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problem-one

Tuesday, 13 November, 2018 20:04

- $Au = \lambda u$ $\qquad\qquad [A, B] = 0$

  $Av = \mu v$

a) $\lambda \neq \mu$ (non-deg.)

$Bu \stackrel{?}{=} \nu u$

$A(Bu) = BAu = B(\lambda u) = \lambda (Bu)$

$\Rightarrow$ Bu is eigenvector of A w/ e.va. λ

λ non-deg. $\Rightarrow$ u is only e.ve. (direction) with λ

$\Rightarrow$ $Bu = \alpha u$ $(\alpha \in \mathbb{R})$

But then u is e.ve. of B w/ e.va. α !

//ly for v.

b) $\lambda = \mu$.

$\rightsquigarrow$ don't need $Bu \parallel u$. spans space: (u, v)

Find eigenvector, $|\psi\rangle$, of B (with eigenvalue b)

$\Rightarrow$ consider $|\psi\rangle = \overset{\text{diff. } \alpha}{\alpha} |u\rangle + \beta |v\rangle$ $\qquad$ recall: $A|u\rangle = \lambda |u\rangle$

(what are α, β ?) $\qquad\qquad\qquad\qquad$ $A|v\rangle = \underset{\lambda = \mu}{\lambda} |v\rangle$

$A|\psi\rangle = \alpha A|u\rangle + \beta A|v\rangle$

$= \alpha \lambda |u\rangle + \beta \lambda |v\rangle$

$$= \alpha\lambda|u\rangle + \beta\lambda|v\rangle$$

$$= \lambda\left(\alpha|u\rangle + \beta|v\rangle\right)$$

$$= \lambda|\psi\rangle$$

$$B|\psi\rangle \stackrel{?}{=} b|\psi\rangle$$

If true:

$$B|\psi\rangle = B\left(\alpha|u\rangle + \beta|v\rangle\right) = \underbrace{\alpha B|u\rangle + \beta B|v\rangle} = b\left(\alpha|u\rangle + \beta|v\rangle\right) = \underbrace{\alpha b|u\rangle + \beta b|v\rangle}$$

side: $\left(\langle u|u\rangle = 1,\ \langle u|v\rangle = 0,\ \langle v|v\rangle = 1\right)$

- $\times\langle u|$: $\alpha\underbrace{\langle u|B|u\rangle}_{B_{uu}} + \beta\underbrace{\langle u|B|v\rangle}_{B_{uv}} = \alpha b$

- $\times\langle v|$: $\alpha\underbrace{\langle v|B|u\rangle}_{B_{vu}} + \beta\underbrace{\langle v|B|v\rangle}_{B_{vv}} = \beta b$

$$\Rightarrow \underbrace{\begin{pmatrix} B_{uu} & B_{uv} \\ B_{vu} & B_{vv} \end{pmatrix}}_{\substack{\text{matrix repr. of} \\ B \text{ in } (u,v) \text{ space}}} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = b \underbrace{\begin{pmatrix} \alpha \\ \beta \end{pmatrix}}_{\substack{\text{vector repr.} \\ \text{of } |\psi\rangle = \alpha|u\rangle + \beta|v\rangle}}$$

Solve e.va, e.ve of $B \Rightarrow$ get $|\psi\rangle$ (get α, β).

problem-two

Monday, 29 October, 2018 18:38

$\langle \Phi | H_0 | \Phi \rangle = ?$

$H_0 = h(\underline{r}_1, \underline{p}_1) + h(\underline{r}_2, \underline{p}_2) \quad ; \quad h(\underline{r}, \underline{p}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r})$

$$\Phi = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_1(\underline{r}_1)\chi_1(1) & \psi_1(\underline{r}_2)\chi_1(2) \\ \psi_2(\underline{r}_1)\chi_2(1) & \psi_2(\underline{r}_2)\chi_2(2) \end{vmatrix}$$

