hbar}\left(\frac{\mu}{2|E|}\right)^{1/2} = Z\alpha\left(\frac{\mu c^2}{2|E|}\right)^{1/2}$$

$$\alpha = e^2/\hbar c = 1/137$$

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \frac{\cancel{\hbar^2}}{4\cancel{8\mu}|E|}\frac{\cancel{2\mu} \overset{-|E|}{E}}{\cancel{\hbar^2}}R + \frac{\cancel{\hbar^2}}{4\cancel{8\mu}|E|}\frac{\cancel{2\mu} Ze^2}{\cancel{\hbar^2}\rho}\left(\frac{8\mu|E|}{\hbar^2}\right)^{1/2}R - \frac{\cancel{\hbar^2}}{\cancel{8\mu|E|}}\frac{l(l+1)}{\rho^2}\frac{\cancel{8\mu|E|}}{\cancel{\hbar^2}} = 0$$

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} - \frac{1}{4}R + \frac{Ze^2}{\rho}\left(\frac{\cancel{8}\mu\cancel{|E|}}{\cancel{16}\hbar^2|E|^{\cancel{2}}}\right)^{1/2}R - \frac{l(l+1)}{\rho^2}R = 0$$

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} - \frac{l(l+1)}{\rho^2}R + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)R = 0$$

BS K

ENERJİ SPEKTRUMU

Büyük ρ'lar için bu denklemin asimtotik biçimine bakalım!!...

$$\frac{d^2R}{d\rho^2} - \frac{1}{4}R \simeq 0$$

$$\Rightarrow \quad R(\rho) \sim e^{\pm\rho/2} \qquad e^{+\rho/2} \xrightarrow{\rho\to\infty} \infty \;\checkmark$$

$$R(\rho) = e^{-\rho/2}\, G(\rho)$$

$$R' = -\frac{1}{2}e^{-\rho/2}G + e^{-\rho/2}G'$$

$$R'' = \frac{1}{4}e^{-\rho/2}G - \frac{1}{2}e^{-\rho/2}G' - \frac{1}{2}e^{-\rho/2}G' + e^{-\rho/2}G''$$

$$= \frac{1}{4}e^{-\rho/2}G - e^{-\rho/2}G' + e^{-\rho/2}G''$$

$$G'' - G' + \cancel{\frac{1}{4}G} - \frac{1}{\rho}G + \frac{2}{\rho}G' - \frac{l(l+1)}{\rho^2}G$$

$$+\left(\frac{\lambda}{\rho} - \cancel{\frac{1}{4}}\right)G = 0$$

$$\frac{d^2G}{d\rho^2} - \left(1 - \frac{2}{\rho}\right)\frac{dG}{d\rho} + \left[\frac{\lambda-1}{\rho} - \frac{l(l+1)}{\rho^2}\right]G = 0$$

$$G(\rho) = \rho^l \sum_{n=0}^{\infty} a_n \rho^n = \rho^l H(\rho)$$

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$$G' = \ell \rho^{\ell-1} H + \rho^{\ell} H'$$

$$G'' = \ell(\ell-1)\rho^{\ell-2} H + \ell \rho^{\ell-1} H' + \ell \rho^{\ell-1} H' + \rho^{\ell} H''$$

$$H'' + 2\ell \rho^{-1} H' + \ell(\ell-1)\rho^{-2} H - \left(1 - \frac{2}{\rho}\right)\left(H' + \ell \rho^{-1} H\right)$$

$$+ \left[\frac{\lambda - 1}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right] H = 0$$

$$\frac{d^2 H}{d\rho^2} + \left(\frac{2\ell + 2}{\rho} - 1\right)\frac{dH}{d\rho} + \left[\frac{\overset{\cancel{\ell^2 - \ell}}{\ell(\ell-1)}}{\rho^2} - \frac{\ell}{\rho} + \cancel{\frac{2\ell}{\rho^2}}\right.$$

$$\left. + \frac{\lambda - 1}{\rho} - \frac{\overset{\cancel{\ell^2 + \ell}}{\ell(\ell+1)}}{\rho^2}\right] H = 0$$

