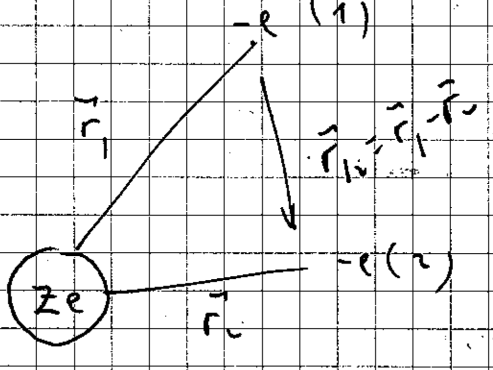
BÖLÜM 18

HELYUM ATOMU



$$H = \frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

$Z = 2$

* Çekirdeğin hareketi
* relativistik etkiler
* S-O etkisi
* bir elektronun hareketinin sebep olduğu alanın diğer elektrona etkisi

gibi etkileri ihmal ediyoruz.

$$H = H^{(1)} + H^{(2)} + V$$

$$H^{(i)} = \frac{\vec{p}_i^{\,2}}{2m} - \frac{Ze^2}{r_i} \quad , \quad V = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

Z ile çalışıp daha sonra $Z = 2$ alacağız.

V'yi ihmal etseydik, özfonksiyonlar

$$u(\vec{r}_1, \vec{r}_2) = \phi_{n_1 l_1 m_1}(\vec{r}_1)\, \phi_{n_2 l_2 m_2}(\vec{r}_2)$$

olacaktı.

$$\left[H^{(1)} + H^{(2)}\right] u(\vec{r}_1, \vec{r}_2) = E\, u(\vec{r}_1, \vec{r}_2)$$

$$E = E_{n_1} + E_{n_2} \qquad E_n = -\frac{1}{2} m c^2 (Z\alpha)^2 \frac{1}{n^2}$$

$$E = -2E_1 = -mc^2 (2\alpha)^2 = -108.8 \text{ ev}$$

$$= 2 \times (Z)^2 E_{Hyd} = 8 E_{Hyd}$$ Taban durumu

İlk uyarılmış durumu $\begin{cases} n = 1 & (1) \\ n = 2 & (2) \end{cases}$

$$E = E_1 + E_2 = \underbrace{-\frac{1}{2} m c^2 (2\alpha)^2 \frac{1}{1^2}}_{4 E^{1}_{Hyd}} - \frac{1}{2} m c^2 (2\alpha)^2 \frac{1}{2^2}$$

$$4 E^{1}_{Hyd} + E^{1}_{Hyd}$$

$$= 5 E^{Hyd}_{1} = -68.0 \text{ ev}$$

İyonizasyon enerjisi bir elektronu taban durumundan ∞'a götürmek için gerekli enerji:

$$E_{iyon} = \left(E_1 + \cancel{E_\infty}_{\,0}\right) - 2E_1$$

$$= -E_1 = -4 E_{Hyd} = 54.4 \text{ ev}$$

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Dışarlama İlkesinin Etkisi:

İki elektron özdeş fermiyonlar olduğu için, toplam dalga fonk.'nun elektronların uzay ve spin koordinatlarının değiş tokuşu altında antisimetrik olmalıdır. Böylece idealleştirilmiş modelin taban durumuna uygun şekil şöyle

$$u_0(\vec{r}_1, \vec{r}_2) = \phi_{100}(\vec{r}_1)\,\phi_{100}(\vec{r}_2)\,\chi_{singlet}$$

dalga fonk.'nun uzaysal kısmı simetrik olduğundan spin durumu singlet olmalı.

$$\chi_{singlet} = \frac{1}{\sqrt{2}}\left(\chi_+^{(1)}\chi_-^{(2)} - \chi_-^{(1)}\chi_+^{(2)}\right)$$

$V=0$ için dejenere olan ilk uyarılmış durum için iki olasılık vardır. Bunlar

$$u_1^{(s)} = \frac{1}{\sqrt{2}}\left[\phi_{100}(\vec{r}_1)\,\phi_{2\ell m}(\vec{r}_2) + \phi_{2\ell m}(\vec{r}_1)\,\phi_{100}(\vec{r}_2)\right]\chi_{sing}$$

$$u_2^{(t)} = \frac{1}{\sqrt{2}}\left[\phi_{100}(\vec{r}_1)\,\phi_{2\ell m}(\vec{r}_2) - \phi_{2\ell m}(\vec{r}_1)\,\phi_{100}(\vec{r}_2)\right]\chi_{trip.}$$

$$\chi_{trip} = \begin{cases} \chi_+^{(1)}\chi_+^{(2)} \\ \frac{1}{\sqrt{2}}\left(\chi_+^{(1)}\chi_-^{(2)} + \chi_-^{(1)}\chi_+^{(2)}\right) \\ \chi_-^{(1)}\chi_-^{(2)} \end{cases}$$

$$\chi_{sing}\,\chi_{trip} = 0.$$

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Elektron-elektron itmesinin etkisi

V'nin varlığı ilk yaklaşımda pertürbasyon olarak alındı ile. İlk olarak taban durumun 1. mertebeden enerji kaymasını hesaplayalım.

$$\Delta E = \int d^3\vec{r}_1\, d^3\vec{r}_2\, u_0^*(\vec{r}_1,\vec{r}_2)\, \frac{e^2}{|\vec{r}_1-\vec{r}_2|}\, u_0(\vec{r}_1,\vec{r}_2)$$

