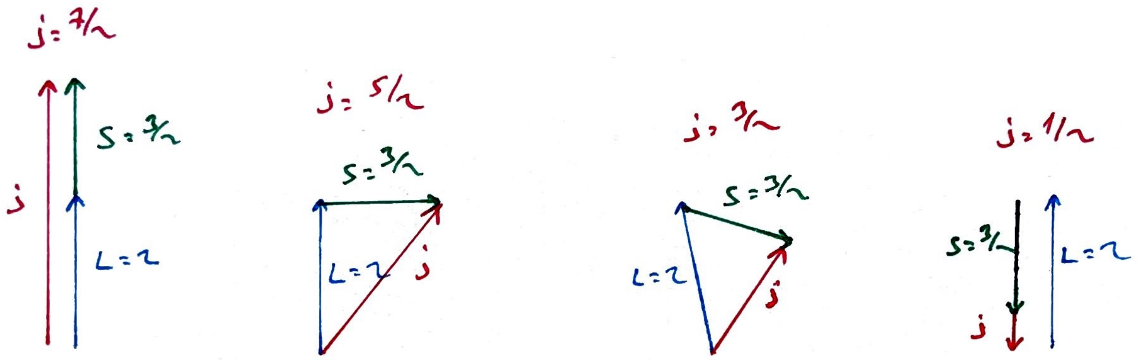
5.1. $L=2$ ve $S=\frac{3}{2}$ olan çok elektronlu bir sistem için mümkün olan j değerlerini vektör gösterimlerini de vererek belirleyiniz.

$$|L-S| \leq j \leq L+S \Rightarrow \left|\frac{3}{2}-2\right| \leq j \leq \left(\frac{3}{2}+2\right) \Rightarrow j: \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$$

$(2S+1) = (2\cdot\frac{3}{2}+1) = 4$ tane



5.2. np^2 yerleşimi için mümkün olan tüm kuantum durumlarını bulunuz.

$np^2 \longrightarrow$ e^- sayısı $= 2$

p: 6 e^- alır $(P_x, P_y, P_z) \longrightarrow l=1, \; m_\ell = 1, 0, -1$

$\uparrow \; \uparrow \; \uparrow$
$P_x \; P_y \; P_z$

$e^- \rightarrow S = 1/2$
$m_s = 1/2, -1/2$
$\uparrow \quad \downarrow$

m_ℓ: 1 0 −1

P_x	P_y	P_z

Pauli dışarlama ilkesi gereği aynı durumda aynı spinli iki e^- olamaz: $\cancel{\boxed{\uparrow\uparrow}}$

	P_x	P_y	P_z
1	↑↓		
2		↑↓	
3			↑↓
4	↑	↑	
5	↓	↓	
6	↑	↓	
7	↓	↑	
8		↑	↑
9		↓	↓
10		↑	↓
11		↓	↑
12	↑		↑
13	↓		↓
14	↑		↓
15	↓		↑

Spektral terim: $^{2|S|+1}L_{j=|L+S|}$

	$m_{\ell 1}$	$m_{\ell 2}$	m_{s1}	m_{s2}	L	S	(Çoklz.T.) Ç.T.	J	Spektral terim
1	1	1	$1/2$	$-1/2$	2	0	1	2	$^1D_2$
2	0	0	$1/2$	$-1/2$	0	0	1	0	$^1S_0$
3	-1	-1	$1/2$	$-1/2$	-2	0	1	2	$^1D_2$
4	1	0	$1/2$	$1/2$	1	1	3	2	$^3P_2$
5	1	0	$-1/2$	$-1/2$	1	-1	3	0	$^3P_0$
6	1	0	$1/2$	$-1/2$	1	0	1	1	$^1P_1$
7	1	0	$-1/2$	$1/2$	1	0	1	1	$^1P_1$
8	0	-1	$+1/2$	$+1/2$	-1	1	3	0	$^3P_0$
9	0	-1	$-1/2$	$-1/2$	-1	-1	3	$\|-2\|$	$^3P_2$
10	0	-1	$1/2$	$-1/2$	-1	0	1	$\|-1\|$	$^1P_1$
11	0	-1	$-1/2$	$1/2$	-1	0	1	$\|-1\|$	$^1P_1$
12	1	-1	$1/2$	$1/2$	0	1	3	1	$^3S_1$
13	1	-1	$-1/2$	$-1/2$	0	-1	3	$\|-1\|$	$^3S_1$
14	1	-1	$1/2$	$-1/2$	0	0	1	0	$^1S_0$
15	1	-1	$-1/2$	$1/2$	0	0	1	0	$^1S_0$