$$\frac{d^2 H}{d\rho^2} + \left(\frac{2\ell + 2}{\rho} - 1\right)\frac{dH}{d\rho} + \frac{\lambda - 1 - \ell}{\rho} H = 0$$

$$H(\rho) = \sum_n a_n \rho^n \qquad H'(\rho) = \sum_n a_n n \rho^{n-1}$$

$$H''(\rho) = \sum_n a_n n(n-1)\rho^{n-2}$$

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$$\sum_{n=1} a_n\, n(n-1)\, \rho^{n-2} + \left(\frac{2\ell+2}{\rho}\right)\sum_{n=1} a_n\, n\, \rho^{n-1} \qquad n \to n+1$$

$$-\sum a_n\, n\, \rho^{n-1} + (\lambda-1-\ell)\sum_n a_n\, \rho^{n-1} = 0$$

$$\sum_{n=0}^{\infty}\left\{ a_{n+1}(n+1)n + (2\ell+2)\,a_{n+1}(n+1) - a_n n + (\lambda-1-\ell)\,a_n \right\}\rho^{n-1} = 0$$

$$\sum_{n=0}^{\infty}\left\{ (n+1)\left[n a_{n+1} + (2\ell+2)\,a_{n+1}\right] + (\lambda-1-\ell-n)\,a_n \right\}\rho^{n-1} = 0$$

$$\frac{a_{n+1}}{a_n} = \frac{n+\ell+1-\lambda}{(n+1)(n+2\ell+2)}$$

Büyük n'ler için $\quad \dfrac{a_{n+1}}{a_n} \simeq \dfrac{1}{n}$

Çözümün sonsuzda iyi davranışlı olabilmesi için serinin bir yerde kesilmesi gerekir.

$$\lambda = \underbrace{n_r+\ell+1} \qquad n_r \text{ pozitif tamsayı}$$

n asal kuantum sayısı.

$$n \geq \ell+1$$

$$\Rightarrow \ell \leq n-1$$

$\lambda = n$ bağıntısı

$$\frac{Ze^2}{\hbar}\left(\frac{\mu}{2|E|}\right)^{1/2} = n = Z\alpha\left(\frac{\mu c^2}{2|E|}\right)^{1/2}$$

$$E = -\frac{1}{2}\mu c^2 \frac{(Z\alpha)^2}{n^2} \qquad \mu = \frac{mM}{m+M}$$

İki uyarılmış durum arasındaki fark,

$$\omega_{ij} = \frac{E_i - E_j}{\hbar} = -\frac{1}{2}(Z\alpha)^2 \mu c^2 \left(\frac{1}{n_i^2} - \frac{1}{n_j^2}\right)\frac{1}{\hbar^3}$$

SPEKTRUMUN ~~DEJENERELİĞİ~~ KATMERLİLİĞİ.

Enerji ℓ'ye bağlı değildir. yani verilen bir $n \geq \ell+1$ için tüm durumları enerjileri katmerlidir

(*) $\lambda = 1$, taban durumu için $n_r = 0$, $\ell = 0$ → tek bir taban durumu.

(*) $\lambda = 2$, $\Big\{$ (i) $n_r = 1$, $\ell = 0$

$$\frac{a_{n+1}}{a_n} = \frac{n - n_r}{(n+1)(n+2\ell+2)} \Rightarrow \frac{a_1}{a_0} = \frac{-1}{1 \times 2}$$

$$H(\rho) = a_0\left(1 - \frac{\rho}{2}\right)$$

açısal dağılım küresel simetrik.

(ii) $n_r = 0$, $\ell = 1$ $\Rightarrow$ $H(\rho) = a_0$ radyal dalga fonk.'u sbt.

Ama açısal kısım $Y_{\ell m}(\theta, \varphi)$ $\Rightarrow$ $2\ell + 1$ katmerlilik var. $\{$ 3 durum.