V pertürbasyonu spini içermediğinden

$$\Delta E = \int d^3\vec{r}_1\, d^3\vec{r}_2\, |\phi_{100}(\vec{r}_1)|^2 \frac{e^2}{|\vec{r}_1-\vec{r}_2|} |\phi_{100}(\vec{r}_2)|^2$$

<u>Fiziksel yorum:</u>

$|\phi_{100}(\vec{r}_1)|^2$: $\vec{r}_1$'deki 1 elektronun bulunma olasılığı

$e|\phi_{100}(\vec{r}_1)|^2$ yük yoğunluğu. Bunun $\vec{r}_2$'de oluşturacağı potansiyel

$$U(\vec{r}_2) = -\int d^3\vec{r}_1 \frac{e|\phi_{100}(\vec{r}_1)|^2}{|\vec{r}_1-\vec{r}_2|}$$

$$\Delta E = -\int d^3\vec{r}_2\, e|\phi_{100}(\vec{r}_2)|^2\, U(\vec{r}_2)$$

2. elektron ile bu potansiyel etkileşiminin elektrostatik enerjisi.

$$\phi_{100} = \left(2/\sqrt{4\pi}\right)\left(Z/a_0\right)^{3/2} e^{-Zr/a_0}$$

$$\Delta E = \left[\frac{1}{\pi}\left(\frac{Z}{a_0}\right)^3\right]^2 e^2 \int_0^\infty r_1^2\, dr_1\, e^{-2Zr_1/a_0} \int_0^\infty r_2^2\, dr_2\, e^{-2Zr_2/a_0}$$

$$\underbrace{\int d\Omega_1}_{4\pi} \int d\Omega_2 \frac{1}{|\vec r_1 - \vec r_2|}$$

$$\frac{1}{|\vec r_1 - \vec r_2|} = \frac{1}{\left(r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta\right)^{1/2}}$$

(a) $\vec r_1 = r_1 \hat z$.

$$\int d\Omega_2 \frac{1}{|\vec r_1 - \vec r_2|} = \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \frac{1}{\left(r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta\right)^{1/2}}$$

$\cancel{= 2Z\pi}$

$$r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta = u$$

$$-2r_1 r_2\, d(\cos\theta) = du$$

$$= -\cancel{2}\pi \frac{1}{\cancel{2}r_1 r_2} \int du/u^{1/2} = -\frac{\pi}{r_1 r_2} \frac{u^{1/2}}{1/2}$$

$$= -2\pi \frac{1}{r_1 r_2} \left(r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta\right)^{1/2} \Big|_{-1}^{+1}$$

$$= -\frac{2\pi}{r_1 r_2} \Big\{ \underbrace{\left(r_1^2 + r_2^2 - 2r_1 r_2\right)^{1/2}}_{|r_1 - r_2|} - \underbrace{\left(r_1^2 + r_2^2 + 2r_1 r_2\right)^{1/2}}_{(r_1 + r_2)} \Big\}$$

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$$= -\frac{2\pi}{r_1 r_2}\left\{ |r_1 - r_2| + (r_1 + r_2) \right\}$$

$$= \frac{2\pi}{r_1 r_2}\left\{ r_1 + r_2 - |r_1 - r_2| \right\}$$

$$\Rightarrow \Delta E = \frac{1}{\pi^2}\,\frac{Z^6}{a_0^6}\,e^2\,\frac{8\pi^2}{1}$$

$$\times \int_0^\infty r_1\,dr_1\,e^{-2Zr_1/a_0}\int_0^\infty r_2\,dr_2\,e^{-2Zr_2/a_0}$$

$$\times \left(r_1 + r_2 - |r_1 - r_2| \right)$$

(b) $r_1 > r_2$

$$(r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta)^{-1/2} = r_1^{-1}\left(1 + \frac{r_2^2}{r_1^2} - 2\frac{r_2}{r_1}\cos\theta\right)^{-1/2}$$

$$= \frac{1}{r_1}\sum_{l=0}^{\infty}\left(\frac{r_2}{r_1}\right)^l P_l(\cos\theta)$$

$r_2 > r_1$ ie $r_1 \leftrightarrow r_2$.

$$\int d\Omega_1 \int d\Omega_2 \frac{1}{|\vec{r}_1 - \vec{r}_2|} = \int d\Omega_1 \int d\Omega_2 \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\theta)$$

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$$\frac{1}{2}\int_{-1}^{+1} d(\cos\theta)\, P_L(\cos\theta) = \delta_{L0}$$

$$\frac{1}{2}\int_{-1}^{+1} d(\cos\theta)\, P_L(\cos\theta)\, P_{L'}(\cos\theta) = \frac{\delta_{LL'}}{2L+1}$$

$$\Delta E = 8e^2\left(\frac{Z}{a_0}\right)^6 \int_0^\infty r_1\, dr_1\, e^{-2Zr_1/a_0}$$

$$\times\left\{ 2\int_0^{r_1} r_2^2\, dr_2\, e^{-2Zr_2/a_0} + 2r_1 \int_{r_1}^{\infty} r_2\, dr_2\, e^{-2Zr_2/a_0}\right\}$$

$$\Delta E = \frac{5}{8}\frac{Ze^2}{a_0} = \frac{5}{4} Z\left(\frac{1}{2}mc^2\alpha^2\right)$$

$$\Delta E\Big|_{Z=2} = 34\ \text{eV}$$

$$E_0 = -108.8 + 34. \cong -74.8\ \text{eV}.$$

$$E_{\text{Den}} = -78.975\ \text{eV}$$

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Dışarlama ilkesi ve değiş tokuş etkileşmesi