$$= \frac{1}{\sqrt{2}} \Big[\psi_1(\underline{r}_1)\psi_2(\underline{r}_2)\chi_1(1)\chi_2(2) - \psi_1(\underline{r}_2)\psi_2(\underline{r}_1)\chi_1(2)\chi_2(1) \Big]$$

so $\langle \Phi | h(\underline{r}_1, \underline{p}_1) | \Phi \rangle$

$$= \frac{1}{2} \iint d\underline{r}_1 d\underline{r}_2 \Big\{ \Big[\psi_1(\underline{r}_1)^* \psi_2(\underline{r}_2)^* \chi_1(1)^\dagger \chi_2(2)^\dagger - \psi_1(\underline{r}_2)^* \psi_2(\underline{r}_1)^* \chi_1(2)^\dagger \chi_2(1)^\dagger \Big] \times h(\underline{r}_1, \underline{p}_1) \times \Big[\psi_1(\underline{r}_1)\psi_2(\underline{r}_2)\chi_1(1)\chi_2(2) - \psi_1(\underline{r}_2)\psi_2(\underline{r}_1)\chi_1(2)\chi_2(1) \Big] \Big\}$$

check notes

$$= \frac{1}{2} \Big\{ \int d^3r_1\, \psi_1^*(\underline{r}_1)\, h(\underline{r}_1, \underline{p}_1)\, \psi_1(\underline{r}_1) \underbrace{\int d^3r_2\, \psi_2^*(\underline{r}_2)\psi_2(\underline{r}_2)}_{=1 \text{ (norm.)}} \underbrace{\chi_1^\dagger(1)\chi_1(1)}_{=1} \underbrace{\chi_2^\dagger(2)\chi_2(2)}_{=1}$$

$$- \int d^3r_1\, \psi_1^*(\underline{r}_1)\, h(\underline{r}_1, \underline{p}_1)\, \psi_2(\underline{r}_1) \underbrace{\int d^3r_2\, \psi_2^*(\underline{r}_2)\psi_1(\underline{r}_2)}_{=0 \text{ (orthog.)}} \chi_1^\dagger(1)\chi_1(2)\, \chi_2^\dagger(2)\chi_2(1)$$

$$- \int d^3r_1\, \psi_2^*(\underline{r}_1)\, h(\underline{r}_1, \underline{p}_1)\, \psi_1(\underline{r}_1) \underbrace{\int d^3r_2\, \psi_1^*(\underline{r}_2)\psi_2(\underline{r}_2)}_{=0 \text{ (orthog.)}} \chi_1(2)^\dagger \chi_1(1)\, \chi_2^\dagger(1)\chi_2(2)$$

$$+ \int d^3r_1\, \psi_2^*(\underline{r}_1)\, h(\underline{r}_1, \underline{p}_1)\, \psi_2(\underline{r}_1) \underbrace{\int d^3r_2\, \psi_1^*(\underline{r}_2)\psi_1(\underline{r}_2)}_{=1 \text{ (norm.)}} \underbrace{\chi_1^\dagger(2)\chi_1(2)}_{=1} \underbrace{\chi_2^\dagger(1)\chi_2(1)}_{=1} \Big\}$$

$$= \frac{1}{2} \Big\{ \int d^3r_1\, \psi_1^*(\underline{r}_1) h(\underline{r}_1, \underline{p}_1)\psi_1(\underline{r}_1) + \int d^3r_1\, \psi_2^*(\underline{r}_1) h(\underline{r}_1, \underline{p}_1)\psi_2(\underline{r}_1) \Big\}$$

$$= \frac{1}{2} \sum_{i=1}^{2} \int d^3 r_1 \; \psi_i^*(\underline{r}_1)\, h(\underline{r}_1, \underline{p}_1)\, \psi_i(\underline{r}_1)$$

