Student Number:______________________ Name: ______________________________

Quiz 9

1. **Write the molecular Hamiltonian for LiH^+ molecular cation, including the dependence on constants like** $\hbar, e, \varepsilon_0, m_e, \ldots$**.**

2,3. Write the electronic and nuclear Schrödinger equations for the *P*-atom *N*-electron molecule. You can use atomic units.

4. **What are the eigenenergies for <u>one</u> electron in a <u>three-dimensional</u> harmonic well with force constant *k*?**

   $E_{n_x n_y n_z} =$

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Quiz 9

1. **Write the molecular Hamiltonian for LiH^+ molecular cation, including the dependence on constants like $\hbar, e, \varepsilon_0, m_e, \ldots$.**

$$\hat{H}_{\mathrm{LiH}^+} \equiv \overbrace{-\tfrac{\hbar^2}{2M_H}\nabla_H^2 - \tfrac{\hbar^2}{2M_{Li}}\nabla_{Li}^2}^{\text{nuclear k.e.}} \overbrace{-\tfrac{\hbar^2}{2m_e}\nabla_1^2 - \tfrac{\hbar^2}{2m_e}\nabla_2^2 - \tfrac{\hbar^2}{2m_e}\nabla_3^2}^{\text{electronic k.e.}} + \overbrace{\frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_1-\mathbf{r}_2|} + \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_1-\mathbf{r}_3|} + \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_2-\mathbf{r}_3|}}^{\text{electron-electron repulsion p.e.}} + \overbrace{\frac{3e^2}{4\pi\varepsilon_0|\mathbf{R}_H-\mathbf{R}_{Li}|}}^{\text{nuclear-nuclear repulsion p.e.}}$$

$$\underbrace{-\frac{3e^2}{4\pi\varepsilon_0|\mathbf{r}_1-\mathbf{R}_{\mathrm{Li}}|} - \frac{3e^2}{4\pi\varepsilon_0|\mathbf{r}_2-\mathbf{R}_{\mathrm{Li}}|} - \frac{3e^2}{4\pi\varepsilon_0|\mathbf{r}_3-\mathbf{R}_{\mathrm{Li}}|} - \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_1-\mathbf{R}_{\mathrm{Li}}|} - \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_2-\mathbf{R}_{\mathrm{Li}}|} - \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_3-\mathbf{R}_{\mathrm{Li}}|}}_{\text{electron-nuclear attraction p.e.}}$$

2,3. **Write the electronic and nuclear Schrödinger equations for the *P*-atom *N*-electron molecule. You can use atomic units.**

$$\left(\sum_{i=1}^{N}\tfrac{-1}{2}\nabla_i^2 + \sum_{i=1}^{N}\sum_{\alpha=1}^{P} -\frac{Z_\alpha}{|\mathbf{r}_i-\mathbf{R}_\alpha|} + \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|} + \frac{1}{2}\sum_{\alpha=1}^{P}\sum_{\substack{\beta=1\\ \beta\neq\alpha}}^{N}\frac{1}{|\mathbf{R}_\alpha-\mathbf{R}_\beta|}\right)\psi_e(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N|\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_P)$$

$$= U(\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_P)\psi_e(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N|\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_P)$$

$$\left(\sum_{\alpha=1}^{P}\frac{-1}{2M_\alpha}\nabla_\alpha^2 + U(\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_P)\right)\chi_n(\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_P) = E_{\mathrm{mol}}\chi_n(\mathbf{R}_1,\mathbf{R}_2,\ldots,\mathbf{R}_P)$$

4. **What are the eigenenergies for <u>one</u> electron in a <u>three-dimensional</u> harmonic well with force constant *k*?**

$$E_{n_x n_y n_z} = \frac{\hbar}{2}\sqrt{\frac{k}{m_e}}\left(2n_x + 2n_y + 2n_z + 3\right)$$

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