He'un ilk uyarılmış durumunu inceleyeceğiz. 18.14 ve 18.15 de singlet ve triplet m=0 durumları enerji kaymasını hesaplamak yeterlidir. Çünkü kayma L_z ile sıradeğiştiren bir pertürbasyon tarafından gerçekleştirilir. Bu gibi bir pertürbasyon için kayma m değerinden bağımsız olmalıdır.

$$\Delta E_1^{(s,t)} = \frac{e^2}{2} \int d^3\vec{r}_1 \int d^3\vec{r}_2$$

$$\times \left[\phi_{100}(\vec{r}_1)\phi_{210}(\vec{r}_2) \pm \phi_{210}(\vec{r}_1)\phi_{100}(\vec{r}_2) \right]^*$$

$$\times \frac{1}{|\vec{r}_1-\vec{r}_2|} \left[\phi_{100}(\vec{r}_1)\phi_{210}(\vec{r}_2) \pm \phi_{210}(\vec{r}_1)\phi_{100}(\vec{r}_2) \right]$$

$$= e^2 \int d^3\vec{r}_1 \int d^3\vec{r}_2 \, |\phi_{100}(\vec{r}_1)|^2 |\phi_{210}(\vec{r}_2)|^2 \frac{1}{|\vec{r}_1-\vec{r}_2|}$$

$$\pm e^2 \int d^3\vec{r}_1 \int d^3\vec{r}_2 \, \phi_{100}^*(\vec{r}_1)\phi_{210}^*(\vec{r}_2) \frac{1}{|\vec{r}_1-\vec{r}_2|}$$

$$\times \phi_{210}(\vec{r}_1)\phi_{100}(\vec{r}_2)$$

<u>1. terim</u>: iki elektronun dalga fonk.'larına göre dağılmış iki "elektron bulutu" arasındaki elektrostatik etkileşme

<u>2. terim</u>: klasik karşılığı yok! İşareti spinin <u>sıfır</u> ya da <u>bir</u> olmasına bağlı. Böylece <u>değiş tokuş</u> etkileşmesinden dolayı triplet ve singlet durumlar farklı değerlere ayrılırlar.

Genel olarak

$$\Delta E^{(t)}_{n,l} = J_{nl} - K_{nl}$$

$$\Delta E^{(s)}_{n,l} = J_{nl} + K_{nl}$$

$e^2/|\vec{r}_1 - \vec{r}_2|$ spine bağlı olmadığı halde, dalga fonk.'unun simetrisi pot.'in sanki simetri bağımlıymış gibi etkidiğini gösterir. 18.36'yı bunu belirleyecek şekilde yazarız.

$$\vec{S}^2 = \vec{S}_1^2 + \vec{S}_2^2 + 2\vec{S}_1 \cdot \vec{S}_2$$

$\vec{S}_1^2$ ve $\vec{S}_2^2$'nin de öz fonk.'ları olan χ_{trip}, $\chi_{sing.}$ etki ettirdiğimiz zaman

$$S(S+1)\hbar^2 = \frac{3}{4}\hbar^2 + \frac{3}{4}\hbar^2 + 2\cdot\vec{S}_1\cdot\vec{S}_2$$

$$\frac{2\,\vec{S}_1\cdot\vec{S}_2}{\hbar^2} = S(S+1) - \frac{3}{2} = \begin{cases} 1/2 & \text{trip.} \\ -3/2 & \text{sing.} \end{cases}$$

$$\vec{S}_i = (\hbar/2)\,\vec{\sigma}_i$$

$$\Delta E_{n,l} = J_{n,l} - \frac{1}{2}\left(1 - \vec{\sigma}_1\cdot\vec{\sigma}_2\right) K_{nl}$$

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VARYASYON İLKESİ

Φ karesi integrallenebilir.

$\langle \Phi | \Phi \rangle = 1$ normalize.

$$H \varphi_n = E_n \varphi_n$$

$$\Phi = \sum_n c_n \varphi_n$$

$$\langle \Phi | H | \Phi \rangle = \sum_n \sum_m c_n^* \langle \varphi_n | H | \varphi_m \rangle c_m$$

$$= \sum_n \sum_m c_n^* c_m E_m \langle \varphi_n | \varphi_m \rangle$$

$$= \sum_n |c_n|^2 E_n$$

$$\geq E_0 \underbrace{\sum_n |c_n|^2}_{1}$$

$$E_0 \leq \langle \Phi | H | \Phi \rangle$$

üst sınır hesaplanacak.