$$= \frac{1}{2} \sum_i \left\{ \int d^3 r_1 \; \psi_i^*(\underline{r}_1) \left[-\frac{\hbar^2}{2m} \nabla^2 \psi_i(\underline{r}_1) \right] + \int d^3 r_1 \; |\psi_i(\underline{r}_1)|^2 \, V(\underline{r}_1) \right\}$$

but r_1 is just a dummy variable:

$$\langle \underline{\Phi} | h(\underline{r}_1, \underline{p}_1) | \underline{\Phi} \rangle$$

$$= \frac{1}{2} \sum_i \left\{ \int d^3 r \; \psi_i^*(\underline{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 \psi_i(\underline{r}) \right] + \int d^3 r \; \rho(\underline{r}) \, V(\underline{r}) \right\}$$

so $\langle \underline{\Phi} | H_0 | \underline{\Phi} \rangle = \langle \underline{\Phi} | \big(h(\underline{r}_1, \underline{p}_1) + h(\underline{r}_2, \underline{p}_2) \big) | \underline{\Phi} \rangle$

$$= \frac{1}{2} \sum_i \left\{ \int d^3 r \; \psi_i^*(\underline{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 \psi_i(\underline{r}) \right] + \int d^3 r \; \rho(\underline{r}) \, V(\underline{r}) \right\}$$

$$+ \frac{1}{2} \sum_i \left\{ \int d^3 r \; \psi_i^*(\underline{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 \psi_i(\underline{r}) \right] + \int d^3 r \; \rho(\underline{r}) \, V(\underline{r}) \right\}$$

$$= \sum_i \left\{ \int d^3 r \; \psi_i^*(\underline{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 \psi_i(\underline{r}) \right] + \int d^3 r \; \rho(\underline{r}) \, V(\underline{r}) \right\} \quad \blacksquare$$

problem-three

Tuesday, 30 October, 2018 9:38

a) Yes, since ϕ_A, ϕ_B are, and there's a $\frac{1}{\sqrt{2}}$ in ψ^{ind}. Explicitly:

$$\langle \psi^{dis}_{AB} | \psi^{dis}_{AB} \rangle = \int d^2r \, |\psi^{dis}_{AB}(\underline{r}, \underline{r}')|^2$$

$$= \iint dr \, dr' \, |\phi_A(\underline{r}) \, \phi_B(\underline{r}')|^2$$

$$= \int dr \, |\phi_A(\underline{r})|^2 \int dr' \, |\phi_B(\underline{r}')|^2$$

$$= 1 \cdot 1 = 1$$

✓ yes.

$$\langle \psi^{ind}_{AB} | \psi^{ind}_{AB} \rangle = \int d^2r \, |\psi^{ind}_{AB}(\underline{r}, \underline{r}')|^2$$

$$\langle \psi | \psi \rangle = \int dx \, |\psi(x)|^2$$

$$= \frac{1}{2} \int d^2r \, | \phi_A(r) \, \phi_B(r') \pm \phi_B(r) \, \phi_A(r') |^2$$

$$= \frac{1}{2} \int d^2r \, \left(\phi_A(r) \, \phi_B(r') \pm \phi_B(r) \, \phi_A(r') \right)^* \left(\phi_A(r) \, \phi_B(r') \pm \phi_B(r) \, \phi_A(r') \right)$$

$$= \frac{1}{2} \int d^2r \, \Big\{ \underbrace{|\phi_A(r)|^2 \, |\phi_B(r')|^2}_{\int dr \, |\phi_A(r)|^2 \int dr' \, |\phi_B(r')|^2 = 1 \cdot 1 = 1} \pm \underbrace{\phi_A^*(r) \, \phi_A(r') \, \phi_B(r) \, \phi_B^*(r')}_{=0} \pm \underbrace{\phi_A^*(r') \, \phi_A(r) \, \phi_B^*(r) \, \phi_B(r')}_{\pm \int dr \, \phi_A(r) \phi_B^*(r) \int dr' \, \phi_A^*(r') \phi_B(r')}$$

$$+ \underbrace{|\phi_B(r)|^2 \, |\phi_A(r')|^2}_{=1} \Big\}$$

$$\underbrace{\int dr \, \phi_A(r) \, \phi_B^*(r)}_{=0}$$

since wfs don't overlap.

