CML 100: 2017-2018
Quantum Tutorial 1

1. In algebra it can be easily shown that $(P + Q)(P - Q) = P^2 - Q^2$. What is the value of $(P + Q)(P - Q)$ if P and Q are operators? Under what conditions will this result be equal to $P^2 - Q^2$.
2. Find $[z^3, \frac{d}{dz}]$ and $[\frac{d^2}{dx^2}, ax^2 + bx + c]$.

3. Which of the following functions cannot be solutions of the Schrödinger equation for all values of x? Why not? (a) $Asec(x)$; (b) $Atan(x)$; (c) $Aexp(x^2)$; (d) $Aexp(-x^2)$.

4. Write down the Hamiltonian for the following systems: (a) a particle of mass m in a cubical box of side a; (b) a particle of mass m in a spherical box of radius a; (c) a particle of mass m moving on the x-axis subjected to a force directed towards the origin, of magnitude proportional to the distance from the origin; (d) an electron moving in the presence of a nuclear charge $+Ze$; (e) two electrons moving in the presence of a fixed nucleus of charge $+Ze$.

5. (a) Evaluate the probability of locating a particle in the middle third of 1-D box. (b) Find the probability that a particle in a box L wide can be found between $x = 0$ and $x = L/n$ when it is in the nth state.

6. Describe the color of carrots using the particle in a box model. (Hint: Consider the π electrons to be confined to a box whose length is the length of the molecule. Use 1.54 Å as a C−C and 1.35 Å as a C=C bond length.)

7. Many proteins contain metal porphyrin molecules. These molecules are approximated as square planar and contain 26 π electrons. If the edge of the molecule is ~1000 pm, then what is the predicted lowest energy absorption of the porphyrin molecule?

8. The possible values obtained from a measurement of a discrete variable, x, are 1, 2, 3, and 4. (a) If the respective probabilities are 1/4, 1/4, 1/4, and 1/4, calculate the expectation values of x and x^2. (b) If the respective probabilities are 1/12, 5/12, 5/12, and 1/12, calculate the expectation values of x and x^2.

9. Why can the electron not be at the nucleus? Using the uncertainty principle, find the value of the Bohr radius for electron in a H-atom in the ground state.

10. The wave function of the first excited state of a harmonic oscillator is $Ax \exp -ax^2$. By substituting in the Schrödinger equation determine a. Determine A from the normalization condition.

11. Verify the recursion relation $H_{n+1}(z) - 2zH_n(z) + 2nH_{n-1}(z) = 0$ using the first four Hermite polynomials.

12. In the vibrational motion of HI, the iodine atom remains stationary because of its large mass. Assume that the hydrogen atom undergoes harmonic motion and that the force constant is $317\ \text{N m}^{-1}$, what is the vibrational frequency ν_0? What is the zero point energy if H is replaced by D? Assume that there is no change in the force constant.