2023

PHYSICS — HONOURS — PRACTICAL

Paper : CC-10P

(Syllabus : 2019-2020)

[Quantum Mechanics]

Full Marks : 30

[Experiment : 20, LNB : 5, viva voce : 5]

Programming Language : Python

[*Instruction : Use proper title, axis label and legends in the plots*]

Day - 1

1. A particle of mass m is in a potential

$$V(x)=\begin{cases}0, & |x|\le a/2\\ V_0, & |x|>a/2\end{cases}.$$

Find the energies of the bound states with *even parity* by graphically solving the given transcendental equation that appears as the eigenvalue condition and plot the corresponding normalized wave functions by numerically solving the time independent Schrödinger equation.

$$\sqrt{\left(u_0^2-v^2\right)}=v\tan(v),\ \text{where}\ u_0=\sqrt{\frac{ma^2V_0}{2\hbar^2}},\ v=\frac{a}{2}\sqrt{\frac{2mE}{\hbar^2}}.\ \text{(Symbols have usual meanings)}$$

[Given : $\frac{m}{\hbar^2}=1$, $V_0=20$ and $a=2$]

Distribution of Marks:

(a) Stating the boundary conditions used 3

(b) Plotting of graphs to solve the transcendental equation 5

(c) Reading of the guess roots viewing the graph 1

(d) Finding and printing of the eigenenergies from refined roots using guess values (any SciPy root searching package may be used) 3

(e) Finding and plotting of the normalized wave functions along with the potential in the same graph (any method may be used for integration). 8

2. A particle of mass m is in a potential

$$V(x)=\begin{cases} 0, & x<0 \\ -V_0, & 0\le x\le a \\ 0, & x>a \end{cases}$$

Solve the time independent Schrödinger equation numerically to find first two bound states. Use shooting algorithm to find Eigenenergies and Euler or Numerov algorithm for solving ODE to find the normalized wave functions.

[Given : $\frac{m}{\hbar^2}=1$, $V_0 = 40$ and $a = 1$]

Distribution of Marks:

(a) Working formula (Time independent Schrödinger's Equation, Formula for Euler/Numerov Method). 4

(b) Finding and printing the energy eigenvalues using shooting method (any SciPy root searching package may be used) along with the shooting curve. 10

(c) Finding and plotting of the normalized wave functions along with the potential in the same graph. 6

3. Solve the time independent Schrödinger equation for a one-dimensional Quantum Harmonic Oscillator to find the ground and first excited state. Use shooting algorithm to find Eigenenergies and Euler or Numerov algorithm for solving ODE to find the normalized wave functions.

Distribution of Marks:

(a) Working formula (Schrödinger equation and its dimensionless form). 3

(b) Finding and printing the energy eigenvalues using shooting method (any SciPy root searching package may be used). 11

(c) Finding and plotting of the normalized wave functions along with the potential in the same graph. 6

4. (a) Write down time independent Schrödinger equation for the following central potential $V(r)$ in dimensionless form or state appropriate energy scale to be chosen to solve the equation numerically.

(b) State the boundary conditions and also the initial conditions deduced from it.

(c) Write a Python program for determining the lowest two eigenvalues and normalized radial wave functions (s-orbital) for the following potential, where the ordinary differential equation (ODE) may be solved using either Euler or Numerov algorithm.

$$V(r)=\frac{1}{2}r^2.$$

4+2+(8+6)

5. A particle of mass m in a one-dimensional triangular well potential

$$V(x) = \begin{cases} \infty, & x < 0 \\ x, & x \geq 0 \end{cases}$$

Solve the time independent Schrödinger equation numerically to find first two bound states. Use shooting algorithm to find Eigenenergies and Euler or Numerov algorithm for solving ODE to find normalized wave functions.

[Given : $\frac{2m}{\hbar^2} = 1$]

Distribution of Marks:

(a) Working formula (time independent Schrödinger equation and formula for Euler/Numerov method). 4

(b) Finding and printing energy eigenvalues using shooting method (any SciPy root searching package may be used) along with the shooting curve. 11

(c) Finding and plotting of the normalized wave functions along with the potential in the same graph. 5

6. (a) In order to study time evolution of wave function by numerically solving time dependent Schrödinger equation in one dimension, write down the Crank-Nicolson operator which evolves the wave function from initial to final state explaining symbols used.