Araş . Gör. Çağlar Çetinkaya
caglarcetinkaya@istanbul.edu.tr

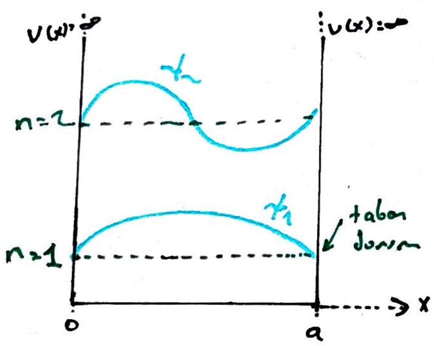
5.3. Birbirleriyle etkileşmeyen iki özdeş parçacık a genişliğinde bir sonsuz kuyu potansiyelinde hareket etmektedirler. Parçacıkların spinsiz olduğunu ve dalga fonksiyonlarının sadece uzay kısmından oluştuğunu varsayarak, parçacıkların;

a) Birer bozon

b) Birer fermiyon

olmaları durumunda taban durum dalga fonksiyonlarını ve enerjilerini ifade ediniz.

Tek parçacık durumu için;



$H|\psi\rangle = E|\psi\rangle \qquad \hat{p} = -i\hbar\vec{\nabla}$

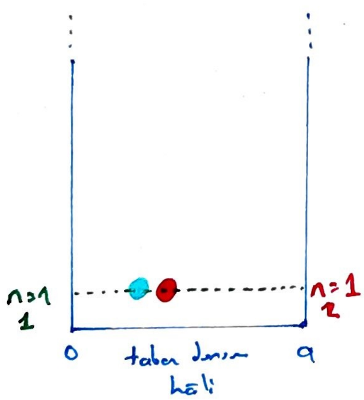
$\frac{p^2}{2m}|\psi\rangle = E|\psi\rangle \quad (0\leq x\leq a) \qquad V(x) = \begin{cases} 0, & 0\leq x\leq a \\ \infty, & \text{other} \end{cases}$

$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}|\psi_n(x)\rangle = E_n|\psi_n\rangle$

$|\psi_n(x)\rangle = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right), \quad E_n = n^2\frac{\pi^2\hbar^2}{2ma^2}, \; n=1,2,\ldots$

$\frac{\pi^2\hbar^2}{2ma^2} = E$

a: Bozonlar: Ayırt edilebilirler. Dalga fonksiyonları simetriktir. Aynı enerji durumunda yığılabilirler.



● 1. bozon : $\psi_{n_1}(x_1) = \sqrt{\frac{2}{a}}\left(\frac{n_1\pi}{a}x_1\right) \rightarrow E_1 = n_1^2 E$

● 2. bozon : $\psi_{n_2}(x_2) = \sqrt{\frac{2}{a}}\left(\frac{n_2\pi}{a}x_2\right) \rightarrow E_2 = n_2^2 E$

$\psi_{n_1n_2}(x_1,x_2) = \psi_{n_1}(x_1)\,\psi_{n_2}(x_2), \quad E_{n_1,n_2} = (n_1^2+n_2^2)E$

$$-\frac{\hbar^2}{2m}\left[\nabla_{x_1}^2\underbrace{\left(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\right)}_{\psi_{n_1n_2}(x_1,x_2)} + \nabla_{x_2}^2\underbrace{\left(\psi_{n_1}(x_1)\psi_{n_2}(x_2)\right)}_{\psi_{n_1n_2}(x_1,x_2)}\right] = \underbrace{E_{n_1n_2}}_{E_{n_1n_2}}\underbrace{\left(\psi_{n_1}\psi_{n_2}\right)}_{\psi_{n_1n_2}(x_1,x_2)}$$

Taban durumunda; $n_1=1$, $n_2=1$

$\psi_{n_1=1}(x_1) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x_1\right), \quad \psi_{n_2=1}(x_2) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x_2\right)$

$E_{n_1=1} = E, \qquad E_{n_2=1} = E$

$\psi_{1,1}^{\text{taban}}(x_1,x_2) = \frac{2}{a}\sin\left(\frac{\pi}{a}x_1\right)\sin\left(\frac{\pi}{a}x_2\right), \quad E_{1,1}^{\text{taban}} = (1^2+1^2)E = 2E$

$\psi_{1,1}^{\text{taban}} \longrightarrow$ simetrik

Araş . Gör. Çağlar Çetinkaya
caglarcetinkaya@istanbul.edu.tr

5.4. Hamilton işlemcisini ve Slater Determinantını,

a) $_{3}Li$

b) $_{6}C$

c) $_{8}O$

elementleri için oluşturunuz.