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$$\Psi(\vec{r}_1, \vec{r}_2) = \psi_{100}(\vec{r}_1)\, \psi_{100}(\vec{r}_2)$$

$$\left(\frac{\vec{p}^{\,2}}{2m} - \frac{Z^* e^2}{r} \right) \psi_{100}(\vec{r}) = \epsilon\, \psi_{100}(\vec{r})$$

$$\epsilon = -(1/2)\, m c^2 \left(Z^* \alpha \right)^2 / 1^2$$

$$\int d^3\vec{r}_1 \int d^3\vec{r}_2\, \psi^*_{100}(\vec{r}_1)\, \psi^*_{100}(\vec{r}_2)$$

$$\left[\frac{\vec{p}_1^{\,2}}{2m} + \frac{\vec{p}_2^{\,2}}{2m} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \right] \psi_{100}(\vec{r}_1)\, \psi_{100}(\vec{r}_2)$$

$$\cancel{= \epsilon + (Z^* - Z) e^2 \int d^3 \vec{r}_1}$$

$$\int d^3\vec{r}_1 \int d^3\vec{r}_2\, \psi^*_{100}(\vec{r}_1)\, \psi^*_{100}(\vec{r}_2) \left(\frac{\vec{p}_1^{\,2}}{2m} - \frac{Ze^2}{r_1} \right) \psi_{100}(\vec{r}_1)\, \psi_{100}(\vec{r}_2)$$

$$= \qquad〃 \qquad \left(\frac{\vec{p}_1^{\,2}}{2m} - \frac{Z^* e^2}{r_1} + \frac{(Z^* - Z) e^2}{r_1} \right) 〃$$

$$= \epsilon + (Z^* - Z) e^2 \int d^3\vec{r}_1\, |\psi_{100}|^2 \frac{1}{r_1}$$

$$= \epsilon + (Z^* - Z) e^2 \frac{Z^*}{a_0}$$

$$= \epsilon + Z^* (Z^* - Z)\, m c^2 \alpha^2$$

$$\langle \Psi | H | \Psi \rangle = -\frac{1}{2} m c^2 \alpha^2 \left(2 Z^{*2} + 4 Z^* (Z - Z^*) - \frac{5}{4} Z^* \right)$$

$$= -\frac{1}{2} m c^2 \alpha^2 \left(4 Z Z^* - 2 Z^{*2} - \frac{5}{4} Z^* \right)$$

$Z' = Z - \frac{5}{16}$

$E_0 \simeq -\frac{1}{2} mc^2\alpha^2 \left[2 \quad \left(Z - \frac{5}{16}\right)^2\right] = -77.8\,eV$

$Z = 2$

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döteron = nötron + proton

$$V(r) = -V_0\, e^{-r/r_0} / (r/r_0) \quad \text{Yukawa pot.}$$

$$\psi(r) = A\, e^{-Br/r_0}$$

$$\int d^3\vec{r}\, |\psi(\vec{r})|^2 = 1 = \int_\Omega d\Omega \int_0^\infty r^2 dr\, A^2 e^{-2Br/r_0}$$

$$\Rightarrow 4\pi A^2 \int_0^\infty r^2 dr\, e^{-2Br/r_0} = 1$$

$$= 4\pi A^2 \left(\frac{r_0}{2B}\right)^3 \underbrace{\int_0^\infty y^2 dy\, e^{-y}}_{2} = 1$$

$$\int_0^\infty \underbrace{y^2}_{u} \underbrace{dy\, e^{-y}}_{dv} = \cancel{-y^2 e^{-y}\Big|_0^\infty} + 2\int_0^\infty y\, dy\, e^{-y}$$

$$= 2\left\{ \cancel{-y e^{-y}}\Big|_0^\infty + \int_0^\infty dy\, e^{-y} \right\}$$

$$= -2\, e^{-y}\Big|_0^\infty = 2$$

$$\Rightarrow \cancel{8}\pi A^2 \frac{r_0^3}{\cancel{8} B^3} = 1 \rightarrow A = \left(B^3/\pi r_0^3\right)^{1/2}$$

$$\psi(r) = \left(\frac{B^3}{\pi r_0^3}\right)^{1/2} e^{-Br/r_0} \qquad B \text{ vary. par.}$$

$$E_0 = \min\left\{ \int d^3\vec{r}\, \psi^*(r) \left\{ -\frac{\hbar^2}{2\mu}\vec{\nabla}^2 + V_0 \frac{e^{-r/r_0}}{r/r_0} \right\} \psi(r) \right\}$$

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2

$$E_0 = \min \left\{ \frac{B^3}{\pi r_0^3} \left[4\pi \int_0^\infty r^2 dr\, e^{-Br/r_0} \left(-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) \right.\right.\right.$$

$$\left.\left.\left. \cancel{+} V_0 \frac{e^{-r/r_0}}{r/r_0} \right) e^{-Br/r_0} \right] \right\}$$

$$\cancel{E = \frac{B^3}{\pi r_0^3} 4\pi}$$

$$\frac{d}{dr} e^{-Br/r_0} = -\frac{B}{r_0} e^{-Br/r_0}$$

$$\frac{d}{dr}\left(r^2 \frac{d}{dr} e^{-Br/r_0} \right) = \frac{d}{dr}\left(r^2 \left(-\frac{B}{r_0}\right) e^{-Br/r_0} \right)$$

$$= -\frac{B}{r_0} \left\{ 2r\, e^{-Br/r_0} - r^2 \frac{B}{r_0} e^{-Br/r_0} \right\}$$

$$= -\frac{B}{r_0} \left(2r - r^2 \frac{B}{r_0} \right) e^{-Br/r_0}$$

$$E_0 = \min \left\{ \frac{B^3}{\pi r_0^3} \left[4\pi \int_0^\infty r^2 dr\, e^{-2Br/r_0} \right.\right.$$