(b) What are the advantages of using Crank-Nicolson algorithm to study time evolution of wave function for solving time dependent Schrödinger equation in one dimension?

(c) Write Python code for solving time dependent Schrödinger equation in one dimension to study time evolution of wave packet moving in free space for a Gaussian wave packet using Crank-Nicolson Algorithm.

The Gaussian wave packet will be of following form :

$$\psi(x, t) = \exp\left\{-\frac{(x - x_0)^2}{a} + ikx\right\},$$

where x_0, a and k are constants and $i = \sqrt{-1}$.

(d) Print the output wave function at appropriately chosen three different instances of time to exhibit time evolution. 3+2+12+3

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Programming Language : Python

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Day - 2

1. A particle of mass m is in a one-dimensional finite square well potential

$$V(x)=\begin{cases}0, & |x|\le\frac{a}{2}\\ V_0, & |x|>\frac{a}{2}\end{cases}$$

Find the energies of the bound states with *odd parity* by graphically solving the given transcendental equation that appears as the eigenvalue condition and plot the corresponding normalized wave functions by numerically solving the time independent Schrödinger equation. Hence, find the probability density of the states.

$$\sqrt{\left(u_0^2-v^2\right)}=-v\cot(v), \text{ where } u_0=\sqrt{\frac{ma^2V_0}{2\hbar^2}}, v=\frac{a}{2}\sqrt{\frac{2mE}{\hbar^2}}.$$ (Symbols have usual meanings)

[Given : $\frac{m}{\hbar^2}=1$, $V_0=30$ and $a=2$]

Distribution of Marks:

(a) Stating the boundary conditions used 3

(b) Plotting of graphs to solve the transcendental equation 5

(c) Reading of the guess roots viewing the graph 1

(d) Finding and printing of the eigenenergies from refined roots using guess values (any SciPy root searching package may be used) 3

(e) Finding and plotting of the normalized wave functions and the probability density in different graphs (any method may be used for integration). 8

2. A particle of mass m is in a potential

$$V(x) = \begin{cases} 0, & x < -a \\ -V_0, & -a \le x \le a \\ 0, & x > a \end{cases}$$

Solve the time independent Schrödinger equation numerically to find first excited state. Use shooting algorithm to find Eigenenergy and Euler or Numerov algorithm for solving ODE to find the normalized wave function. Hence, find the probability of finding the particle in the region $x < -a$.

[Given : $\frac{m}{\hbar^2} = 1$, $V_0 = 30$ and $a = 1$]

Distribution of Marks:

(a) Working formula (Time independent Schrödinger's Equation, Formula for Euler/Numerov Method). 4

(b) Finding and printing energy eigenvalues using shooting method (any SciPy root searching package may be used). 9

(c) Finding and plotting of the normalized wave function along with the potential in the same graph. 5

(d) Finding and printing the probability. 2

3. Solve the time independent Schrödinger equation for a one-dimensional Quantum Harmonic Oscillator to find the ground state. Use shooting algorithm to find Eigenenergy and Euler or Numerov algorithm for solving ODE to find the normalized wave function.

Distribution of Marks:

(a) Working formula (Schrödinger equation and its dimensionless form). 3

(b) Finding and printing the energy eigenvalue using shooting method (any SciPy root searching package may be used) along with the shooting curve. 12

(c) Finding and plotting of the normalized wave function. 5

4. (a) Write down time independent Schrödinger equation in one dimension for the potential $V(x) = D(-1 + \alpha^2x^2)$. Here D and α are constants.

(b) State the boundary conditions and also the initial conditions deduced from it.

(c) Write a Python program for determining the lowest two eigenvalues and normalized wave functions for the following potential, where the ordinary differential equation (ODE) may be solved using either Euler or Numerov algorithm : $V(x) = D\left(-1+\alpha^2x^2\right)$. 2+2+10+6

Data Supplied : $D = (37244/10.5930)$ and $\alpha = 2.380$ are dimensionless numbers, use $\frac{\hbar^2}{2m} = 1$.

