This question paper contains 4 printed pages

6992 *Your Roll No*

M.Tech. / II Sem. **J**

NANOSCIENCE AND NANOTECHNOLOGY

PAPER NSNT-202 Computational Methods

Time 3 hours *Maximum Marks* 38

(Write your Roll No on the top immediately on receipt of this question paper.)

Attempt any ***four*** *questions*
All questions carry equal marks

1 (*a*) Explain Newton-Raphson method of finding a root of the equation $f(x)=0$. Show that it has a second order convergence. Use the method to find root of the equation $x \sin x - 1 \cdot 0 = 0$, starting with $x = 1 \cdot 0$ and use three iterations only. 5½

(*b*) Explain Ramanujan's iterative method which can be used to determine the smallest root of the equation $f(x)=0$. Use this method to find the smallest root of $x^3 - 6x^2 + 11x - 6 = 0$. 4

2 (*a*) Establish Newton's forward difference interpolation formula and the remainder terms (error in the formula) in terms of appropriate derivatives. Find the value of $e^{1.17}$ using Gauss

P.T.O.

forward formula from the following data (for x and e^x): (1 . 2 7183), (1 05 2 8577); (1 10 3 0042), (1 15 3 1582), (1 20 3 3201), (1 25 3 4903) and (1 30 3 6693) 5½

(*b*) Define the operators Δ, ∇, δ, E and μ and show:

(*i*) $\mu E = E\mu$

(*ii*) $\mu^2 = 1 + \frac{1}{4}\delta^2$ 4

3 (*a*) Use Gauss Quadrature method based on intervals of unequal width to calculate a definite integral Calculate the weights and abscissae for $n=2$. Obtain the first four Legendre polynomials using recurrence relation

$$(n+1)P_{n+1}(u) = (2n+1)uP_n(u) - nP_{n-1}(u).$$

Take $P_0(u)=1$ and $P_1(u)=u$ 6

(*b*) Use four point Gauss-Legendre formula to evaluate the integral $\int_0^{1/2} \frac{1}{\sqrt{1-x^2}}\,dx$

Abscissae and weights are

$\pm u_i = 0{\cdot}33998 \quad w_i = 0{\cdot}65215$

$\pm u_i = 0\ 86114 \quad w_i = 0{\cdot}34785$ 3½

4 (*a*) Discuss the finite difference method in a two point linear boundary value problem in an ordinary differential equation and estimate the error involved in this method

Use second order Runge-Kutta formula to evaluate $\frac{dy}{dx} = x+y$; where $y(0)=1$; for $x=0\cdot3$, take $h=0\cdot1$ $5_{1/2}$

(*b*) Describe with equation Adams-Moulton method (Predictor-Corrector formula) to find the solution of a differential equation 4

5 (*a*) Obtain the expressions for the best value of the slope and intercept and their standard errors using least square method $5_{1/2}$

(*b*) Discuss different types of errors in an experimental data, standard error in a single and a set of observations 4

6 Attempt any *two* of the following $9_{1/2}$

(*i*) Obtain Trapezoidal formula for the evaluation of a definite integral Work out the error involved in this method

(*ii*) Obtain the electron-density equation for a crystal in terms of scattering amplitude and location of the atoms in a crystal using Fourier transforms

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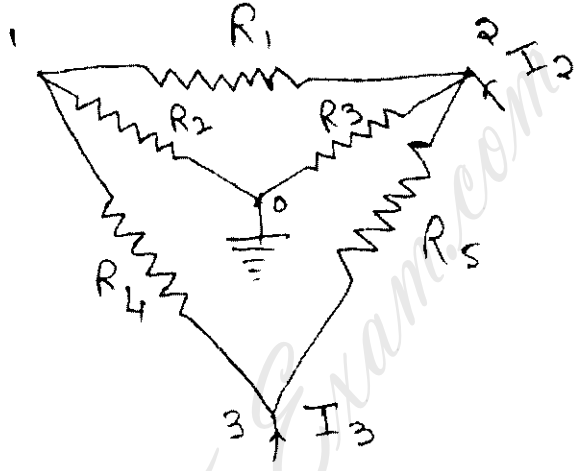
(*iii*) Write the admittance and current matrix of the following circuit and find the voltage vector using matrix operations



$R_1 = R_2 = R_3 = 1\ \Omega$

$R_4 = R_5 = 2\ \Omega$

$I_2 = 1$ amp

$I_3 = 2$ amp