a: $_{3}Li : 1s^2\, 2s^1$ ($\uparrow\downarrow$ $\uparrow$)

$$|\alpha\rangle = |\tfrac{1}{2}, \tfrac{1}{2}\rangle \;:\; \text{spin up} \qquad (s \;\; m_s)$$

$$|\beta\rangle = |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \;:\; \text{spin down}$$

$$\Psi_{tüm} = \Psi_{nem_\ell}\, \Psi_{spin}$$

$$|\Psi_{tüm}\rangle = |n\, \ell\, m_\ell\rangle\, |s\, m_s\rangle$$

n=2 --- $\uparrow$ → $\phi_{2s}(i)\,\alpha(i)$

n=1 --- $\uparrow$ $\downarrow$ → $\phi_{1s}(i)\,\alpha(i)$, $\phi_{1s}(i)\,\beta(i)$

$$\Psi_{Tüm} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{1s}\,\alpha(1) & \cdots & \phi_{1s}(N)\,\alpha(N) \\ \vdots & & \\ \phi_{n\ell}\,\alpha(1)\,/\,\beta(1) & \cdots & \phi_{n\ell}\binom{\alpha}{\beta} \end{vmatrix}_{N\times N}$$

$N=3$

$$\Psi_{tüm}^{taban} = \frac{1}{\sqrt{3.2.1}} \begin{vmatrix} \phi_{1s}(1)\,\alpha(1) & \phi_{1s}(2)\,\alpha(2) & \phi_{1s}(3)\,\alpha(3) \\ \phi_{1s}(1)\,\beta(1) & \phi_{1s}(2)\,\beta(2) & \phi_{1s}(3)\,\beta(3) \\ \phi_{2s}(1)\,\alpha(1) & \phi_{2s}(2)\,\alpha(2) & \phi_{2s}(3)\,\alpha(3) \end{vmatrix}$$

Hamiltonyen;
$$H = -\frac{\hbar^2}{2m_e}\sum_{i=1}^{N} \nabla_i^2 - \sum_{i=1}^{N} \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{r_i} + \sum_{j>i}^{N}\sum_{i=1}^{N} \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_{ij}}$$

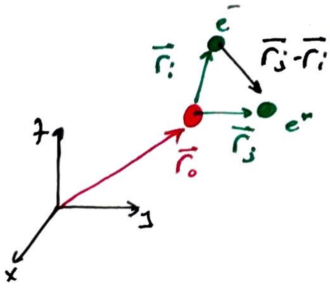
$$H = -\frac{\hbar^2}{2m_e}\sum_{i=1}^{N}\left[\nabla_i^2 + \left(\frac{-Ze^2}{4\pi\varepsilon_0}\right)\frac{1}{r_i}\right] + \frac{1}{2}\sum_{\substack{i\neq j\\ i=1}}^{N} \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r_{ij}}$$

$$r_{ij} = |\vec{r}_i - \vec{r}_j|$$
$$r_i = |\vec{r}_i - \vec{r}_0| = |\vec{r}_i|$$

i. elektronun kinetik enerjisi

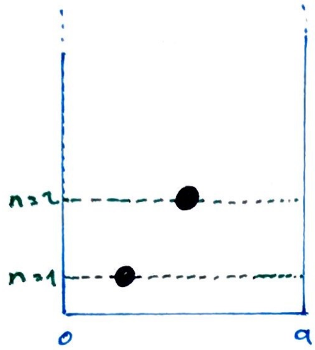
i. elektronun potansiyel enerjisi

i. ve j. elektronlar arasındaki itme potansiyeli



$$H = -\frac{\hbar^2}{2m}\left[\nabla_1^2 + \nabla_2^2 + \nabla_3^2\right] + \left(\frac{-3e^2}{4\pi\varepsilon_0}\right)\left(\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3}\right)$$
$$+ \frac{e^2}{8\pi\varepsilon_0}\left(\frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}}\right) //$$

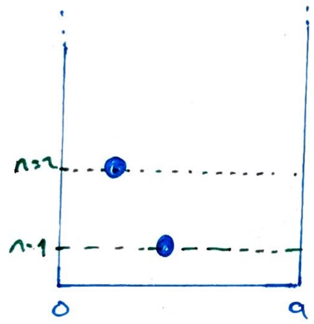
6: Fermiyonlar: Ayırt edilemezler, dalga fonksiyonları asimetriktir. Aynı enerji düzeyinde aynı dalga fonksiyonuna sahip birden fazla fermiyon bulunamaz. (Pauli ilkesi)