$\Leftrightarrow$ orthogonal.

$$= \frac{1}{2} \{ 1 + 1 \}$$

$$= 1$$

b) $\hat{O}_1 = O_1(\underline{r}) + O_1(\underline{r}')$

i) $\langle \psi^{ind}_{AB} | \hat{O}_1 | \psi^{ind}_{AB} \rangle$

$$= \int d^2\underline{r} \;\; \psi^{ind\,*}_{AB}(\underline{r},\underline{r}')\, \hat{O}_1(\underline{r},\underline{r}')\, \psi^{ind}_{AB}(\underline{r},\underline{r}')$$

$$= \frac{1}{2}\int d^2\underline{r} \;\left(\phi_A(\underline{r})\,\phi_B(\underline{r}') \pm \phi_B(\underline{r})\,\phi_A(\underline{r}')\right)^* \left[O_1(\underline{r}) + O_1(\underline{r}')\right]\left(\phi_A(\underline{r})\,\phi_B(\underline{r}') \pm \phi_B(\underline{r})\,\phi_A(\underline{r}')\right)$$

again, cross terms vanish due to orthogonality of ϕ_A & ϕ_B,

$$= \frac{1}{2}\Big[\int d^2\underline{r} \;\; \phi_A^*(\underline{r})\,\phi_B^*(\underline{r}')\,\left(O_1(\underline{r}) + O_1(\underline{r}')\right)\phi_A(\underline{r})\,\phi_B(\underline{r}')$$
$$+ \int d^2\underline{r} \;\; \phi_B^*(\underline{r})\,\phi_A^*(\underline{r}')\,\left(O_1(\underline{r}) + O_1(\underline{r}')\right)\phi_B(\underline{r})\,\phi_A(\underline{r}')\Big]$$

and one integral goes to unity by normalisation:

$$= \frac{1}{2}\Big[\int dr\;\phi_A^*(\underline{r})\,O_1(\underline{r})\,\phi_A(\underline{r}) + \int dr'\;\phi_B^*(\underline{r}')\,O_1(\underline{r}')\,\phi_B(\underline{r}')$$
$$+ \int dr'\;\phi_A^*(\underline{r}')\,O_1(\underline{r}')\,\phi_A(\underline{r}') + \int dr\;\phi_B^*(\underline{r})\,O_1(\underline{r})\,\phi_B(\underline{r})\Big]$$

$$= \sum_{I\in\{A,B\}} \int dr\;\phi_I^*(\underline{r})\;O_1(\underline{r})\;\phi_I(\underline{r})$$

ii) $\langle \psi^{dis}_{AB} | \hat{O}_1(\underline{r},\underline{r}') | \psi^{dis}_{AB} \rangle$

$$= \iint d^3\underline{r} \;\; \phi_A^*(\underline{r})\,\phi_B^*(\underline{r}')\,\left(O_1(\underline{r}) + O_1(\underline{r}')\right)\phi_A(\underline{r})\,\phi_B(\underline{r}')$$

Similarly,

$$= \int d\underline{r}\ \phi_A^*(\underline{r})\, O_1(\underline{r})\, \phi_A(\underline{r}) + \int d\underline{r}'\ \phi_B^*(\underline{r}')\, O_1(\underline{r}')\, \phi_B(\underline{r}')$$

ie the same expression.

