Name : .....

Roll No. : .....

Invigilator's Signature : .....

CS/INTPCS (CH-Sc.)/SEM-3/CH-512/2011-12

2011

CHEMICAL DYNAMICS OF ATOMS, MOLECULES & SOFT CONDENSED MATTER

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.

1. Considering nuclear and electronic coordinate dependent molecular wavefunction.

   a) define the adiabatic and the diabatic representation and the corresponding nuclear Schrö dinger equation (SE)

   b) transform the adiabatic SE to diabatic one. 4 + 6

2. a) Show that non-adiabatic coupling terms could be singular at the degenerate point of two electronic states.

   b) Derive Curl equation for non-adiabatic coupling terms starting from adiabatic-diabatic transformation (ADT) condition.

   c) While integrating the non-adiabatic coupling term over an angular co-ordinate φ (0, 2π), why is it expected to find a residue of π for a degenerate electronic system ?

   4 + 4 + 2

3. Considering collinear arrangement,

   a) write the reagent and product coordinates of any tri-atomic chemical reaction,

   b) derive the relation between the two sets of coordinates,

   c) define skewed angle and its value in case of collinear reaction. 2 + 6 + 2

4. a) Write the generalized form of Gaussian Wave Packet (GWP) for 1-d dynamical process and define its parameters.

   b) Find its normalization in terms of width parameter.

   c) Derive the classical equation of motion for the parameters of GWP to obtain its time dependence.

   2 + 4 + 4

5. Considering any tri-atomic chemical reaction,

   a) show the reactants, products and interaction regions on the potential energy contour.

   b) write down the wavefunction for those three regions considering Particle In a Box (PIB) model.

   c) find the reactant to product ratio / probability for any state-to-state reaction. 2 + 4 + 4