5. Radial part of time independent Schrödinger equation for hydrogen atom is given by

$$\frac{d^2u(r)}{dr^2} = \left[\frac{l(l+1)}{r^2} - \frac{2}{r} - E_n\right]u(r)$$

$R(r) = \frac{u(r)}{r}$ = Radial wave function

r = Dimensionless radial distance

E_n = Dimensionless Energy for principal quantum number n

l = Angular momentum quantum number.

Numerically solve the given equation to find the energy and radial wave function for 2s electron using shooting algorithm along with Euler or Numerov algorithm for solving ODE.

Distribution of Marks:

(a) Finding and printing the energy eigenvalue using shooting algorithm (any SciPy root searching package may be used) along with the shooting curve. 12

(b) Finding and plotting of the radial wave function along with probability density in same graph. 8

6. (a) In order to study time evolution of wave function by numerically solving time dependent Schrödinger equation in one dimension, write down the Crank-Nicolson operator which evolves the wave function from initial to final state explaining symbols used.

(b) What are the advantages of using Crank-Nicolson algorithm to study time evolution of wave function for solving time dependent Schrödinger equation in one dimension?

(c) Write Python code for solving time dependent Schrödinger equation in one dimension to study tunnelling through a barrier of finite height for a Gaussian wave packet using Crank-Nicolson Algorithm.

The initial Gaussian wave packet will be of following form :

$$\psi(x,t) = e^{\left\{-\frac{(x-x_0)^2}{a}+ikx\right\}},$$

where x_0, a and k are constants, may be chosen judiciously by the student.
The barrier potential function will be of following form :

$$V(x) = \alpha \quad \text{for} \quad x_b \leq x \leq x_b + \delta$$
$$= 0 \quad \text{otherwise}$$

where, x_b and δ are constants.

(d) Print the output wave function at appropriately chosen three different instances of time to exhibit time evolution.

3+2+12+3

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Day - 3

1. A particle of mass m is in a one-dimensional finite square well potential

$$V(x)=\begin{cases} V_0, & x<0 \\ 0, & 0\le x\le a \\ V_0, & x>a \end{cases}$$

Find the energy of the *first excited state* by graphically solving the given transcendental equation that appears as the eigenvalue condition and plot the corresponding normalized wave function numerically solving the time independent Schrödinger equation [Consider $\frac{m}{\hbar^2}=1$, $V_0 = 50$ and $a = 1$]. Hence, find the probability density.

$\sqrt{u_0^2-v^2}=-v\cot(v)$, where $u_0=\sqrt{\frac{ma^2V_0}{2\hbar^2}}$, $v=\frac{a}{2}\sqrt{\frac{2mE}{\hbar^2}}$. (Symbols have usual meanings)

Distribution of Marks:

(a) Stating the boundary conditions used 3

(b) Plotting of graphs to solve the transcendental equation 5

(c) Reading of the guess root viewing the graph 1

(d) Finding and printing of the eigenenergy from refined root using guess value (any SciPy root searching package may be used) 3

(e) Finding and plotting of the normalised wave function along with the probability density in the same graph (any method may be used for integration). 8

2. Solve the time independent Schrödinger equation for a one-dimensional Quantum Harmonic Oscillator to find the ground state. Use shooting algorithm to find Eigenenergy and Euler or Numerov algorithm for solving ODE to find the normalized wave function. Hence, find the average position of the particle in ground state.

Distribution of Marks:

(a) Working formula (Schrödinger equation and its dimensionless form) 3

(b) Finding and printing energy eigenvalues using shooting method (any SciPy root searching package may be used). 10

(c) Finding and plotting of the normalized wave functions along with the potential in the same graph. 5

(d) Finding and printing the average position. 2

3. A particle of mass m is in a potential

$$V(x) = \begin{cases} 0, & |x| \le a \\ \infty, & |x| > a \end{cases}$$

Solve the time independent Schrödinger equation numerically to find first two bound states. Use shooting algorithm to find Eigenenergies and Euler or Numerov algorithm for solving ODE to find normalized wave functions. Hence, show that the states are orthogonal.

