

2. A suitable Hamiltonian 'H' which takes into account the mutual interactions of the electrons as well as spin orbit interaction is,

$$(a) H = \sum_{i=1}^z \left[ \frac{-\hbar^2}{2m} \nabla_i^2 - \frac{ze^2}{r_i} - \sum_i (r_i) \vec{l}_i \cdot \vec{s}_i \right] + \sum_{i,j} \frac{l^2}{r_{ij}}$$

$$(b) H = \sum_{i=1}^z \left[ \frac{-\hbar^2}{2m} \nabla_i^2 - \frac{ze^2}{r_i} \right] + \sum_{i,j} \frac{e^2}{r_{ij}}$$

$$(c) H = \sum_{i=1}^z \left[ \frac{-\hbar^2}{2m} \nabla_i^2 - \frac{ze^2}{r_i} \right] - \sum_i (r_i) \vec{l}_i \cdot \vec{s}_i$$

$$(d) H = \sum_{i=1}^z \left[ \frac{-\hbar^2}{2m} \nabla_i^2 + \frac{e^2}{r_i} \right] - \sum_i \frac{ze^2}{r_i}$$

3. The spectroscopic value for the internuclear distance for H<sub>2</sub>-molecule is

- (a) 2.5 Å<sup>o</sup>                      (b) 0.02 Å<sup>o</sup>  
 (c) 0.74 Å<sup>o</sup>                      (d) 0.002 Å<sup>o</sup>

4. If 'ρ' is density matrix and  $\hat{F}$  is any operator then  $\langle \hat{F} \rangle$  is

- (a) Trace  $\left( \frac{\rho}{\hat{F}} \right)$                       (b) Trace (ρ)  
 (c) Trace  $\left( \frac{\hat{F}}{\rho} \right)$                       (d) Trace ( $\hat{F} \rho$ )

5. Lagrangian equation for the generalised co-ordinate  $\bar{a}_i$  is,

$$(a) \frac{\partial L}{\partial \bar{a}_i} - \frac{\partial L}{\partial a_i} = 0$$

$$(b) \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{\bar{a}}_i} \right) - \frac{\partial L}{\partial \bar{a}_i} = 0$$

$$(c) \frac{\partial L}{\partial a_i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{\bar{a}}_i} \right) = 0$$

$$(d) \frac{d}{dt} \left( \frac{\partial L}{\partial a_i} \right) - \left( \frac{\partial L}{\partial \dot{\bar{a}}_i} \right) = 0$$

Answer ALL questions in 1 or 2 sentences :

- Give the connecting relation between scattering amplitude and scattering cross section.
- What is the type of atoms for which Thomas Fermi method is suited to?
- Give the meaning of 'self-consistent'.
- How will you represent spin  $\frac{1}{2}$ -density matrix?
- Define Hermitian operator  $N_i$  through creation operator  $a_i$  and annihilation operator  $a_i^*$ .