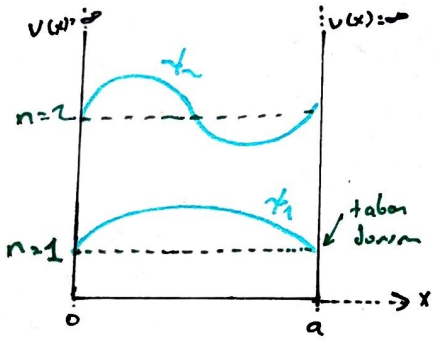
10. Ek1. Birbirleriyle etkileşmeyen iki özdeş parçacık a genişliğinde bir sonsuz kuyu potansiyelinde hareket etmektedirler. Parçacıkların spinsiz olduğunu ve dalga fonksiyonlarının sadece uzay kısmından oluştuğunu varsayarak, parçacıkların;

a) Birer boson

b) Birer fermiyon

olmaları durumunda taban durum dalga fonksiyonlarını ve enerjilerini ifade ediniz.

Tek parçacık durumu için;



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

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

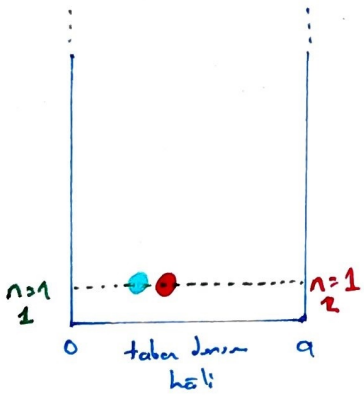
$(0 \le x \le a)$

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

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

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

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



- 1. boson: $\psi_{n_1}(x_1) = \sqrt{\frac{2}{a}}\left(\frac{n_1\pi}{a}x_1\right) \rightarrow E_{n_1} = n_1^2 E$
- 2. boson: $\psi_{n_2}(x_2) = \sqrt{\frac{2}{a}}\left(\frac{n_2\pi}{a}x_2\right) \rightarrow E_{n_2} = n_2^2 E$

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

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

$\psi_{n_1 n_2}(x_1, x_2)$ $\psi_{n_1 n_2}(x_1, x_2)$ E_{n_1,n_2} $\psi_{n_1 n_2}(x_1, x_2)$

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

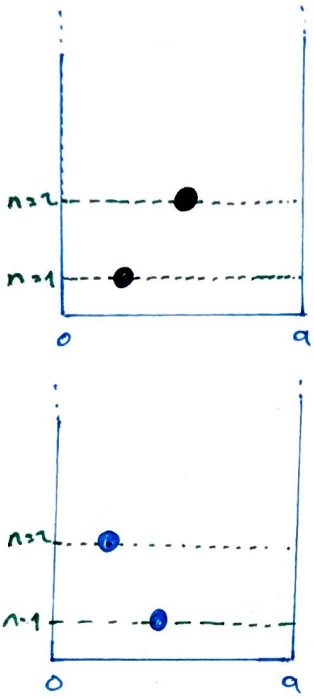
$$\psi_{n_1=1}(x_1) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x_1\right), \quad \psi_{n_2=1}(x_2) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x_2\right)$$

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

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

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

b: Fermiyonlar: Aynı edilenler, dalga fonksiyonları asimetriktir. Aynı enerji durumunda aynı dalgafonksiyonuna sahip birden fazla fermiyon bulunamaz. (Pauli ilkesi)



● : Fermiyonlar

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

$$= \frac{2}{a}\sin\left(\frac{\pi}{a}x_1\right)\sin\left(\frac{2\pi}{a}x_2\right), \quad E_{12} = (1^2+2^2)E_0 = 5E_0$$

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

$$= \frac{2}{a}\sin\left(\frac{2\pi}{a}x_1\right)\sin\left(\frac{\pi}{a}x_2\right), \quad E_{21} = (2^2+1^2)E_0 = 5E_0$$