$\lambda = n = 2$ için toplam dejenerelik $3 + 1 = 2^2$

(*) $\lambda = 3$:

$n_r = 2, \ell = 0$ $\Rightarrow$ $a_2/a_1 = -1/6$ ve $a_1/a_0 = -1$ $H(\rho) = a_0\left(1 - \rho + \frac{1}{6}\rho^2\right)$

$n_r = 1, \ell = 1$ $H(\rho) = a_0(1 - \rho/4)$ 3 durum

$n_r = 0$, $\ell = 2$ 5 durum.

$$1 + 3 + 5 = 9 = 3^2$$

Genel olarak

$$1 + 3 + 5 + \ldots + \left[2(n-1) + 1\right] = n^2$$

Verilen bir n için ℓ'nin mümkün değerleri : $0, 1, 2, \ldots n-1$

Herbiri $2\ell + 1$ katlı katmerli

$$\sum_{\ell=0}^{n-1} (2\ell + 1) = n^2$$

Spin de gözönüne alınırsa $2n^2$ katmerli.

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RADYAL ÖZFONKSİYONLAR:

$$a_{k+1} = \frac{k+l+1-n}{(k+1)(k+2l+2)} a_k$$

$$k=0 \Rightarrow \quad a_1 = \frac{l+1-n}{1\cdot(2l+2)} a_0 = -\frac{n-(l+1)}{1\cdot(2l+2)} a_0$$

$$k=1 \Rightarrow \quad a_2 = \frac{l+2-n}{2(2l+3)} a_1 = -\frac{n-(l+2)}{2(2l+3)} a_1$$

$$\vdots$$

$$a_{k+1} = (-1)^{k+1} \frac{n-(k+l+1)}{(k+1)(k+2l+2)} \cdots \frac{n-(l+1)}{1\cdot(2l+2)} a_0$$

$$H(\rho) = L^{2l+1}_{n-l-1}(\rho) \quad \text{Birleşik Laguerre pol.}$$

Örneğin taban durumuna bakalım

$$n=1, \quad l=0 \quad : 1S$$

$$a_{k+1} = \frac{k}{(k+1)(k+2)} a_k$$

$$\Downarrow$$

$$H(\rho) = \sum_{k=0}^{\infty} a_k \rho^k \qquad a_0 \neq 0, \quad a_1 = a_2 = \ldots = a_k = 0$$

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$H(\rho) = a_0$

$\Rightarrow R_{n\ell}(\rho) = C e^{-\rho/2} \rho^{\ell}$

$C^2 \int_0^\infty r^2 dr \, R_{n\ell}^2(r) = 1 \qquad d^3r = \underbrace{d\Omega}_{Y_{\ell m}\text{'ye normalize edildi}} r^2 dr$

$\rho = \left(\frac{8\mu|E|}{\hbar^2}\right)^{1/2} r \qquad E = -\frac{1}{2}(Z\alpha)^2 \frac{\mu c^2}{n^2}$

$\Rightarrow \rho^2 = r^2 \frac{\overset{4}{\cancel{8}}\mu}{\hbar^2} \cdot \frac{1}{\cancel{2}} (Z\alpha)^2 \frac{\mu c^2}{\hbar^2 n^2}$

$= r^2 \left(\frac{2\mu Z\alpha c}{\hbar^2 n}\right)^2 \Rightarrow \rho = r \frac{2Z}{a_0 n}, \quad a_0 = \frac{\hbar}{\mu c \alpha}$

$R_{n\ell}(r) = C e^{-Zr/na_0}$

$C^2 \int_0^\infty r^2 e^{-2Zr/a_0} dr = 1$

$C^2 \cdot \left(\frac{a_0}{2Z}\right)^3 \int_0^\infty \underbrace{r'^2}_{u} \underbrace{dr' e^{-r'}}_{dv} = 1$

$\cancel{-r'^2 e^{-r'}\Big|_0^\infty} + 2\int_0^\infty \underbrace{r'}_{u} \underbrace{dr' e^{-r'}}_{dv}$

$2\left\{\cancel{-r' e^{-r'}\Big|_0^\infty} + \underbrace{\int_0^\infty dr' e^{-r'}}_{-e^{-r'}\big|_0^\infty = 1}\right.$

$C^2 \left(\frac{a_0}{2Z}\right)^3 \cdot 2 = 1$

$C = 2\left(\frac{Z}{a_0}\right)^{3/2}$

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$$R_{10}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

(A) r'nin küçük değerleri için r^{ℓ} baskındır. Bu davranış elektronların çekirdeğe yapışmasını engelleyen davranıştır.

