Lecture 19-QM_II (06/09/00)

Saturday, November 27, 2021 2:50 PM

اتم هلیوم :

^4He

^3He

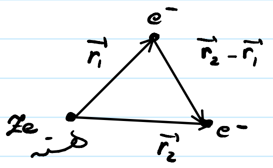
$Z = 2$

$$H = H_1 + H_2 + V_{12}(|\vec{r}_1 - \vec{r}_2|)$$

$$H_1 = \frac{\vec{P}_1^{\,2}}{2m_e} - \frac{Ze^2}{r_1}$$

$$H_2 = \frac{\vec{P}_2^{\,2}}{2m_e} - \frac{Ze^2}{r_2}$$

$$V_{12} = + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$



طیف اتم هلیوم بدون دافعه الکترون-الکترون

$$H_i|\psi\rangle_{(i)} = E_i|\psi\rangle_{(i)} \; ; \; |\psi\rangle_{(i)} = |n \ell m_\ell\rangle_{(i)} \qquad i = 1, 2$$

$$|\psi\rangle = |\psi\rangle_{(1)} |\psi\rangle_{(2)}$$

$$H|\psi\rangle = E|\psi\rangle$$

$$H|\psi\rangle = (H_1 + H_2)(|\psi\rangle_1 \otimes |\psi\rangle_2) = (E_1 + E_2)\; |\psi_1\rangle \otimes |\psi_2\rangle = (E_1 + E_2)|\psi\rangle = E|\psi\rangle$$

$$E = E_1 + E_2 \qquad E_i = -\frac{1Ry}{n_i^2} Z^2$$

$Z = 2$

$$E_{n_1 n_2} = -4Ry\left(\frac{1}{n_1^2} + \frac{1}{n_2^2}\right) \qquad 1Ry = \frac{1}{2} m_e c^2 \alpha^2 = 13.6\,eV$$

1) $n_1 = 1$, $n_2 = 1$

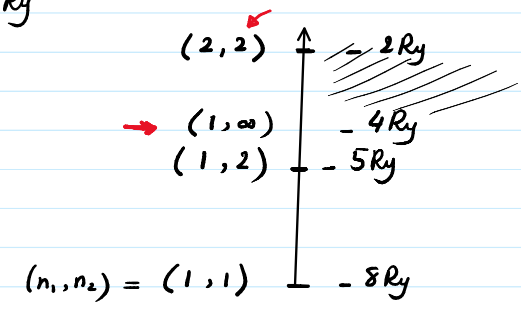
$E_{11} = -8Ry \quad \rightarrow \quad E_{Ion} = -E_1 = 4Ry$, $E_1 = -4Ry$

2) $n_1 = 1$, $n_2 = 2$

$E_{12} = -4Ry\left(1 + \frac{1}{4}\right) = -5Ry$

3) $n_1 = 2$, $n_2 = 2$

$E_{22} = -4Ry\left(2 \times \frac{1}{4}\right) = -2Ry$



تابع موج کل = تابع موج مکانی ⊗ تابع موج اسپینی

singlet $|s, m_s\rangle = |0,0\rangle \qquad \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = |0,0\rangle$

triplet $|s, m_s\rangle = |1, m_s\rangle \qquad |1,1\rangle = |\uparrow\uparrow\rangle$ ✓

$m_s = 0, \pm 1 \qquad |1,0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$

$|1,-1\rangle = |\downarrow\downarrow\rangle$

$|n \ell m_\ell\rangle \qquad |100\rangle$ (n, ℓ, m_ℓ) ✓ اربیتال s

$|100\rangle\;|100\rangle$ تابع موج متقارن

$(|100\rangle_{(1)}|2\ell m_\ell\rangle_{(2)} \pm |2\ell m_\ell\rangle_{(1)}|100\rangle_{(2)})$ → متقارن / پادمتقارن

Ortho He: تابع موج اسپینی متقارن (triplet) ⊗ تابع موج مکانی پادمتقارن = پادمتقارن — ^3He فرمیون

Para He: تابع موج اسپینی پادمتقارن ⊗ تابع موج مکانی متقارن = پادمتقارن — → ^4He بوزون

^3He فرمیون

(triplet)

Para He — تابع موج اسپین پادمتقارن (singlet) ⊗ تابع موج فضا متقارن = پادمتقارن → ^4He بوزون

Ortho He $\quad \frac{1}{\sqrt{2}} \left(|100\rangle |n\ell m\rangle - |n\ell m\rangle |100\rangle \right) |1, m_s\rangle \quad n>1$