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

$$E^{taban} = 5E_0$$

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

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

$N=2 \Rightarrow$

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

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

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

10.Ek2. Hamilton işlemcisini ve Slater Determinantını,

a) ${}_3Li$

b) ${}_6C$

c) ${}_8O$

Not: Bu örnek için verilen atomların elektronik konfigürasyonlarının verildiğini kabul edin. Sadece çok elektronlu bir sistemde Slater determinantının ve Hamiltonyenin nasıl oluştuğuna odaklanın. Örnek bütünlüğünü bozmamak adına Atom Fiziği konularını içerecek şekilde çözümü verdim.

elementleri için düşünelim.

a: ${}_3Li : 1s^2\ 2s^1$ (↑↓ ↑)

$|\alpha\rangle = |1/2, 1/2\rangle$: spin up

$|\beta\rangle = |1/2, -1/2\rangle$: spin down

S m_s

$\psi_{tam} = \psi_{mek} \psi_{spin}$

$|\psi_{tam}\rangle = |n\ l\ m_l\rangle |s\ m_s\rangle$

n=2 ---↑------ $\phi_{2s}(i)\alpha(i)$

n=1 --↑-↓----- $\phi_{1s}(i)\beta(i)$

$\phi_{1s}(i)\alpha(i)$

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

$N = 3$

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

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

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

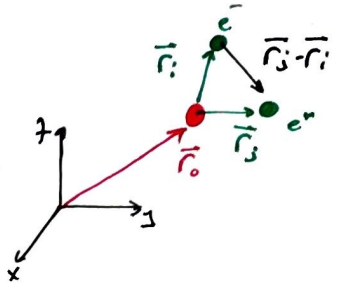
$r_{ij} = |\vec{r}_i - \vec{r}_j|$

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

↑ i. elektronun kinetik enerjisi

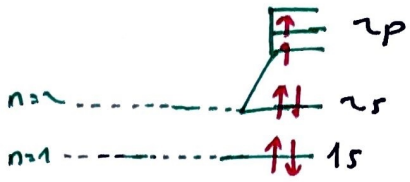
↑ i. elektronun potansiyel enerjisi

↑ i. ve j. elektronlar arasındaki itme potansiyeli



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

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



$N = 6$

$$\psi_{ton}^{taban} = \frac{1}{\sqrt{6!}} \begin{vmatrix} \phi_{1s}(1)\alpha(1) & \phi_{1s}(2)\alpha(1) & \cdots & \phi_{1s}(6)\alpha(6) \\ \phi_{1s}(1)\beta(1) & \phi_{1s}(2)\beta(1) & \cdots & \phi_{1s}(6)\beta(6) \\ \phi_{2s}(1)\alpha(1) & \phi_{2s}(2)\alpha(2) & \cdots & \phi_{2s}(6)\alpha(2) \\ \phi_{2s}(1)\beta(1) & \phi_{2s}(2)\beta(1) & \cdots & \phi_{2s}(6)\beta(2) \\ \phi_{2p_x}(1)\alpha(1) & \phi_{2p_x}(2)\alpha(2) & \cdots & \phi_{2p_x}(6)\alpha(6) \\ \phi_{2p_3}(1)\alpha(1) & \phi_{2p_3}(2)\alpha(2) & \cdots & \phi_{2p_3}(6)\alpha(6) \end{vmatrix}$$

Hamiltonyen;

$$H = -\frac{\hbar^2}{2m_e}\left[\nabla_1^2 + \nabla_2^2 + \cdots + \nabla_6^2\right] - \frac{6e^2}{4\pi\varepsilon}\left[\frac{1}{r_1} + \frac{1}{r_2} + \cdots + \frac{1}{r_6}\right] + \frac{e^2}{4\pi\varepsilon}\left[\frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{14}}\right.$$

$$+ \frac{1}{r_{15}} + \frac{1}{r_{16}} + \frac{1}{r_{23}} + \frac{1}{r_{24}} + \frac{1}{r_{25}} + \frac{1}{r_{26}} + \frac{1}{r_{34}} + \frac{1}{r_{35}} + \frac{1}{r_{36}} + \frac{1}{r_{45}} + \frac{1}{r_{46}}$$

$$\left. + \frac{1}{r_{56}}\right]\frac{1}{2}$$