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UG/5th Sem/Phys(H)/Pr/19

2019

B.Sc. (Honours)

5th Semester Examination

PHYSICS

Paper - C11P

(Python Computing)

Full Marks : 20

Time : 3 Hours

*The figures in the margin indicate full marks.  
Candidates are required to give their answers  
in their own words as far as practicable.*

Answer any *one* question from the following.

15×1=15

1. Consider Schrodinger equation for 1D harmonic oscillator :

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi$$

Reduce the energy terms in appropriate dimensionless forms to solve it numerically. Write a Python script

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to solve with the help of the modules and functions taken from Scipy package. Obtain the first three eigen energies by looking at the zero crossing from graphical display. Use Matplotlib package for graph plots.

2. Write a Python script for the following. Starting with the reduced form of the 1D Schrodinger equation for harmonic oscillator, determine numerically the normalized eigen function for a given eigen energy (to be supplied). Plot the wave function with the help of Matplotlib package. Also, take a slightly different energy value than the given eigen energy and graphically check what the resulting wave function looks like.
3. For the problem in (2), plot the normalized eigen function for a given energy along the potential energy. Write a Python script for this. Use Numpy, Scipy and Matplotlib packages as and when necessary.
4. The reduced form of the radial part  $R(r)$  of the 3D Schrodinger equation in spherical polar coordinate system is given by :

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

where  $u(r) = rR(r)$  and  $k^2 = 2mE / \hbar^2$

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Solve this numerically to find out any one eigen energy for a chosen  $l$  and the corresponding eigen function. Write a Python script for this with the help of modules and functions from Scipy and Matplotlib packages.

5. For the problem in (3), determine the normalized eigen function (as a list) for a given eigen energy and plot. Consider that the eigen function turns out to be  $R(r) \sim j(kr)$ . Now, plot this spherical Bessel function (for the given order  $l$ ) along with the solution obtained. Take the Bessel function from Scipy special module.
6. The radial part from the Schrodinger equation (in spherical polar coordinates) for the Hydrogen atom problem is the following :

$$\frac{d^2u}{d\rho^2} = \left[ 1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right] u$$

where,  $\rho = kr$ ,  $k = \frac{\sqrt{-2mE}}{\hbar^2}$  ( $E$  is negative)

Write a Python script to obtain  $R_{20}(r)$  and compare this graphically with the analytic solution,

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$$R_{20}(r) = \frac{c_0}{2a} \left( 1 - \frac{r}{2a} \right) e^{-r/2a}$$

where,  $k = \frac{1}{an}$ ,  $\rho = \frac{r}{an}$ ,  $a =$  Bohr radius. Consider

$\rho_0 = 2n$ ,  $n$  being the principal quantum number.  
[Use modules and functions from Scipy, Numpy and Matplotlib packages.]

7. For the problem as in (5), write a Python script to obtain  $R_{21}(r)$  and do graphical comparison with the

analytical result  $R_{21}(r) = \frac{c_0}{4a^2} r e^{-r/2a}$ .

[LNB : 2 Viva-Voce : 3]

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