Tutorial 5 - Answers

1. $$\hat{H} = \frac{-\hbar^2}{2m_N}\nabla_N^2 - \frac{\hbar^2}{2m_e}\sum_i^n \nabla_i^2 - \frac{Ze^2}{4\pi\varepsilon_0}\sum_i^n \frac{1}{r_i} + \frac{e^2}{4\pi\varepsilon_0}\sum_i^{n-1}\sum_{j>i}^{n}\frac{1}{r_{ij}}$$

2. Orbital approximation:

The wavefunction of an n-electron system can be written as the product of n one-electron wavefunctions.

$$\psi(1,2,\dots n) = \phi(1)\cdot\phi(2)\cdot\phi(3)\dots\phi(N)$$

It doesn't neglect inter-electronic repulsion.

3. $\alpha(1)\beta(2)$, $\beta(1)\alpha(2)$

↓

both are not acceptable as they violates indistinguishability condition.

→ The given slater determinant for excited state of He is also not acceptable as it also violates indistinguishability condition.

As per the wavefunction, electron in 2s orbital can only have α spin and electron in 3s orbital can only have β spin.

4.

$$\psi_1 = \frac{1}{2}\begin{vmatrix} 1s(1)\alpha(1) & 2s(1)\beta(1) \\ 1s(2)\alpha(2) & 2s(2)\beta(2) \end{vmatrix} - \frac{1}{2}\begin{vmatrix} 1s(1)\beta(1) & 2s(1)\alpha(1) \\ 1s(2)\beta(2) & 2s(2)\beta(2) \end{vmatrix}$$

$$\psi_2 = \frac{1}{\sqrt{2}}\begin{vmatrix} 1s(1)\alpha(1) & 2s(1)\alpha(1) \\ 1s(2)\alpha(2) & 2\,(2)\alpha(2) \end{vmatrix}$$

$$\psi_3 = \frac{1}{\sqrt{2}}\begin{vmatrix} 1s(1)\beta(1) & 2s(1)\beta(1) \\ 1s(2)\beta(2) & 2s(2)\beta(2) \end{vmatrix}$$

$$\psi_4 = \frac{1}{2}\begin{vmatrix} 1s(1)\alpha(1) & 2s(1)\beta(1) \\ 1s(2)\alpha(2) & 2s(2)\beta(2) \end{vmatrix} + \frac{1}{2}\begin{vmatrix} 1s(1)\beta(1) & 2s(1)\alpha(1) \\ 1s(2)\beta(2) & 2s(2)\alpha(2) \end{vmatrix}$$

5. (a) $\alpha(1)\alpha(2)$

(b) The spin wavefunction is an eigenfunction of $\hat{S}^2_{total}$ operator.