(B) $H(\rho)$ lar $n_r = n-\ell-1$. inci mertebeden polinomlardır. Yani n_r tane düğüm noktası (sıfır) vardır. $n-\ell$ tane tümsek vardır.

Olasılık yoğunluğu,

$$P(r) = r^2 \left[R_{n\ell}(r)\right]^2$$

n verilmiş iken ℓ'nin max. değeri: $\ell_{max} = n-1$ bunda da bir adet tepe vardır.

$$R_{n,n-1}(r) \sim r^{n-1} e^{-Zr/a_0 n}$$

$$\Rightarrow P(r) \propto r^{2n} e^{-2Zr/a_0 n}$$

$$\frac{dP(r)}{dr} = 0 \Rightarrow 2n\cancel{r^{2n-1}}\cancel{e^{-2Zr/a_0 n}} + \cancel{r^{2n}}\left(-\frac{2Z}{a_0 n}\right)\cancel{e^{-2Zr/a_0 n}} = 0$$

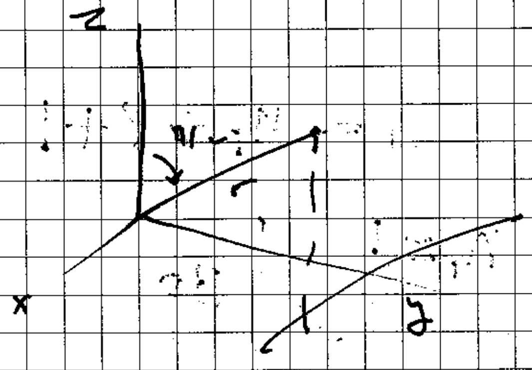
$$\frac{2n}{r} = \frac{2Z}{a_0 n} \Rightarrow r = \frac{n^2 a_0}{Z}$$

(C) Dalga fonk.'nın P_ℓ^m ile orantılı olduğunu biliyoruz.

bu olasılık yoğunluğunda $\left[P_\ell^m(\cos\theta)\right]^2$ olur.

$m=\ell$ olursa $\left[P_\ell^m\right]^2 \propto \left(\sin\theta\right)^{2\ell}$ olur.

Bu, $\theta=\frac{\pi}{2}$ ise $\sin\theta \to max$.



bu düzlemde sivri tepe var.

$$|m|=\ell \Rightarrow L_z = \ell^2$$

$$L_x^2+L_y^2+L_z^2 = L^2$$

$$L^2-L_z^2 = L_x^2+L_y^2 = \ell(\ell+1)-\ell^2 = \ell.$$

Açısal mom. vektörü belli bir eksen boyunca yönelmez denebilir.

(D) $R_{n\ell}(r)$'ler belli ise

$$\langle r^k\rangle = \int_0^\infty dr\, r^2 r^k \left[R_{n\ell}(r)\right]^2$$

$$R_{n\ell}(r) = N_{n\ell}\, r^\ell\, e^{-Zr/na_0}\, L_{n-\ell-1}^{2\ell+1}(r)$$

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$l = 0 \quad 1 \quad 2 \quad 3$

$s \quad p \quad d \quad f$

$n=1 \begin{cases} n_r = 0 \\ l = 0 \end{cases}$ 1s

$n=2 \begin{cases} n_r = 0 \quad \cancel{2s} \\ l = 1 \quad 2p \end{cases}$ $\left.\begin{matrix} n_r = 1 \\ l = 0 \end{matrix}\right\}$ 2s

$n=3 \begin{cases} n_r = 1 \\ l = 0 \end{cases}$ 3s

$n = n_r + l + 1$

$\begin{matrix} n_r = 0 \\ l = 2 \end{matrix}$ 3d $\qquad \left.\begin{matrix} n_r = 1 \\ l = 1 \end{matrix}\right\}$ 3p

n	Yörünge	l	orbital	R_{nl}
1	K	0	1s	R_{10}
2	L	0	2s	R_{20}
		1	2p	R_{21}
3	M	0	3s	R_{30}
		1	3p	R_{31}
		2	3d	R_{32}

