Section 1. True/False: Write T(rue)/F(alse) in the space provided (4×2 pts.)

True Maximum electron probability density in the ground state of H_2^+ occurs at each nucleus.

False For $2p_x$ and $2p_y$ atomic orbitals, the three quantum numbers – principal, orbital angular momentum, and magnetic – are 2, 1, and ± 1, respectively.

False The Born-Oppenheimer approximation will introduce more error for diatomic Cs_2 than for diatomic H_2.

False The ground-state energy of H atom calculated using a trial wavefunction $\phi = e^{-\alpha r}$ is greater than the true ground-state energy of H atom.

Section 2. Fill in the blanks (4 pts. per blank)

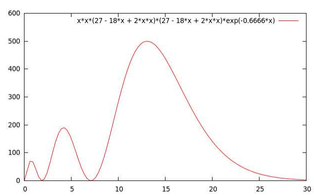
1. The normalization constant, N, for $\phi_+ = N\left(\psi_{1s_A} + \psi_{1s_B}\right)$ is $\frac{1}{\sqrt{2(1+S)}}$.
2. The Hamiltonian operator for H_2^+ (in atomic units) in the Born-Oppenheimer approximation is $-\frac{1}{2}\nabla^2 - \frac{1}{r_A} - \frac{1}{r_B} + \frac{1}{R}$.
3. The spherical harmonic $Y_{3,-1}(\theta, \phi)$ is an eigenfunction of the $\hat{L}_x^2 + \hat{L}_y^2$ operator with the eigenvalue $11\hbar^2$.
4. An example of a quantum-mechanical system for which the spacing between energy (E) levels (a) increases as E increases is particle-in-a-box, rotation in 2D, rotation in 3D, (b) remains the same as E increases is harmonic oscillator, and (c) decreases as E increases is the hydrogen atom.
5. In H_2^+ the integral representing the interaction of the electron density of the electron around nucleus A with the nucleus B has the form $-\int \frac{1s_A * 1s_A}{r_B} d\tau$. The form of the integral responsible for chemical bonding is $-\int \frac{1s_B * 1s_A}{r_B} d\tau$.

Section 3. Answer in the space provided (2×5 pts.)

Consider a H atom in the state $\psi = \frac{1}{81\sqrt{3\pi a_0^3}}\left(27 - \frac{18r}{a_0} + \frac{2r^2}{a_0^2}\right) e^{-r/3a_0}$.

1. Sketch the radial distribution function versus r.

Answer:



2. Sketch the radial wave function versus r.

Answer: