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1. Untuk molekul $HeH^+$ terdiri dari 2 Nuclei (He dan H) dan 2 elektron ($Z_{He} = 2$, $Z_H = 1$)

$$\hat{H}_{HeH^+} = \underbrace{-\frac{1}{2M_{He}}\nabla^2_{R_{He}}}_{\text{Kinetic energi of He}} - \underbrace{\frac{1}{2M_H}\nabla^2_{R_H}}_{\text{Kinetik energi of H}} - \underbrace{\sum_{i=1}^{2}\frac{1}{2}\nabla^2_{r_i}}_{\text{kinetik energi of elektron i}}$$

$$- \underbrace{\sum_{i=1}^{2}\frac{2}{|r_i - R_{He}|}}_{\text{electron attraction of He}} - \underbrace{\sum_{i=1}^{2}\frac{1}{|r_i - R_H|}}_{\text{electron attraction to H}} + \underbrace{\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{1}{|r_i - r_j|}}_{\text{electron-electron Repulsion}}$$

$$+ \underbrace{\sum_{i=1}^{2}\sum_{J=1}^{2}\frac{Z_i Z_j}{|R_i - R_j|}}_{\text{nuclei-nuclei Repulsion}} \rightarrow \text{asumsi}$$

$Z_i = Z_{He}$

$Z_j = Z_H$

2. Fungsi gelombang Elektronik anti simetrik $HeH^+$

•) Fungsi gelombang Electronik $HeH^+$

$$\Phi_1 HeH^+ = \chi_i(\vec{r}_1, \sigma_1)\, \chi_j(r_i, \sigma_i) \rightarrow \text{Simetrik}$$

•) Sesuai prinsip pauli, Fungsi yang anti simetrik menjadi

$$\Phi_2 HeH^+ = \chi_i^{\circ}(\vec{r}_1 \sigma_2)\, \chi_j^{\circ}(\vec{r}_1 \sigma_1) \rightarrow \text{anti simetrik}$$

•) fungsi lengkapnya menjadi (dengan normalisasi $\frac{1}{\sqrt{2}}$)

$$\Phi = \frac{1}{\sqrt{2}} [\chi_i(\vec{r}_1, \sigma_1)\chi_j(\vec{r}_2, \sigma_2) - \chi_i(\vec{r}_2 \sigma_2)\chi_j(\vec{r}_1 \sigma_1)]$$

•). dalam bentuk determinan Slater

$$\Phi = \frac{1}{\sqrt{2}} \begin{vmatrix} \chi_i(\vec{r}_1, \sigma_1) & \chi_j(\vec{r}_1 \sigma_1) \\ \chi_i(\vec{r}_2, \sigma_2) , & \chi_j(r_2, \sigma_2) \end{vmatrix}$$

3. Fungsi kerapatan elektron dan HeH⁺ berdasarkan no 2.

contoh : $\Psi(\vec{r}, \omega, \vec{r}_2, \omega_2 \ldots r_H, \omega_n)$

$$\rightarrow n(r) = He_{+}s \int \ldots \int \Psi(\vec{r}, \omega, \vec{r}_2 \omega_2 \ldots r_{Hei}, \omega_{Hei})$$

$$\Psi(\vec{r}_1 \omega_1 \vec{r}_2 \omega_2), \ldots\ldots \vec{r}_{nd}, \omega_{He}) d\omega d\vec{r}_2 d\omega_2$$

$$\ldots d\vec{r}_{Hed} d\omega_{Hel})$$

untuk HeH⁺, wave fungcion

$$\Psi(\vec{r}_1, \sigma_1, r_2 \sigma_2)$$

maka fungsi kerapatan elektron menjadi

$$n(r) = \iint \Psi^*(\vec{r}_1, \sigma_1, \vec{r}_2, \sigma_2) \Psi(\vec{r}_1, \sigma_2, \vec{r}_2 \sigma_2)$$

$$d\vec{r}_1 d\sigma_1, d\vec{r}_2, d\sigma_2.)$$

4. Buktikan (dengan menganggap elektron tidak terbedakan)

$$\int \ldots \int \psi^* \left( \sum_{i=1}^{N_{el}} V_{ext}(r_i) \psi \, dx_1 \ldots dx_{N_e} \right.$$

dapat di reduksi menjadi

$$= \int V_{ext}(\vec{r}) n(\vec{r}) \, dr$$

dengan $N_{el} = \int n(\vec{r}) dr$

$dN_{el} = n(\vec{r}) d\vec{r})$

External potential contribution to energy expectation value depend on electron density

$$H = \sum_{i=1}^{n} \frac{\vec{\nabla}_i^2}{2m_e} + \sum_{i=j}^{n} \frac{e^2}{|r_i - r_j|} + \sum_{i}^{n} V_{ext}(r_i \{R\})$$

$$\langle H \rangle = \langle \psi | T | \psi \rangle + \langle \psi | V | \psi \rangle + \sum_{i}^{n} | V_{ext}(r_i) | \psi \rangle$$

$$\langle \psi | V_{ext}(r_k) | \psi \rangle = \int dx_1 dx_2 \ldots dx_n \psi^* (\{r_i\}) V(r_k) \psi(\{r_i\})$$

$$\langle \psi | V_{ext}(r_k) | \psi \rangle = \int V_{ext}(r_k) dr_k \int dx \, |\psi(\{r_i\})|^2$$

$$\langle \psi | V_{ext}(r) | \psi \rangle = \int V_{ext}(r) n(r) \, dr$$