BS K

BÖLÜM 12

PROBLEMLER

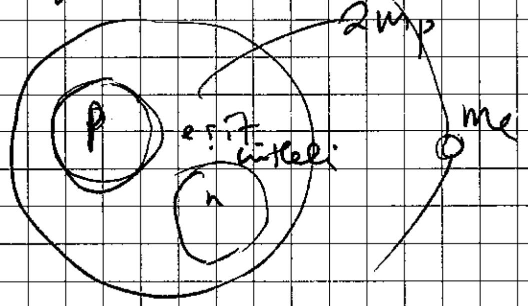
Prb. 12.1. $$E_n = -\frac{1}{2}\mu c^2 \frac{(Z\alpha)^2}{n^2}$$

$$\omega_{ij} = \frac{1}{2\hbar}\frac{mc^2}{1+m/M}(Z\alpha)^2\left(\frac{1}{n_i^2}-\frac{1}{n_j^2}\right)$$

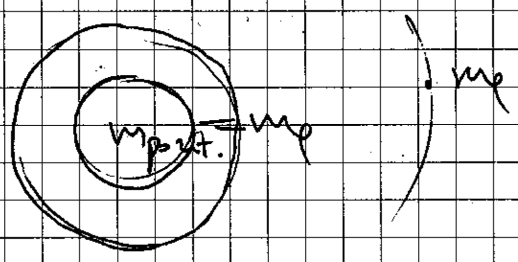
$$\lambda = 2\pi c / \omega_{ij}$$

i) Hidrojen: $Z=1$; $n_i=1$, $n_j=2$ $\lambda = 1215.69\ \mathring{A}$

ii) Döteryum : $Z=1$; $n_i=1$, $n_j=2$ $\lambda = 1215.36\ \mathring{A}$



iii) Pozitronyum : $Z=1$; $n_i=1$, $n_j=2$, $\lambda = 2430\ \mathring{A}$



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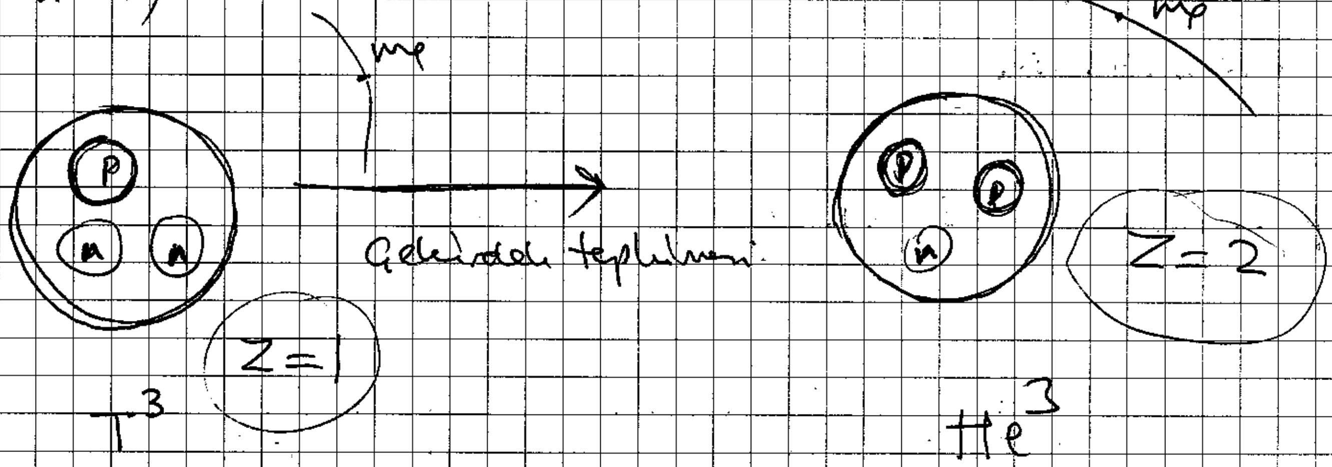
Prb. 12.2.) Trityum



$$\psi_{100}(\vec r) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}\, Y_{00}(\theta,\varphi)$$

$$\psi^{T}_{100} = 2\, a_0^{-3/2}\, e^{-r/a_0}\,\frac{1}{\sqrt{4\pi}} \qquad a_0=\frac{\hbar}{\mu c\alpha}\ ,\ \mu=\frac{m}{1+\frac{m}{M}}$$

$$\psi^{He}_{100} = 2^{5/2}\, a_0^{-3/2}\, e^{-2r/a_0}\,\frac{1}{\sqrt{4\pi}}$$

$$\text{Olasılık} = \int d^3r\, \psi^{He*}_{100}\,\psi^{T}_{100} = \langle \psi^{He}_{100} | \psi^{T}_{100}\rangle$$

$$= 4\left(2/a_0\right)^{3/2}\int_0^\infty r^2 dr\, e^{-3r/a_0} = \ldots$$

Elektronun serbest parçacık durumuna gelme olasılığı.

