CH4102-2018. Mid Semester Examination.

$2 \times 10 = 20$. Time 1 hr.

(Please answer to the point and avoid round-about routes.)

1. Indicate which of the following functions are "acceptable" ($-\infty \leq x \leq \infty$). If one is not, give a reason: (i) $\psi = x$ (ii) $\psi = x^2$ (iii) $\psi = \sin x$ (iv) $\psi = \exp(-x)$ (v) $\psi = \exp(-x^2)$.

2. Let S and A be respectively symmetric and antisymmetric functions for the operator R, with $RS = S$ and $RA = -A$. Evaluate the following, where R operates on every function to its right. (i) RSS (ii) RAA (iii) RAS (iv) $RSASA$ (v) $RSASAS$ (vi) $RSASASA$ (vi) $RAASASSA$ (vii) $RAASASAA$. Can you think of a simple general rule for telling when a product of symmetric and antisymmetric functions will be antisymmetric?

3. An unnormalized eigenfunction for the H atom is given by: $\psi = (27 - 18r + 2r^2)\exp(-r/3)$ (i) write l, m values (ii) how many radial nodes does this function possess? (iii) find out the energy of this state in Hartree unit (atomic unit).

4. Without comparing to tabulated formulas, state whether each of these functions could reasonably be expected to be eigenfunctions (unnormalized) of the Hamiltonian for an H-like atom:
   (i) $(27 - 18Zr + 2Z^2r^2)\exp(-2Zr/3)$ (ii) $r\exp(Zr/2)\sin\theta\cos\theta$ (iii) $r\sin\theta\exp(-i\phi)$.

5. Suppose a particle is capable of being in any one of the *three* states (α, β, γ). Suppose you have two such particles in a molecule. (i) Write down all the spin functions you can that are symmetric for exchange of these two particles. (ii) Also the antisymmetric cases. Do not worry about normalization.

6. Evaluate the following integrals (over all space) using labor-saving approaches. (i) $\int \psi_{2p_x} L_z \psi_{2p_x} d\tau$ (ii) $\int \psi_{2p_x} L^2 \psi_{2p_x} d\tau$. (iii) $\int \psi_{2p_x} L_x \psi_{2p_x} d\tau$ (iv) $\int_0^{2\pi} \exp(2i\phi)\exp(-3i\phi) d\phi$.

7. Evaluate each of the followings in a.u. (by inspection): $\psi_{n,l,m}$ stands for an H-atom eigenfunction of the Hamiltonian operator. (i) $L^2\psi_{3,2,1}$ (ii) $L^2\psi_{2p_x}$ (iii) $H\psi_{3p_x}$ (iv) $(1/i)\,\frac{\partial}{\partial\phi}\psi_{2p_{-1}}$. [Hint: $\psi_{2p_{-1}} \propto R_{2p}(r)\sin\theta\ \exp(-i\phi)$.]

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8. For each of the following operators, indicate by "yes" or "no", whether ψ_{3p_x} (with $Z = 1$) is an eigenfunction. If it is, then also give eigenvalues in a.u. (i) $\frac{1}{2}\nabla^2$ (ii) $-\frac{1}{2}\nabla^2 - \frac{1}{r}$ (iii) $-\frac{1}{2}\nabla^2 - \frac{3}{r}$ (iv) L_z (v) L_x (vi) L^2 (vii) r (viii) $1/r$.

9. Which of the following functions are eigenfunctions of $\frac{d^2}{dx^2}$ operator? (a) e^x (b) x^2 (c) $\sin x$ (d) $3\cos x$ (e) $\sin x + \cos x$. Give eigenvalue for each eigenfunctions.

10. Evaluate the commutators: (a) $[x, p_x]$ (b) $[x, p_x^2]$ (c) $[x, p_y]$ (d) $[x, V(x, y, z)]$ (e) $[x, H]$, where H represents the Hamiltonian operator for a single particle in 3D.