$$\left.\left. \left[+ \frac{\hbar^2}{2m} \frac{1}{r^2} \frac{B}{r_0} \left(2r - r^2 \frac{B}{r_0} \right) \cancel{+} V_0 \frac{e^{-r/r_0}}{r/r_0} \right] \right] \right\}$$

$$= \min \left\{ \frac{4\cancel{\pi} B^3}{\cancel{\pi} r_0^3} \frac{\hbar^2}{2m} \frac{B}{r_0} \int_0^\infty dr\, e^{-2Br/r_0} \left(2r - r^2 \frac{B}{r_0} \right) \right.$$

$$\left. \cancel{+} V_0 r_0 \int_0^\infty r\, dr\, e^{-2Br/r_0} e^{-r/r_0} \right\}$$

$$2Br/r_0 = y$$

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$$E_0 = \min \Big\{ \frac{\cancel{4}B^3}{r_0^3} \frac{\hbar^2}{\cancel{2}m} \frac{1}{\cancel{4}} \frac{r_0}{B} \int_0^\infty dy\, e^{-y} \left(y - \frac{1}{4} y^2 \right)$$

$$+ V_0 r_0 \int_0^\infty r\, dr\, e^{-r/r_0 (1+2B)} \Big\}$$

$$\int_0^\infty y^2 dy\, e^{-y} = 2$$

$$\int_0^\infty y\, dy\, e^{-y} = 1$$

$$= \min \Big\{ \frac{B^2 \hbar^2}{2m r_0^2} - 4\pi V_0 \frac{B^3}{\pi r_0^3} r_0 \int_0^\infty r\, e^{-(1+2B) r / r_0} dr \Big\}$$

$$= \min \Big\{ \frac{B^2 \hbar^2}{2m r_0^2} - 4\pi V_0 \frac{B^3}{\pi \cancel{r_0^3}} \cancel{r_0} \frac{\cancel{r_0^2}}{(1+2B)^2} \underbrace{\int_0^\infty y\, dy\, e^{-y}}_{1} \Big\}$$

$$= \min \Big\{ \frac{B^2 \hbar^2}{2m r_0^2} - 4\cancel{\pi} V_0 B^3 \frac{1}{(1+2B)^3} \Big\}$$

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prb. 18.11.) $H = \frac{P^2}{2m} + \lambda x^4$

$$\psi = N e^{-\alpha x^2}$$

$$\langle\psi|\psi\rangle = 1 \Rightarrow N^2 \int_{-\infty}^{+\infty} dx\, e^{-2\alpha x^2} = 1$$

$$N^2 \frac{1}{\sqrt{2\alpha}} \underbrace{\int_{-\infty}^{+\infty} dy\, e^{-y^2}}_{\sqrt{\pi}} = 1$$

$$N = \left(\frac{2\alpha}{\pi}\right)^{1/4}$$

$$\psi = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2}$$

$$\langle H\rangle_0 = E_0 = \min \left\{ \left(\frac{2\alpha}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} \left\{ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \lambda x^4 \right\} \right.$$

$$e^{-\alpha x^2}$$

$$= \left(\frac{2\alpha}{\pi}\right)^{1/2} \left\{ \frac{\hbar^2}{2m} \int_{-\infty}^{+\infty} dx \right.$$

$$\frac{d}{dx}\left(e^{-\alpha x^2}\right) = -2x\alpha e^{-\alpha x^2}$$

$$\int_0^{\infty} x^m e^{-ax^2} dx = \frac{\Gamma((m+1)/2)}{2a^{\frac{m+1}{2}}}$$

$$\frac{d^2}{dx^2}(\psi) = -2\alpha e^{-\alpha x^2} + 4\alpha^2 x^2 e^{-\alpha x^2}$$

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Prb. 18.5 $\Psi = N e^{-\alpha r}$ deneme dalga fonk.'unu kullanarak

3 boyutlu harmonik osilatörün taban durum enerjisini bulunuz.

$$\langle \psi | \psi \rangle = 1 = N^2 \int d\Omega \int_0^\infty r^2 dr\, e^{-2\alpha r}$$

$$\Rightarrow 4\pi \cdot \frac{1}{(2\alpha)^3} \int_0^\infty y^2 dy\, e^{-y} = 1$$

$$4\pi \frac{1}{(2\alpha)^3} \left\{ \cancel{- y^2 e^{-y} \Big|_0^\infty} + 2 \int_0^\infty y\, dy\, e^{-y} \right\} = 1$$

$$\frac{\cancel{\pi}}{\cancel{2}\alpha^3} \left\{ \cancel{- y e^{-y} \Big|_0^\infty} + \int_0^\infty dy\, e^{-y} \right\} = \frac{1}{\alpha^3} \left(- e^{-y} \right)_0^\infty = \frac{1}{\alpha^3}$$

$$\psi = \alpha^{-3/2} e^{-\alpha r}$$

$$E_1 = \min \left\{ \int \Psi^* \left[-\frac{\hbar^2}{2m} \vec\nabla^2 + \frac{1}{2} m \omega^2 r^2 \right] \psi \, d^3\vec r \right\}$$

$$= \min \left\{ \alpha^{-3} \int_0 d\Omega \int_0^\infty r^2 dr\, e^{-\alpha r} \left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{1}{2} m \omega^2 r^2 \right] \times e^{-\alpha r} \right\}$$

$$\frac{d}{dr} e^{-\alpha r} = -\alpha e^{-\alpha r}$$

$$\frac{d}{dr} \left(r^2 (-)\alpha e^{-\alpha r} \right) = -\alpha \left[2r e^{-\alpha r} - \alpha r^2 e^{-\alpha r} \right]$$

$$= \min \left\{ \alpha^{-3} 4\pi \int_0^\infty r^2 dr\, e^{-\alpha r} \left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \left(-\alpha \left(2r e^{-\alpha r} - \alpha r^2 e^{-\alpha r} \right) \right) \right] \right.$$