$$= (2\pi\hbar)^{-3/2}\langle e^{i\vec k\cdot\vec r} | \psi^{T}_{100}\rangle = (2\pi\hbar)^{-3/2}\frac{2}{\sqrt{4\pi}\, a_0^{3/2}}\int d^3r\, e^{-i\vec k\cdot\vec r}\, e^{-r/a_0}$$

$$= \frac{\sqrt{4\pi}}{(2\pi\hbar a_0)^{3/2}\, ik}\int_0^\infty dr\, r\, e^{-r/a_0}\left(e^{ikr} - e^{-ikr}\right)$$

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Prob. 12.5.)

$$\Psi = \frac{1}{6}\left[4\,\psi_{100}(\vec{r}) + 3\,\psi_{211}(\vec{r}) - \psi_{210}(\vec{r}) + \sqrt{10}\,\psi_{21-1}(\vec{r})\right]$$

$$\int d^3\vec{r}\,|\Psi|^2 = 1$$

(a) $$E = \int d^3r\,\Psi^* H \Psi = \langle \Psi | H | \Psi \rangle$$

$$= \left(\frac{4}{6}\right)^2 \langle \psi_{100} | H | \psi_{100} \rangle + \left(\frac{3}{6}\right)^2 \langle \psi_{211} | H | \psi_{211} \rangle$$

$$+ \left(\frac{1}{6}\right)^2 \langle \psi_{210} | H | \psi_{210} \rangle + \frac{10}{6^2} \langle \psi_{21-1} | H | \psi_{21-1} \rangle$$

$$= \left(\frac{4}{6}\right)^2 E_1 + \left[\left(\frac{3}{6}\right)^2 + \left(\frac{1}{6}\right)^2 + \frac{10}{6^2}\right] E_2$$

$$= \frac{4}{9} E_1 + \frac{5}{9} E_2$$

b) $$\langle L^2 \rangle = \langle \Psi | \vec{L}^2 | \Psi \rangle = \langle \Psi | \vec{L}^2 \Psi \rangle$$

$$= \frac{1}{6^2}\left[0 + 9 \cdot 2\hbar^2 + 2\hbar^2 + 10 \cdot 2\hbar^2\right]$$

$$= \frac{40}{36}\hbar^2 = \frac{10}{9}\hbar^2$$

c) $$\langle L_z \rangle = 0$$

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4.

prb. 12.6.) $\psi(r) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{3/2} e^{-\alpha^2 r^2/2}$

$$\langle r \rangle = a_0 = \int_0^\infty r^2 dr \int_\Omega d\Omega \, \psi^* r \psi$$

$$= 4\pi \left(\frac{\alpha}{\sqrt{\pi}}\right)^3 \int_0^\infty r^3 dr \, e^{-\alpha^2 r^2/2} e^{-\alpha^2 r^2/2}$$

$$= 4\pi \left(\frac{\alpha}{\sqrt{\pi}}\right)^3 \frac{1}{2} \int_0^\infty r^2 e^{-\alpha^2 r^2} d(r^2) \, \frac{\alpha^4}{\alpha^4}$$

$$= \frac{\cancel{4}^{2}\pi}{\alpha^4} \frac{1}{\cancel{2}} \left(\frac{\alpha}{\sqrt{\pi}}\right)^3 \underbrace{\int_0^\infty r e^{-r} dr}_{=1} \qquad \cancel{-re^{-r}\Big|_0^\infty} + \int_0^\infty e^{-r} dr$$

$$a_0 = \frac{2}{\alpha\sqrt{\pi}} \Rightarrow \alpha = \frac{2}{a_0\sqrt{\pi}}.$$

