Name :	
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Invigilator's Signature :	

## CS/INT.PBIR(PHY)/SEM-2/PHY-205/2010 2010

## **COMPUTATIONAL METHODS IN PHYSICS**

*Time Allotted* : 3 Hours

Full Marks : 50

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

Answer *all* questions.  $5 \times 10 = 50$ 

1. Write a program to find out the solution for the transcendental equation :

 $e^{-x} = \tan x.$ 

- 2. Write a program to check the range of *x* where the following approximation is valid within a given error bar :  $\sin x \approx x$ .
- 3. Write a program in FORTRAN for the Hamiltonian matrix elements of a one-dimensional chain having alternate site potentials ( $\varepsilon_A$  and  $\varepsilon_B$ ) with nearest ( $t_1$ ) and next nearest neighbour hoppings ( $t_2$ ). Assume  $\varepsilon_A = -0.5$  eV,  $\varepsilon_B = 0.5$  eV,  $t_1 = 1$  eV and  $t_2 = 0.2$  eV.
- 4. Write the subroutine to assign the Hamiltonian matrix elements for a two-dimensional square lattice with periodic boundary condition along *X* direction. Consider only nearest neighbour hopping (t = 1 eV).

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5. Write the expression for the energy spectrum in three dimensions for the tight binding approximation for the Hamiltonian of a cubic lattice. What is the maximum degeneracy possible ? Write a subroutine for the assignment of Hamiltonian matrix elements for a cubic lattice with only nearest neighbour hopping, t = 1 eV.