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2

$$E_0 = \mathrm{Min}\left\{ 4\pi\alpha^{-3} \left[\int_0^\infty r^2 dr \left\{ -\frac{\hbar^2}{2m}\frac{1}{r^2}\left[-\alpha\left(2r e^{-\alpha r} - \alpha r^2\right)\right]\right.\right.\right.$$

$$+ \frac{1}{2} m\omega^2 r^2 \Big\} e^{-2\alpha r}$$

$$= \mathrm{Min}\left\{ 4\pi\alpha^{-3}\left[+ \frac{\hbar^2}{2m}\alpha \int_0^\infty dr \left(2r e^{-\alpha r} - \alpha r^2\right) e^{-2\alpha r}\right.\right.$$

$$+ \frac{1}{2} m\omega^2 \int_0^\infty r^4 e^{-2\alpha r} \Big]\Big\}$$

$$= 4\pi\alpha^{-3}\left\{ \frac{\hbar^2\alpha}{\cancel{2}m}\cancel{2}\int_0^\infty dr\, r e^{-2\alpha r} - \frac{\hbar^2\alpha^2}{2m}\int_0^\infty r^3 e^{-2\alpha r} dr\right.$$

$$\left. + \frac{1}{2} m\omega^2 \int_0^\infty r^4 e^{-2\alpha r} dr \right\}$$

$$= 4\pi\alpha^{-3}\left\{ \frac{\hbar^2\alpha}{m}\frac{1}{(2\alpha)^2}\int_0^\infty y\, dy\, e^{-y} - \frac{\hbar^2\alpha^2}{2m}\frac{1}{(2\alpha)^4}\int_0^\infty y^3 e^{-y} dy\right.$$

$$\left. + \frac{1}{2} m\omega^2 \frac{1}{(2\alpha)^5}\int_0^\infty y^4 dy\, e^{-y}\right\}$$

$$I1 = \int_0^\infty y\, dy\, e^{-y} = 1$$

$$I2 = \int_0^\infty y^3 e^{-y} dy = \cancel{-y^3 e^{-y}\Big|_0^\infty} + 3\int_0^\infty y^2 dy\, e^{-y}$$

$$= 3\left\{\cancel{-y^2 e^{-y}\Big|_0^\infty} + 2\underbrace{\int_0^\infty y\, dy\, e^{-y}}_{1}\right\} = 6$$

$$I3 = \int_0^\infty y^4 dy\, e^{-y} =$$

BS K $= \cancel{-y^4 e^{-y}\Big|_0^\infty} + 4\int_0^\infty y^3 e^{-y} dy = 24.$

$$E_0 = \cancel{4}\pi\alpha^{-3}\left\{\frac{\hbar^2}{\cancel{4}\alpha m} - \frac{\hbar^2}{\cancel{32}\alpha^2 m}\cdot\cancel{8}^{3} + \frac{1}{2}m\omega^2\frac{1}{\cancel{32}\alpha^5}\cdot\cancel{24}^{3}\right\}$$

$$= \frac{\pi\hbar^2}{m}\left\{\frac{1}{\alpha^4} - \frac{3}{4}\frac{1}{\alpha^5} + \frac{3}{2}\left(\frac{m\omega}{\hbar}\right)^2\frac{1}{\alpha^8}\right\}$$

$$\frac{\partial E_0}{\partial\alpha} = 0 \Rightarrow -\frac{4}{\alpha^5} + \frac{3}{4}\cdot\frac{5}{\alpha^6} - \frac{3}{\cancel{2}}\left(\frac{m\omega}{\hbar}\right)^2\frac{\cancel{8}^{1}}{\alpha^9} = 0$$

$$\cancel{-4 + \frac{15}{4}2}$$

$$-4\alpha^4 + \frac{15}{4}\alpha^3 - 12\left(\frac{m\omega}{\hbar}\right)^2 = 0$$

$$\int_0^\infty x^n e^{-ax}\,dx = \frac{\Gamma(n+1)}{a^{n+1}}$$

BS K

4

18.6.) $V(r) = V_0 e^{-r/r_0} \big/ (r/r_0)$

$$\psi = \sqrt{\alpha^3/\pi r_0^3}\; e^{-\alpha r/r_0}$$

$$E_0 = \min \left\{ \frac{\alpha^2 \hbar^2}{2m r_0^2} + \frac{\alpha^3}{\pi r_0^3} 4\pi V_0 \underbrace{\int_0^\infty r^2 \frac{e^{-r/r_0}}{r/r_0} e^{-2\alpha r/r_0} dr}_{-4V_0 \alpha^3 / (1+2\alpha)^2} \right\}$$

$$\frac{dE_0}{d\alpha} = \frac{\alpha \hbar^2}{m r_0^2} - 4V_0 \frac{3\alpha^2 + 6\alpha^3 - 4\alpha^3}{(1+2\alpha)^3}$$

