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Minor I

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The 6 π-electrons of benzene can be modeled as independent, free particles on a ring with a radius of 134 pm. The Hamiltonian for a π-electron is $-\frac{\hbar^2}{2mr^2}\frac{\partial^2}{\partial\phi^2}$.

1. What are the boundary conditions satisfied by the solutions to the Schrödinger equation?
2. What are the solutions to the Schrödinger equation satisfying the boundary condition in 1? [5]
3. Write the energies of the three lowest levels and identify the quantum numbers of the states in these levels. [5]
4. According to this model, at what wavelength (in nm) does the lowest energy absorption occur? ($m_e = 9.109 \times 10^{-31}$ kg, $h = 6.626 \times 10^{-34}$ J s^{-1}, $c = 3.0 \times 10^8$ m s^{-1}) [10]

An electron in H-atom is in the state $\psi(r,\theta,\phi) = \frac{1}{4\sqrt{2\pi a_0^3}}\frac{r}{a_0}e^{-\frac{r}{2a_0}}\cos\theta$.

5. Plot ψ as a function of z. [5]
6. Find $\langle x\rangle$. Information you might need: $\int_0^\infty x^n e^{-ax}\,dx = \frac{n!}{a^{n+1}}$ [10]
7. What is the most probable radius? [5]
8. In this state, what is the orbital angular momentum and its z-projection? [5]

Two electrons are confined on a square sheet with a unit positive charge fixed in the center.

9. Write the Hamiltonian for the system. [10]
10. Do you expect the solution to the Schrödinger equation to be of the form $\psi(x_1,y_1,x_2,y_2) = \phi_1(x_1,y_1)\phi_2(x_2,y_2)$? Why or why not? [5]

Consider the molecule, H_3^{2+}, composed of three protons (A, B, and C) and one electron with the protons at the corners of an equilateral triangle.

11. Write down the complete Hamiltonian for this system in atomic units. [5]
12. A possible LCAO MO for the system is $\psi = c(1s_A + 1s_B + 1s_C)$, where $1s_A$, $1s_B$, and $1s_C$ denote the normalized H-atom 1s state at A, B, and C respectively. Normalize ψ. What is the physical significance of the integrals that appear in your expression? [10]
13. Decide, with a justification, whether ψ is a bonding or antibonding MO. Marks only if the justification is correct. [5]

Obtain an expression for the approximate energy of ψ. Use standard notation for the integrals. Which of these integrals is responsible for bond formation? [15]