[Given : $\frac{m}{\hbar^2} = 1$, and $a = 1$]

Distribution of Marks:

(a) Working formula (Time independent Schrödinger equation and formula for Euler/Numerov method). 4

(b) Finding and printing energy eigenvalues using shooting method (any SciPy root searching package may be used). 10

(c) Finding and plotting of the normalized wave functions. 4

(d) Checking of the orthogonality condition. 2

4. A particle of mass m is in a potential

$$V(x) = \begin{cases} \infty, & x < 0 \\ \frac{1}{2}x, & x \geq 0 \end{cases}$$

Solve the time independent Schrödinger equation numerically to find first two bound states. Use shooting algorithm to find Eigenenergies and Euler or Numerov algorithm for solving ODE to find normalized wave functions. Hence, show that the states are orthogonal.

[Given : $\frac{2m}{\hbar^2} = 1$]

Distribution of Marks:

(a) Working formula (Time independent Schrödinger equation and formula for Euler/Numerov method). 4

(b) Finding and printing energy eigenvalues using shooting method (any SciPy root searching package may be used) along with the shooting curve. 10

(c) Finding and plotting of the normalized wave functions along with the potential in same graph. 4

(d) Checking of the orthogonality condition. 2

5. Radial part of time independent Schrödinger equation for hydrogen atom is given by

$$\frac{d^2u(r)}{dr^2} = \left[\frac{l(l+1)}{r^2} - \frac{2}{r} - E_n\right]u(r)$$

$R(r) = \frac{u(r)}{r}$ = Radial wave function

r = Dimensionless radial distance

$E_n = -\frac{1}{n^2}$ = Dimensionless Energy for principal quantum number n

l = Angular momentum quantum number.

Numerically solve the given equation to find the radial part of wave function for 1s electron using Euler or Numerov algorithm and hence find the electron probability density. Also evaluate the average and most probable radial distance of the 1s electron from the nucleus and compare with their theoretical values.

Distribution of Marks:

(a) Finding and plotting of the radial wave function. 8

(b) Plotting of electron probability density. 3

(c) Finding and printing the average and most probable radial distance. 5

(d) Comparison with theoretical values. 4

6. (a) In order to study time evolution of wave function by numerically solving time dependent Schrödinger equation in one dimension, write down the Crank-Nicolson operator which evolves the wave function from initial to final state explaining symbols used.

(b) What are the advantages of using Crank-Nicolson algorithm to study time evolution of wave function for solving time dependent Schrödinger equation in one dimension?

(c) Write Python code for solving time dependent Schrödinger equation in one dimension to study time evolution of wave packet moving in free space for a Gaussian wave packet using Crank-Nicolson Algorithm.

The Gaussian wave packet will be of following form :

$$\psi(x,t) = \exp\left\{ -\frac{(x-x_0)^2}{a} + ikx \right\},$$

where x_0, a and k are constants and $i = \sqrt{-1}$.

(d) Print the output wave function at appropriately chosen three different instances of time to exhibit time evolution. 3+2+12+3

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Programming Language : Python

[*Instruction : Use proper title, axis label and legends in the plots*]

Day - 4

1. A particle of mass m is in a potential

$$V(x)=\begin{cases} V_0, & x<-\frac{a}{2} \\ 0, & -\frac{a}{2}\le x\le\frac{a}{2} \\ V_0, & x>\frac{a}{2} \end{cases}$$

Find the energy of the *ground state* by graphically solving the given transcendental equation that appears as the eigenvalue condition and plot the corresponding normalized wave function numerically solving the time independent Schrödinger equation. [Consider $\frac{2m}{\hbar^2}=1$, $V_0=40$ and $a=2$]

$\sqrt{u_0^2-v^2}=v\tan v$, where $u_0=\sqrt{\frac{ma^2V_0}{2\hbar^2}}, v=\frac{a}{2}\sqrt{\frac{2mE}{\hbar^2}}$. (Symbols have usual meanings)

Distribution of Marks:

(a) Stating the boundary conditions used 3

(b) Plotting of graphs to solve the transcendental equation 5

(c) Reading of the guess root viewing the graph 1

(d) Finding and printing of the eigenenergy from refined root using guess value (any SciPy root searching package may be used) 3

(e) Finding and plotting of the normalized wave function along with the potential in the same graph (any method may be used for integration). 8

2. Solve the time independent Schrödinger equation for a one-dimensional Quantum Harmonic Oscillator to find the ground and first excited state. Use shooting algorithm to find Eigenenergies and Euler or Numerov algorithm for solving ODE to find the normalized wave functions. Hence, show that the states are orthogonal.