Para He $\quad \begin{cases} \frac{1}{\sqrt{2}} \left(|100\rangle |n\ell m\rangle + |n\ell m\rangle |100\rangle \right) |0\,0\rangle & n>1 \\ \to |100\rangle|100\rangle \; |00\rangle_{s\,m_s} \end{cases}$

$$H = H_1 + H_2 + V(r_{12}) \qquad r_{12} = |\vec r_1 - \vec r_2| \qquad V = \frac{e^2}{r_{12}}$$

$$\Delta E^{(1)}_{n_1=1,n_2=1} = \langle 100|\langle 100| \frac{e^2}{r_{12}} |100\rangle|100\rangle \underbrace{\langle 00|00\rangle}_{1}$$

$$= e^2 \int d^3r_1\, d^3r_2 \frac{|\psi_{100}(\vec r_1)|^2 \, |\psi_{100}(\vec r_2)|^2}{|\vec r_1 - \vec r_2|}$$

$$\psi_{100}(\vec r_i) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0} \qquad \boxed{Z=2}$$

$$\Delta E^{(1)}_{11} = e^2 \left(\frac{(Z/a_0)^3}{\pi}\right)^2 \int r_1^2\, dr_1\, r_2^2\, dr_2\, e^{-Zr_1/a_0} e^{-Zr_2/a_0}$$
$$\times \int d\Omega_1\, d\Omega_2 \frac{1}{|\vec r_1 - \vec r_2|}$$

$$d^3r_i = r_i^2\, dr_i\, d\Omega_i \qquad d\Omega_i = d\varphi_i\, d(\cos\theta_i) \qquad i=1,2$$

$$\boxed{\int d\Omega_1\, d\Omega_2 \frac{1}{|\vec r_1 - \vec r_2|} = (4\pi)^2 \frac{1}{\max(r_1, r_2)}}$$

$r_1 > r_2 \quad \max = r_1$

$r_1 < r_2 \quad \max = r_2$

$$\Delta E^{(1)}_{11} = 2.5\ Ry \qquad Z=2$$

$$E^{(0)}_{11} = -8\ Ry$$
$$E_{11} = (-8 + 2.5)\ Ry = -5.5\ Ry$$
$$E^{exp}_{11} = -5.8\ Ry \quad \text{تجربی}$$

روش وردشی $\begin{cases} \tilde{Z} = Z - \frac{5}{16} \cong 1.7 \\ E_{11} = -5.7\ Ry \end{cases}$

اثبات :

$$\int d\Omega_2 \frac{1}{|\vec r_1 - \vec r_2|} = \int_0^{2\pi} d\varphi_2 \int_{-1}^{1} d(\cos\theta_2) \frac{1}{(r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2)^{1/2}}$$

$$= 2\pi \frac{1}{(r_1 r_2)^{1/2}} \int_{-1}^{1} dz \frac{1}{\left(\frac{r_1^2 + r_2^2}{2r_1 r_2} - z\right)^{1/2}}$$

$$= \text{〃} \quad \text{〃} \quad (-2) \sqrt{\frac{r_1^2 + r_2^2}{2r_1 r_2} - z}\ \Big|_{-1}^{1}$$

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

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

$$\int d\Omega_1\, d\Omega_2 \frac{1}{|\vec r_1 - \vec r_2|} = \frac{8\pi^2}{r_1 r_2} \left(r_1 + r_2 - |r_1 - r_2| \right) \quad *$$

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

$$\underbrace{\int d\Omega_1}_{4\pi} \; d\Omega_2 \; \frac{1}{|r_1 - r_2|} = \frac{8\pi^2}{r_1 r_2} \left(r_1 + r_2 - |r_1 - r_2| \right) \quad *$$

$$= (4\pi)^2 \; \frac{1}{\max(r_1, r_2)} \quad \checkmark$$

$$* \quad r_1 > r_2 \qquad \frac{16\pi^2}{r_1}$$

$$r_1 < r_2 \qquad \frac{16\pi^2}{r_2}$$

روش وردشی :

$$H|n\rangle = E_n |n\rangle$$

$$\rightarrow H|\psi\rangle = E|\psi\rangle$$

$$\sum_n |n\rangle\langle n| = 1$$

$$\langle \psi | H | \psi \rangle = \sum_n \langle \psi | H | n \rangle \langle n | \psi \rangle$$

$$= \sum_n E_n \langle \psi | n \rangle \langle n | \psi \rangle \geqslant E_0 \sum_n \langle \psi | n \rangle \langle n | \psi \rangle$$

$$= E_0 \langle \psi | \psi \rangle$$

$$E_0 \leqslant \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \qquad |\psi(\mu)\rangle$$

$$E_0 \leqslant \frac{\langle \psi(\mu) | H | \psi(\mu) \rangle}{\langle \psi(\mu) | \psi(\mu) \rangle} = E(\mu)$$

$$\left. \frac{\partial E(\mu)}{\partial \mu} \right|_{\mu^*} = 0$$

$$\mu^* \rightarrow E(\mu^*) \quad \min$$