Ex/PG/SC/CBS/PHY/TH/304/2022

M. Sc. Physics Examination, 2022

(2nd Year, 2nd Semester)

Computational Physics

Paper – 304

Time : Two hours | Full Marks : 40

Answer ***any four*** questions : 4×10=40

1. a) SIR model is defined by the set of nonlinear equations,

$$\begin{cases} \dfrac{dS}{dt} = -\alpha SI, \\ \dfrac{dI}{dt} = \alpha SI - \beta I, \\ \dfrac{dR}{dt} = \beta I, \end{cases}$$

where $S(t)$, $I(t)$, $R(t)$ are the susceptible, infected and recovered populations at time t, and the total population $N = S(t) + I(t) + R(t)$. What is the significance of the parameters α and β? Determine the units of α and β.

b) Find the integral form of $S(t)$ and $I(t)$.

c) Find the approximate form of $\dfrac{dR}{dt}$, (Riccati equation) when $\alpha R(t)/\beta < 1$.

d) i) Write down the set of differential equations for the SEIQR model.

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ii) What do you mean by the term "exposed population"?

iii) Explain the significance of additional parameters used in this model.

2+2+2+(1+1+2)=10

2. a) Derive the expression for equation of motion for the oscillation of simple pendulum:

$$\dot{\theta} = \sqrt{2}\omega_0\sqrt{\cos\theta - \cos\theta_c} ,$$

where the symbols have their usual meaning.

b) Find the solution of the above differential equation, and obtain the expression for time period of oscillation in terms of complete elliptic integral of first kind.

c) Usig the binomial expansion of complete elliptic integral of first kind, show that time period of simple pendulum is always greater than that of the corresponding simple harmonic motion.

d) Draw the variation of time period with energy for oscillation and rotation in the same plot.

2+4+3+1=10

3. a) Define fixed point for a nonlinear dynamical system described by the pair of coupled differential equations,

be the real time simulation in sec if a MD simulation runs for 2000 steps with a reduced time step $\Delta t = 0{\cdot}01$?

(5+2)+(1+2)=10

7. Describe Numerov's method for numerical solution of second order differential equation. What kind of differential equations can be solved using this method?

10

8. Write an algorithm for solving the Schrödinger equation for a linear harmonic oscillator in Numerov's method to obtain the wave function. 10

c) With proper θ-t diagrams describe the phenomena: (i) period one, (ii) period two, (iii) period three and (iv) period four.

d) Define Feigenbaum constant. Why it is called universal?

e) Define Liapunov exponent. 2+1+4+(1+1)+1=10

5. a) Write down the expression for Lennard-Jones potential and explain the terms therin with a sketch.

b) Consider the motion of N argon atoms in a two dimensional box. Derive an expression for acceleration of the *i*-th atom if the interaction potential between any two atoms is given by the Lennard-Jones potential.

c) How do you initialize positions of N number of atoms in a two dimensional MD simulation using a random number generator? 2+5+3=10

6. a) Derive Verlet algorithm which is used to find subsequent position and velocity of the atoms in MD simulation. Discuss its accuracy, advantage and disadvantage.

b) Explain the practical reason behind using reduced units in MD simulation. Typical values of the parameters for argon atoms are $\sigma = 3{\cdot}41\times10^{-10}$ m, $\varepsilon = 1{\cdot}65\times10^{-21}$ J and $m = 6{\cdot}69\times10^{-26}$ kg. What will

$$\dot{x}_1 = P(x_1, x_2),$$
$$\dot{x}_2 = Q(x_1, x_2),$$

where the symbols have their usual meaning.

b) Find the expression of Jacobian matrix at the fixed point.

c) Derive the equation of motion for damped simple pendulum in terms of a pair of coupled first order differential equations.

d) Identify the coordinates of fixed points in the phase space.

e) Characterize the fixed points by finding the eigenvalues of Jacobian matrix when damping is comparatively low. 1+2+3+1+3=10

4. a) Derive the equation of motion for a driven-damped simple pendulum:

$$\ddot{\theta} = -2\beta\dot{\theta} - \omega_0^2 \sin\theta + \gamma\omega_0^2 \cos(\omega t),$$

where symbols have their usual meaning.

b) Show that the above second-order nonlinear differential equation can be decomposed as

$$\begin{cases} \dot{\theta} = \phi, \\ \dot{\phi} = -2\beta\phi - \omega_0^2 \sin\theta + \gamma\omega_0^2 \cos\eta, \\ \dot{\eta} = \omega, \end{cases}$$

where $\eta = \omega t$.