Ek.1. Varyasyon yöntemi kullanarak H atomundaki elektron 2S durumundaki enerjisini bulun.

$$\psi_{2s} = A(1-\gamma r)\, e^{-\beta r}$$

$$\langle \psi_{2s} | \psi_{1s} \rangle = 0 \qquad \langle \psi_{2s} | \psi_{2s} \rangle = 1$$

$$\gamma = (\beta+1)/3 \qquad A = \left[3\beta^5 / \pi(\beta^2 - \beta + 1) \right]^{1/2}$$

$$\int \psi_{2s}^* \left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{d}{dr}\right) - \frac{e^2}{r} \right] \psi_{2s}\, d^3r = E_1$$

$$E_1 = -e^2/8.$$

BS K

#1 Varyasyon yöntemi kullanarak bir boyutlu harmonik salınıcının taban durumu enerjisini bulunuz.

$$\psi_0(x) = A e^{-Bx^2} \qquad B>0 \qquad \psi_0(x\to\pm\infty)\to 0.$$

$$\int_{-\infty}^{+\infty} |\psi_0|^2 dx = 1 = A^2 \int_{-\infty}^{+\infty} e^{-2Bx^2} dx \qquad A = \left(\frac{2B}{\pi}\right)^{1/4}$$

$$\psi_0(x) = \left(\frac{2B}{\pi}\right)^{1/4} e^{-Bx^2}$$

$$E_0 = \mathrm{Min}\left\{ \int_{-\infty}^{+\infty} \psi_0^*(x) \left\{ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \right\} \psi_0(x)\, dx \right.$$

$$= \mathrm{Min}\left\{ +\frac{\hbar^2}{2m} B + \frac{m\omega^2}{8B} \right\} \Rightarrow B = \frac{m\omega}{2\hbar}$$

$$E_0 = (\hbar/2)\,\omega.$$

#2. Varyasyon yöntemi kullanarak, bir boyutlu harmonik salınıcının ilk uyarılmış enerji düzeyini belirleyiniz.

$$\psi_1(x) = C x e^{-Dx^2} \qquad D>0$$

$$\langle \psi_1 | \psi_0 \rangle = 0 \; ; \quad \int_{-\infty}^{+\infty} |\psi_1(x)|^2 dx = 1 \Rightarrow C = \left(\frac{32 D^3}{\pi}\right)^{1/4}$$

$$E_1 = \mathrm{Min}\left\{ \frac{3\hbar^2 D}{2m} + \frac{3m\omega^2}{8D} \right\} \Rightarrow D = \frac{m\omega}{2\hbar} \Rightarrow E_1 = \frac{3\hbar\omega}{2}$$

BS K

7. Hidrojen atomundaki elektronun 2S durumundaki enerjisini varyasyon yöntemi ile belirleyiniz.

$\ell = 0$: r bağımlılığı

$$\psi_{2s} = A\,(1- \quad r)\,e^{-\beta r}$$

$$\langle \psi_{2s} | \psi_{1} \rangle = 0 \qquad \langle \psi_{2s} | \psi_{2s} \rangle = 1$$

$$\alpha = \frac{\beta+1}{3} \qquad A = \left(\frac{3\beta^5}{\pi\,(\beta^2-\beta+1)} \right)^{1/2}$$

$$E_{2s} = \mathrm{Min} \left\{ \int \psi_{2s}^{*} \left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{d}{dr} \right) - \frac{e^2}{r} \right] \psi_{2s} \, d^3\vec{r} \right.$$

$$\beta = 1/2 \Rightarrow E_{2s} = -e^2/8$$

$$\psi_{2s} = \frac{1}{\sqrt{8\pi}} \left(1 - \frac{r}{2}\right) e^{-r/2}$$

BS K

(#) 4.) Hidrojen atomundaki elektronun taban durum enerjisini varyasyon yöntemi ile hesaplayın.

$$\psi_1 = A e^{-Br/a_0}$$

$$\int |\psi_1|^2 d^3 r = 1 \Rightarrow A^2 \int_0^\infty e^{-2Br/a_0} r^2 dr \int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\varphi = 1$$

$$4\pi A^2 \frac{2!}{(2B/a_0)^3} = 1 \Rightarrow A = \left(B^3/\pi a_0^3\right)^{1/2}$$

$$E_0 = \min\left\{ \frac{B^3}{\pi a_0^3} \left[\int e^{-Br/a_0} \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} \right) e^{-Br/a_0} d^3 r \right] \right\}$$

$$E_0 = \min\left\{ \frac{B^2 \hbar^2}{2 a_0^2 m} - \frac{B e^2}{a_0} \right\} \qquad B = \frac{e^2 m a_0}{\hbar^2}$$

$$E_0 = -e^2/2a_0$$

BS K

4

(11) 5.) Bir nötron ile bir proton'un bağlanması

$$V(r) = V_0 \, e^{-r/r_0} / (r/r_0) \qquad r_0 = \hbar/mc$$

potansiyeli aracılığı ile olur. (Döteron)'un taban durumu enerjisini varyasyon yöntemi ile hesaplayınız.