Distribution of Marks:

(a) Working formula (Schrödinger equation and its dimensionless form). 3

(b) Finding and printing energy eigenvalues using shooting method (any SciPy root searching package may be used). 10

(c) Finding and plotting of the normalized wave functions. 5

(d) Checking of orthogonality condition. 2

3. A particle of mass m is in a one-dimensional infinite square well potential

$$V(x) = \begin{cases} 0, & |x| \leq \pi/2\sqrt{2} \\ \infty, & |x| > \pi/2\sqrt{2} \end{cases}$$

Solve the time independent Schrödinger equation numerically to find the ground state. Use shooting algorithm to find Eigenenergy and Euler or Numerov algorithm for solving ODE to find the normalized wave function. Compare the ground state energy with its theoretical value.

[Given : $\frac{m}{\hbar^2} = 1$]

Distribution of Marks:

(a) Working formula (Time independent Schrödinger equation, formula for energy eigenvalue and formula for Euler/Numerov method). 4

(b) Finding and printing energy eigenvalues using shooting method (any SciPy root searching package may be used). 10

(c) Finding and plotting of the normalized wave function. 4

(d) Comparison of the ground state energy. 2

4. A particle of mass m is in a one-dimensional triangular well potential

$$V(x) = \begin{cases} 100, & x < 0 \\ x, & x \geq 0 \end{cases}$$

Solve the time independent Schrödinger equation numerically to find first two bound states. Use shooting algorithm to find Eigenenergies and Euler or Numerov algorithm for solving ODE to find wave functions. Hence, find the probability of finding the particle in ground state in the region $x \leq 0$.

[Given : $\frac{2m}{\hbar^2} = 1$]

Distribution of Marks:

(a) Working formula (Time independent Schrödinger equation and formula for Euler / Numerov method). 4

(b) Finding and printing energy eigenvalues using shooting method (any SciPy root searching package may be used). 10

(c) Finding and plotting of the normalized wave functions along with the potential in same graph. 4

(d) Finding and printing the probability. 2

5. Radial part of time independent Schrödinger equation for hydrogen atom is given by

$$\frac{d^2u(r)}{dr^2} = \left[\frac{l(l+1)}{r^2} - \frac{2}{r} - E_n\right]u(r)$$

$R(r) = \frac{u(r)}{r}$ = Radial wave function

r = Dimensionless radial distance

E_n = Dimensionless Energy for principal quantum number n

l = Angular momentum quantum number.

Numerically solve the given euqation to find the energies and radial wave functions for 1s and 2s electrons using shooting algorithm along with Euler or Numerov algorithm for solving ODE. Hence, check whether the states are orthogonal or not.

Distribution of Marks:

(a) Finding and printing energy eigenvalues using shooting algorithm (any SciPy root searching package may be used). 11

(b) Finding and plotting of the radial wave functions. 7

(c) Checking of orthogonality. 2

6. (a) In order to study time evolution of wave function by numerically solving time dependent Schrödinger equation in one dimension, write down the Crank-Nicolson operator which evolves the wave function from initial to final state explaining symbols used.

(b) What are the advantages of using Crank-Nicolson algorithm to study time evolution of wave function for solving time dependent Schrödinger equation in one dimension?

(c) Write Python code for solving time dependent Schrödinger equation in one dimension to study tunnelling through a barrier of finite height for a Gaussian wave packet using Crank-Nicolson Algorithm.

The Gaussian wave packet will be of following form :

$$\psi(x,t) = e^{\left\{-\frac{(x-x_0)^2}{a}+ikx\right\}},$$

where x_0, a and k are constants.

The barrier potential function will be of following form :

$$V(x) = \alpha \quad \text{for } x_b \le x \le x_b + \delta$$
$$= 0 \quad \text{otherwise}$$

where, x_b and δ are constants.

(d) Print the output wave function at appropriately chosen three different instances of time to exhibit time evolution. 3+2+12+3