$$\Rightarrow \psi = \left(\frac{2}{\pi a_0}\right)^{3/2} e^{-2r^2/\pi a_0}$$

olasılık yoğunluğu $= \left[\left(\frac{2}{\pi a_0}\right)^{3/2}\right]^2$

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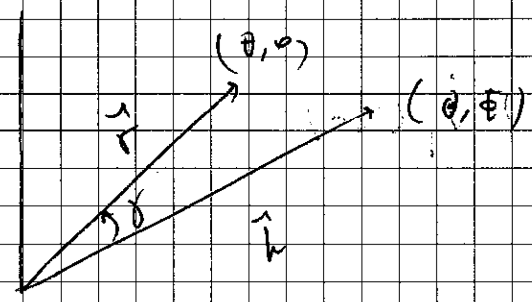
prb. 12.7.) $\psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{k}\, e^{i\vec{k}\cdot\vec{r}} f(\vec{k})$

$$f(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{r}\, e^{-i\vec{k}\cdot\vec{r}} \psi(\vec{r})$$

$$e^{-i\vec{k}\cdot\vec{r}} = \sum_{\lambda=0}^{\infty} \sqrt{4\pi(2\lambda+1)}\, i^{-\lambda} \frac{j_\lambda(kr)}{kr} Y^*_{\lambda 0}(\cos\gamma)$$

$$\psi(\vec{r}) = \frac{u_{nl}(\vec{r})}{r} Y_{lm}(\theta,\varphi)$$



$$Y_{\lambda 0}(\cos\gamma) = \sqrt{\frac{4\pi}{2l+1}} \sum_{\mu=-\lambda}^{+\lambda} Y^*_{\lambda\mu}(\Theta,\Phi) Y_{\lambda\mu}(\theta,\varphi)$$

$$\Rightarrow e^{-i\vec{k}\cdot\vec{r}} = 4\pi \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{+\lambda} i^{-\lambda} \frac{j_\lambda(kr)}{kr} Y^*_{\lambda\mu}(\Theta,\Phi) Y_{\lambda\mu}(\theta,\varphi)$$

$$f(\vec{k}) = \frac{4\pi}{(2\pi)^{3/2}} \int d^3\vec{r}\, \frac{u(r)}{r} Y_{lm}(\theta,\varphi) \sum\sum i^{-\lambda} \frac{j_\lambda(kr)}{kr} Y^*_{\lambda\mu}(\Theta,\Phi) Y_{\lambda\mu}(\theta,\varphi)$$

$$k f(\vec{k}) = \sqrt{\frac{2}{\pi}}\, i^{-l} \int_0^\infty u(r)\, j_l(kr)\, Y_{lm}(\Theta,\Phi)\, dr$$

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$$f(\vec{k}) = \frac{1}{k}\, g_\ell(k)\, Y_{\ell m}(\theta, \Phi)$$

$$\begin{cases} g_\ell(k) = \sqrt{\dfrac{2}{\pi}}\, i^{-\ell} \displaystyle\int_0^\infty dr\, u_\ell(r)\, j_\ell(kr) \\ u_\ell(r) = \sqrt{\dfrac{2}{\pi}}\, i^{\ell} \displaystyle\int_0^\infty dk\, j_\ell(kr)\, g_\ell(k) \end{cases}$$

Hankel Dönüşümü

$$\int_0^\infty dr\, |u_\ell(r)|^2 = 1 \quad , \quad \int_0^\infty dk\, |g_\ell(k)|^2 = 1$$

$n=2$, $\ell=1$, $m=0$ aldığımızda;

$$g_{21}(\vec{k}) = \sqrt{\frac{2}{\pi}}\, \frac{1}{i} \int_0^\infty dr\, u_1(r)\, j_1(kr)$$

$$j_1(kr) = \frac{\sin kr}{(kr)^2} - \frac{\cos kr}{kr}$$

$$R_{21} = \frac{1}{\sqrt{2}} \left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{a_0}\, e^{-Zr/2a_0}$$

$$g_{21}(k) = -i\, \frac{128}{\sqrt{3\pi}}\, \frac{k^2}{(1+4k^2)^3}$$

$$f(\vec{k}) = -i\, \frac{128}{\sqrt{3\pi}}\, \frac{k^2}{(1+4k^2)^3}\, Y_{10} \sim (3\cos^2\theta - 1)$$

