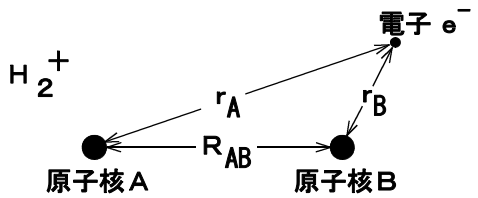
ＸＸＸＩＶ 水素分子の波動関数

【水素分子イオン】

［水素分子イオンのＳｃｈｒ$\ddot{o}$ｄｉｎｇｅｒの方程式］

$$\frac{\hbar^2}{2m_e}\nabla^2\phi + (E-V)\phi = 0 \qquad (34\cdot1)$$

$$V = -\frac{e^2}{4\pi\varepsilon_o r_A} - \frac{e^2}{4\pi\varepsilon_o r_B} + \frac{e^2}{4\pi\varepsilon_o R_{AB}} \qquad (34\cdot2)$$



$$H\phi = E\phi \qquad (34\cdot3)$$

$$H \equiv -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{4\pi\varepsilon_o r_A} - \frac{e^2}{4\pi\varepsilon_o r_B} + \frac{e^2}{4\pi\varepsilon_o R_{AB}} \qquad (34\cdot4)$$

［波動関数］

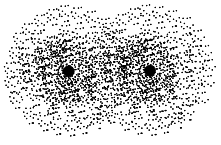
$$\chi_A = \frac{1}{\sqrt{\pi a_o^3}}\exp(-r_A/a_o) \qquad H_A + H_B^+ \qquad (34\cdot5)$$

$$\chi_B = \frac{1}{\sqrt{\pi a_o^3}}\exp(-r_B/a_o) \qquad H_A^+ + H_B \qquad (34\cdot6)$$

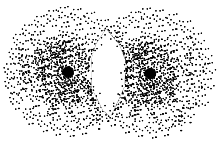
$$\phi = c_A\chi_A + c_B\chi_B \qquad (34\cdot7)$$

$$\int\phi^2 d\tau = 1 \qquad (34\cdot8)$$

$$\phi_S = \frac{1}{\sqrt{2(1+S_{AB})}}(\chi_A+\chi_B) \qquad (34\cdot9)$$



$$\phi_A = \frac{1}{\sqrt{2(1-S_{AB})}}(\chi_A-\chi_B) \qquad (34\cdot10)$$



$$S_{AB} \equiv \exp(-\rho)\cdot\left(1+\rho+\frac{1}{3}\rho^2\right) \quad : 重なり積分 \qquad (34\cdot11)$$

$$\rho \equiv \frac{R_{AB}}{a_o} \qquad (34\cdot12)$$

［エネルギー］

$$E_S = E_o + \frac{e^2}{4\pi\varepsilon_o R_{AB}} + \frac{1}{4\pi\varepsilon_o}\frac{J+K}{1+S_{AB}} \qquad (34\cdot13)$$

$$E_A = E_o + \frac{e^2}{4\pi\varepsilon_o R_{AB}} + \frac{1}{4\pi\varepsilon_o}\frac{J-K}{1-S_{AB}} \qquad (34\cdot14)$$

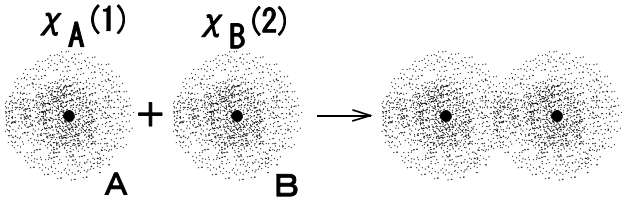
$$J \equiv -\frac{\{1-\exp(-2\rho)\cdot(1+\rho)\}e^2}{R_{AB}} \quad : クーロン積分 \qquad (34\cdot15)$$

$$K \equiv -\frac{-\exp(-\rho)\cdot(\rho+\rho^2)\}e^2}{R_{AB}} \quad : 交換積分 \qquad (34\cdot16)$$

【水素分子】

［原子軌道法 atomic orbital method］

$$\phi = c_1\chi_A(1)\chi_B(2) + c_2\chi_A(2)\chi_B(1) \qquad (34\cdot17)$$



$$\phi_S = \frac{1}{\sqrt{2(1+S^2)}}\{\chi_A(1)\chi_B(2) + \chi_A(2)\chi_B(1)\} \qquad (34\cdot18)$$

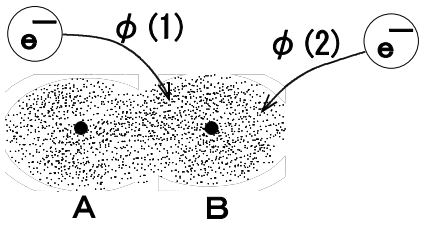
$$\phi_T = \frac{1}{\sqrt{2(1-S^2)}}\{\chi_A(1)\chi_B(2) + \chi_A(2)\chi_B(1)\} \qquad (34\cdot19)$$

［分子軌道法 molecular orbital method］

$$\phi(1) = c_1\chi_A(1) + c_2\chi_B(1) \qquad (34\cdot20)$$

$$\phi(2) = c_1\chi_A(2) + c_2\chi_B(2) \qquad (34\cdot21)$$

$$\phi = \phi(1)\cdot\phi(2) \qquad (34\cdot22)$$



$$\phi_g = \frac{1}{2(1+S)}\{\chi_A(1)+\chi_B(1)\}\{\chi_A(2)+\chi_B(2)\} \qquad (34\cdot23)$$

$$\phi_u = \frac{1}{2(1-S)}\{\chi_A(1)-\chi_B(1)\}\{\chi_A(2)-\chi_B(2)\} \qquad (34\cdot24)$$