$$\psi = A e^{-\beta r/r_0}$$

$$\int_{-\infty}^{+\infty} |\psi|^2 d^3r = 1 \Rightarrow A = \left(\beta^3/\pi r_0^3\right)^{1/2}$$

$$E_0 = \min \left\{ \frac{\beta^2 \hbar^2}{2m r_0^2} - \frac{\beta^3}{\pi r_0^3} 4\pi V_0 \underbrace{\int_0^\infty r^2 \frac{e^{-r/r_0}}{r/r_0} e^{-2\beta r/r_0} dr}_{} \right\}$$

$$= r_0 \int_0^\infty r \, e^{-(1+2\beta) r/r_0} dr$$

$$= r_0 \Big/ \left[\frac{1+2\beta}{r_0}\right]^2 = \frac{r_0^3}{(1+2\beta)^2}$$

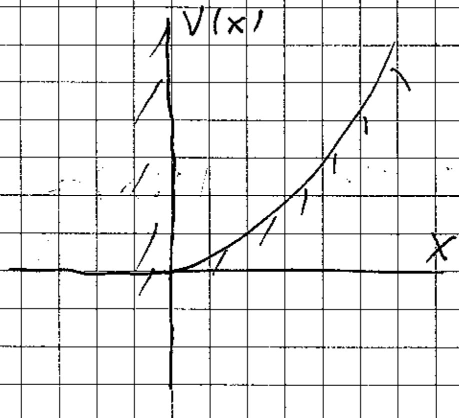
$$E_0 \quad \frac{\beta \hbar^2}{m r_0^2} = 4 V_0 \frac{3\beta^2 + 2\beta^3}{(1+2\beta)^3}$$

$$E_0 = \frac{\beta^2 \hbar^2}{2m r_0^2} - 4 V_0 \frac{\beta^3}{(1+2\beta)^2}$$

BS K

(7) 6.)

$$V = \begin{cases} \dfrac{\hbar^2}{2mb^4} x^2 & x > 0 \\ \infty & x < 0 \end{cases}$$



$$\psi = \left(\frac{(2\alpha)^{2n+1}}{(2n)!} \right)^{1/2} x^n e^{-\alpha x}$$

$$E_a = \min \left\{ \frac{\hbar^2 \alpha^2}{(2n-1)\, 2m} + \frac{(2n+1)(n+1)\hbar^2}{(2\alpha)^2\, m b^4} \right.$$

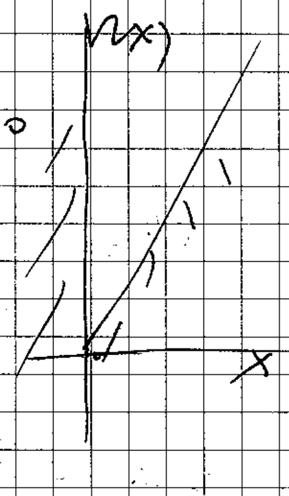
$$\alpha^4 = \frac{(4n^2-1)(n+1)}{2b^4} \qquad \partial E / \partial \alpha = 0$$

$$4\alpha^4 b^4 = (4n+3)(2n-1)^2 \qquad \partial E / \partial n = 0$$

$$E(n) = \left[\frac{(2n+1)(n+1)}{2(2n-1)} \right]^{1/2} \hbar^2 / mb^2$$

(7) 7.)

$$V(x) = \begin{cases} Ax & x > 0 \\ \infty & x < 0 \end{cases} \qquad A > 0$$



$$\psi = \left[1/b\sqrt{\pi} \right]^{1/2} \frac{2x}{b} e^{-x^2/2b^2}$$

$$E_b = \frac{3\hbar^2}{4mb^2} + \frac{2Ab}{\sqrt{\pi}} \Rightarrow b^3 = 3\sqrt{\pi}\,\hbar^2 / 4mA$$

$$E = \left(\frac{81}{4\pi} \right)^{1/3} \left(\frac{A^2 \hbar^2}{m} \right)^{1/3}$$ yukarıdakini de kullanacağız.

BS K

8.)

$$V(x) = \begin{cases} \frac{1}{2} m\omega^2 x^2 + \frac{\alpha}{x^2} ; & x \geq 0 \\ \infty & x < 0 \end{cases}$$

$$\psi = \left(\frac{m\omega'}{\hbar}\right)^{3/4} \frac{2x}{\pi^{1/4}} e^{-m\omega' x^2/2\hbar}$$

1d. [illegible] [illegible]

$$E = \frac{3}{2}\hbar\omega' + \frac{2m\omega'\cancel{\alpha}}{\hbar} + \left(\frac{\omega^2}{\omega'^2} - 1\right)\frac{3}{4}\hbar\omega'$$

$$\omega' = \omega \Big/ \sqrt{1 + \frac{8m\alpha}{3\hbar^2}} \ldots$$

9.)

$$V = \begin{cases} -\alpha\hbar c / x & x \geq 0 \\ \infty & x < 0 \end{cases}$$

$$\psi = \frac{2}{b}\left(1/b\sqrt{\pi}\right)^{1/2} \cancel{x}\, e^{-x^2/2b^2}$$

$$E = \frac{3\hbar^2}{4mb^2} - \frac{2\hbar\alpha c}{b\sqrt{\pi}} \qquad b = 3\hbar\sqrt{\pi} / 4mc\alpha$$

$$E = -\frac{4}{3\pi} mc^2\alpha^2$$

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