c) $\hat{O}_2 = O_2(|\underline{r}-\underline{r}'|)$

i) $\langle \Psi_{AB}^{dis} | \hat{O}_2 | \Psi_{AB}^{dis} \rangle$

$$= \int d^2\underline{r}\ \phi_A^*(\underline{r})\, \phi_B^*(\underline{r}')\ O_2(|\underline{r}-\underline{r}'|)\ \phi_A(\underline{r})\, \phi_B(\underline{r}')$$

$$= \int d^2\underline{r}\ |\phi_A(\underline{r})|^2\, |\phi_B(\underline{r}')|^2\ O_2(|\underline{r}-\underline{r}'|)$$

ii) $\langle \Psi_{AB}^{ind} | \hat{O}_2 | \Psi_{AB}^{ind} \rangle$

$$= \frac{1}{2}\int d^2\underline{r}\ \left(\phi_A(\underline{r})\, \phi_B(\underline{r}') \pm \phi_B(\underline{r})\, \phi_A(\underline{r}')\right)^*\ O_2(|\underline{r}-\underline{r}'|)\ \left(\phi_A(\underline{r})\, \phi_B(\underline{r}') \pm \phi_B(\underline{r})\, \phi_A(\underline{r}')\right)$$

similarly: cross terms vanish leaving

$$= \int d^2\underline{r}\ |\phi_A(\underline{r})|^2\, |\phi_B(\underline{r}')|^2\ O_2(|\underline{r}-\underline{r}'|)$$

so $\langle \Psi_{AB}^{ind} | \hat{O}_i | \Psi_{AB}^{ind} \rangle = \langle \Psi_{AB}^{dis} | \hat{O}_i | \Psi_{AB}^{dis} \rangle$ for $i \in \{1,2\}$.

indistinguishable

ie. we have identical particles, so their wfs must respect exchange symmetry. But since they are localised (seperately), the symmetry (fermionic/bosonic) doesn't affect observable quantities (expectation values of operators) & can be treated as distinguishable.

distinguishable.

which means simpler expressions.

problem-four

Monday, 29 October, 2018 18:12

a) H atom : 1 electron : $\psi(x, y, z) = \psi(\underline{r})$

10^3 points (coarse grid ; cube of side length 10) [10 points per cartesian axis]

$\Rightarrow 10^3$ numbers to be stored (32 bit integers)

$\Rightarrow 4 \times 10^3$ bytes

$\Rightarrow \underline{\underline{4\,kB}}$

b) Li atom : 3 electrons : $\psi(\underline{r}_1, \underline{r}_2, \underline{r}_3) = \psi(x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3)$

$\Rightarrow$ now we need 10^9 numbers

$\Rightarrow$ 4GB (fits on DVD ✓)

c) atom with N electron requires : $(10^3)^N$ numbers $\Rightarrow 4 \times 10^{3N}$ bytes

$m_{DVD} \sim 1g = 10^{-3}\,kg$

i) $M_{earth} \sim 6 \times 10^{24}\,kg = 6 \times 10^{27}$ DVDs

DVD stores $\sim 10GB = 10 \times 10^9$ bytes $= 10^{10}$ bytes

$\Rightarrow 6 \times 10^{37}$ bytes

$$\frac{4 \times 10^{3N}}{6 \times 10^{37}} > 1$$

$$\Rightarrow \tfrac{2}{3} \times 10^{3N-37} = 1 \quad \text{crit}$$

$$10^{3N-37} = 1.5$$

$$3N - 37 = \log_{10} 1.5$$

$$N = \frac{37 + \log 1.5}{3} = 12.4 \quad (3sf)$$

$\Rightarrow$ $N = 13$ exceeds M_{earth} (Al)

ii) $M_{\odot} \sim 2 \times 10^{30}$ kg $= 2 \times 10^{33}$ DVDs $= 2 \times 10^{43}$ bytes

so $N > \frac{43 + \log 1.5}{3} = 14.4$

$\Rightarrow$ $N = 15$ (P)

iii) $M_{MW} \sim 5 \times 10^{11} M_{\odot} = 10^{42}$ kg $= 10^{45}$ DVDs $= 10^{55}$ bytes

$$N > \frac{55 + \log 1.5}{3} = 18.4$$

$\Rightarrow$ $N = 19$ (K)