BS K

prb. 12.8.)

$$[H, \vec{r}\cdot\vec{p}] = \left[\frac{\vec{p}^2}{2m} + V(r), \vec{r}\cdot\vec{p}\right]$$

$$= \left[\frac{\vec{p}^2}{2m}, \vec{r}\cdot\vec{p}\right] + [V(r), \vec{r}\cdot\vec{p}]$$

$$= \vec{r}\cdot\left[\frac{\vec{p}^2}{2m}, \vec{p}\right] + \left[\frac{\vec{p}^2}{2m}, \vec{r}\right]\cdot\vec{p}$$

$$+ \vec{r}\cdot[V(r), \vec{p}] + [V(r), \vec{r}]\cdot\vec{p}$$

$$[V, \vec{p}]\psi = V\vec{p}\psi - \vec{p}(V\psi) = \cancel{V\vec{p}\psi} - \psi\vec{p}V - \cancel{V\vec{p}\psi}$$

$$= -\psi\vec{p}V$$

$$[V, \vec{p}] = -\vec{p}V = i\hbar\vec{\nabla}V$$

$$[\vec{p}^2, \vec{r}] = \vec{p}\cdot\underbrace{[\vec{p}, \vec{r}]}_{\hbar/i} + \underbrace{[\vec{p}, \vec{r}]}_{\hbar/i}\vec{p} = 2\frac{\hbar}{i}\vec{p}$$

$$\therefore [H, \vec{r}\cdot\vec{p}] = -i2\hbar\frac{\vec{p}^2}{2m} + i\hbar\vec{r}\cdot\vec{\nabla}V = 0$$

$$\left\langle\frac{\vec{p}^2}{m}\right\rangle = \langle\vec{r}\cdot\vec{\nabla}V\rangle$$

$$2\langle T\rangle = \langle\vec{r}\cdot\vec{\nabla}V\rangle$$

BS K

prb.12.9.) $H = \frac{\vec{p}^{\,2}}{2m} + \frac{1}{2} m\omega^2 r^2$

$R = u/r$

$$\frac{d^2u}{dr^2} + \left[\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2} r^2 - \frac{\ell(\ell+1)}{r^2}\right] u = 0$$

$\ell = 0 \Rightarrow$ basit 1D'lu harmonik salınıcı

$$\frac{2mE}{\hbar^2} = k^2 \qquad \frac{m\omega}{\hbar} = \lambda \qquad \frac{k^2}{2\lambda} = \frac{E}{\hbar\omega} = \mu$$

$$\frac{d^2u}{dr^2} + \left[k^2 - \lambda^2 r^2 - \frac{\ell(\ell+1)}{r^2}\right] u = 0$$

$$u(r) = r^{\ell+1} e^{-\lambda r^2/2} v(r) \qquad \lambda r^2 = t$$

$$t\frac{d^2v}{dt^2} + \left[\left(\ell+\frac{3}{2}\right) - t\right]\frac{dv}{dt} - \left[\frac{1}{2}\left(\ell+\frac{3}{2}\right) - \frac{\mu}{2}\right] v = 0$$

$$v = C\, {}_1F_1\left(\frac{1}{2}\left(\ell+\frac{3}{2}-\mu\right);\ \ell+\frac{3}{2};\ \lambda r^2\right)$$

$$\cancel{+ C_2 r^{-(2\ell+1)}}\, {}_1F_1\left(\frac{1}{2}\left(-\ell+\frac{1}{2}-\mu\right);\ -\ell+\frac{1}{2};\ \lambda r^2\right)$$

$(r \to 0) \to \infty$

$$u \sim r^{\ell+1} e^{-\lambda r^2/2} e^{\lambda r^2} r^{-\left(\underbrace{\ell+\frac{3}{2}-\mu}_{-n_r}\right)/2} \Rightarrow \mu = 2n_r + \ell + \frac{3}{2}$$

$$E = \left(n + \frac{3}{2}\right)\hbar\omega \qquad n = 2n_r + \ell.$$