**Designette Project: Computing Schrödinger’s Equations**

Deadline: Week 8 Monday, 14 March, 5 pm

Submit the completed .py file/graph plot/interactable 3D plot and worksheet

Name: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Team Members: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

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Assigned Quantum Numbers:

\_\_\_\_\_\_\_\_\_\_\_\_n \_\_\_\_\_\_\_\_\_\_\_\_l \_\_\_\_\_\_\_\_\_\_\_\_ml

For this assignment, you are required to work in groups of 2 or 3.

**Objectives**

1. Calculating and understanding the energy level formula.
2. Calculating the probability of particle location within a box.
3. Understanding the application of coordinate conversion in the Schrödinger’s equation.
4. Understanding the application of separation of variables to solve the Schrödinger’s equation into radial and angular forms.
5. Application of both the Legendre and Laguerre polynomials to solve the angular and radial forms of the Schrodinger’s equation respectively.
6. Calculating the complete wave function solution from the radial and angular solutions.

**Contents and Weightage**

Part A: Theory Segments (attached here – Pages 2 to 6)

Part B: Coding Segments (will be released later on both Digital World and Chemistry eDimension websites)

**Timeline Checklist**

☐ Week 2: Basic functions and Schrodinger’s equations (Part 2a-c, Part 3a)

☐ Week 3/4: Basic loops and Schrodinger’s equations (Part 2d-g, Part 3b)

☐ Week 5/6: Listing and generating 2D plots (Part 3c)

☐ Week 7: Generating 3D plots (Part 3d)

**References**

**It is highly recommended that you read References (b) to (f) as it may prove to be very useful for this assignment.**

1. Introduction to Quantum Mechanics (Second Edition), David J.Griffths
2. From the time independent Schrödinger’s equation in 3d to spherical harmonics, <https://www.youtube.com/watch?v=bqYMUDxD3WQ>
3. Time independent Schrödinger’s equation in 3d radial behavior, <https://www.youtube.com/watch?v=Nq72tUEtbfM>
4. Matplotlib 2D/3D plotting tutorials,
5. <http://matplotlib.org/users/pyplot_tutorial.html>, <http://matplotlib.org/mpl_toolkits/mplot3d/tutorial.html>
6. Atom in a box simulation tool, <http://daugerresearch.com/orbitals/index.shtml#download>

**1. List of Constants**

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| --- | --- | --- | --- |
| **Property** | **Symbol** | **Value** | **Units** |
| Mass Of Electron | *m* | 9.109 × 10−31 | kg |
| Reduced Plank’s Constant | *ħ* | 1.055 × 10−34 | J·s |
| Elementary Charge | *e* | 1.602 × 10−19 | C |
| Permittivity Of Free Space | *ε0* | 8.854 × 10−12 | F/m |

**2. Chemistry Theory Segments**

**Answer the following questions after Week 2 Cohort Lesson 1.**

a. Given the formula for the energy levels below, calculate the energy level including units for your assigned principle quantum number.

Answer and Workings:

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b. Calculate the probability that a particle will be found between 0.49*L* and 0.51*L* in a box of length *L* when it has (i) *n* = 1 and (ii) *n* = 2 on all directions. The wavefunction of a particle in the box is:

Answer and Workings:

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| --- |
| (i)  (ii) |

**Answer the following questions after Week 2 Cohort Lesson 2.**

c. Given the transformation from **Cartesian (x, y, z) to spherical (r, θ, ϕ)** coordinates are as follows, derive the formula to transform **spherical (r, θ, ϕ) to Cartesian (x, y, z)** coordinates. Convert the point (3, 25°, 60°) from **spherical (r, θ, ϕ) to Cartesian (x, y, z)** coordinates.

Answer and Workings:

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d. The Schrödinger equation is:

Use the Laplaican operator to transform the above Schrödinger equation from Cartesian coordinates to spherical coordinates through the use of the Laplacian operator. The Laplacian operator in Cartesian coordinates is as follows:

For a system in spherical coordinates (r, θ, ϕ), which is what we are interested here, the Laplacian operator in spherical coordinates is:

Answer and Workings

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e. Apply separation of variables to derive the expressions for both the angular component (equation written in terms of θ and ϕ only) and radial component (equation written in terms of r only) to be solved. Do not substitute the assigned quantum numbers into the Schrödinger equation.

Hint:

We are looking at solutions that are separable into products in the form of:

*Ψ(r,θ,ϕ) = R(r) ·Y(θ,ϕ)*

You will need to use:

Answer and Workings

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**Answer the following questions together with Digital World after Week 3.**

f. Given the normalized angular solution for Y(θ,ϕ), associated Legendre function and the Legendre polynomial, find the specific normalized solution for your assigned quantum numbers.

Answer and Workings:

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g. Given the normalized radial solution for R(r), associated Laguerre function and the Laguerre polynomial, find the specific normalized solution for your assigned quantum numbers.

Answer and Workings:

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