● : Fermiyonlar

$$\psi_{12}(x_1,x_2) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x_1\right)\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x_2\right)$$

$$= \frac{2}{a}\sin\left(\frac{\pi}{a}x_1\right)\sin\left(\frac{2\pi}{a}x_2\right), \quad E_{12} = (1^2+2^2)E = 5E$$



$$\psi_{21} = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x_1\right)\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x_2\right)$$

$$= \frac{2}{a}\sin\left(\frac{2\pi}{a}x_1\right)\sin\left(\frac{\pi}{a}x_2\right), \quad E_{21} = (2^2+1^2)E = 5E$$

$$\psi^{taban}(x_1 x_2) = \frac{1}{\sqrt{2}}\left(\psi_{12} - \psi_{21}\right)$$

$$E^{taban} = 5E$$

$$\psi^{taban}(x_1,x_2) = \frac{1}{\sqrt{2}}\left(\frac{2}{a}\sin\left(\frac{\pi}{a}x_1\right)\sin\left(\frac{2\pi}{a}x_2\right) - \frac{2}{a}\sin\left(\frac{2\pi}{a}x_2\right)\sin\left(\frac{\pi}{a}x_2\right)\right)$$

anti-simetrik

✱ Eğer N tane fermiyon olsaydı, taban durum dalga fonksiyonu;

$$\psi^{taban}(x_1,\dots x_n) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \cdots & \psi_1(x_N) \\ \vdots & & & \\ \psi_N(x_1) & \psi_N(x_2) & \cdots & \psi_N(x_N) \end{vmatrix}_{N\times N}$$

Slater Determinantı

$N=2 \Rightarrow$

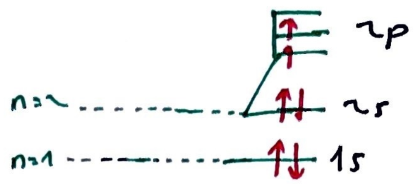
$$\psi^{taban}(x_1,x_2) = \frac{1}{\sqrt{2!}}\begin{vmatrix} \psi_1(x_1) & \psi_2(x_1) \\ \psi_2(x_1) & \psi_2(x_2) \end{vmatrix} = \frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)\right]$$

$$= \frac{1}{\sqrt{2}}\left[\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x_1\right)\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x_1\right) - \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x_1\right)\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x_2\right)\right]$$

$$= \frac{2}{a\sqrt{2}}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi}{a}x_1\right) - \sin\left(\frac{2\pi}{a}x_1\right)\sin\left(\frac{\pi}{a}x_2\right)\right]$$

b: $\,_6C : 1s^2\ 2s^2\ 2p^2$

$\uparrow\downarrow \quad \uparrow\downarrow \quad \uparrow\ \uparrow$



$N=6$

$$\psi^{taban}_{ton} = \frac{1}{\sqrt{6!}} \begin{vmatrix} \phi_{1s}(1)\alpha(1) & \phi_{1s}(2)\alpha(1) & \cdots & \phi_{1s}(6)\alpha(6) \\ \phi_{1s}(1)\beta(1) & \phi_{1s}(2)\beta(2) & \cdots & \phi_{1s}(6)\beta(6) \\ \phi_{2s}(1)\alpha(1) & \phi_{2s}(2)\alpha(2) & \cdots & \phi_{2s}(6)\alpha(2) \\ \phi_{2s}(1)\beta(1) & \phi_{2s}(2)\beta(2) & \cdots & \phi_{2s}(6)\beta(2) \\ \phi_{2p_x}(1)\alpha(1) & \phi_{2p_x}(2)\alpha(2) & \cdots & \phi_{2p_x}(6)\alpha(6) \\ \phi_{2p_y}(1)\alpha(1) & \phi_{2p_y}(2)\alpha(2) & \cdots & \phi_{2p_y}(6)\alpha(6) \end{vmatrix}$$

Hamiltonyen;

$$H = -\frac{\hbar^2}{2m_e}\left[\nabla_1^2 + \nabla_2^2 + \cdots + \nabla_6^2\right] - \frac{6e^2}{4\pi\varepsilon}\left[\frac{1}{r_1} + \frac{1}{r_2} + \cdots + \frac{1}{r_6}\right] + \frac{e^2}{4\pi\varepsilon}\left[\frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{14}} + \frac{1}{r_{15}} + \frac{1}{r_{16}} + \frac{1}{r_{23}} + \frac{1}{r_{24}} + \frac{1}{r_{25}} + \frac{1}{r_{26}} + \frac{1}{r_{34}} + \frac{1}{r_{35}} + \frac{1}{r_{36}} + \frac{1}{r_{45}} + \frac{1}{r_{46}} + \frac{1}{r_{56}}\right]\frac{1}{2}$$

Araş . Gör. Çağlar Çetinkaya
caglarcetinkaya@istanbul.edu.tr