Assignment (18)

① $\left(-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{e^2}{4\pi\varepsilon_0|\vec{r}_1-\vec{R}_A|} - \frac{e^2}{4\pi\varepsilon_0|\vec{r}_1-\vec{R}_B|} - \frac{e^2}{4\pi\varepsilon_0|\vec{r}_2-\vec{R}_A|} - \frac{e^2}{4\pi\varepsilon_0|\vec{r}_2-\vec{R}_B|} + \frac{e^2}{4\pi\varepsilon_0|\vec{r}_1-\vec{r}_2|} + \frac{e^2}{4\pi\varepsilon_0|\vec{R}_A-\vec{R}_B|}\right)\psi_{el}(\vec{r}_1,\vec{r}_2|\vec{R}_A,\vec{R}_B) = U(\vec{R}_A,\vec{R}_B)\,\psi_{el}(\vec{r}_1,\vec{r}_2|\vec{R}_A,\vec{R}_B)$

$\left(-\frac{\hbar^2}{2M}\nabla_A^2 - \frac{\hbar^2}{2M}\nabla_B^2 + U(\vec{R}_A,\vec{R}_B)\right)\chi_n(\vec{R}_A,\vec{R}_B) = E\,\chi_n(\vec{R}_A,\vec{R}_B)$

② $\langle\psi|\hat{A}\hat{B}|\psi\rangle = \langle\psi|\hat{A}\hat{B}\psi\rangle^* = \langle\hat{B}\hat{A}\psi|\psi\rangle$

$\langle\psi|\hat{A}\hat{B}\psi\rangle = \langle\hat{B}\hat{A}\psi|\psi\rangle$ only if $(\hat{A}\hat{B}=\hat{B}\hat{A}) \longrightarrow [\hat{A},\hat{B}]=0$

③ $\left[-\frac{1}{2}\nabla^2 + V_{3D\text{-}box} + V_{light}\right]\Psi = E\Psi$

④ $\sigma_{S_x}^2 = \langle\psi|\hat{S}_x^2|\psi\rangle - (\langle\psi|\hat{S}_x|\psi\rangle)^2 = \langle\psi|\hat{S}_x^2|\psi\rangle$

$\sigma_{S_y}^2 = \langle\psi|\hat{S}_y^2|\psi\rangle - (\langle\psi|\hat{S}_y|\psi\rangle)^2 = \langle\psi|\hat{S}_y^2|\psi\rangle$

> because average spin is zero about x an y if the atom is an eigenstate of $\hat{S}_z$

$\sigma_{S_x}\sigma_{S_y} \geq \frac{1}{2}\hbar|\langle\psi|[\hat{S}_x,\hat{S}_y]|\psi\rangle| = \frac{1}{2}\hbar|\langle\psi|\hbar\hat{S}_z|\psi\rangle|$

$\sigma_{S_x}^2\sigma_{S_y}^2 \geq \frac{1}{4}\hbar^2|\langle\psi|\hbar\hat{S}_z|\psi\rangle|^2 = \frac{1}{4}\hbar^4\left|\frac{3}{2}\hbar\right|^2 = \frac{9}{16}\hbar^6$

$\langle\psi|\hat{S}_x^2|\psi\rangle\langle\psi|\hat{S}_y^2|\psi\rangle \geq \frac{9}{16}$ a.u.

⑤ $[Xe]4f^{11}6s^2$, ^4I

a) $L = 6$

b) $M_L = \pm6, \pm5, \pm4, \pm3, \pm2, \pm1, 0$

c) $S = \frac{4-1}{2} = \frac{3}{2}$

d) $M_S = \pm\frac{3}{2}, \pm\frac{1}{2}$