MA06326
All candidates

DO NOT OPEN THE QUESTION PAPER UNTIL INSTRUCTED TO DO SO BY THE CHIEF INVIGILATOR	
Department	CDISE
Module Code	MA06326
Module Title	Foundation of Multi-Scale Modelling: Kinetics (Mock Exam)
Exam Duration	Two hours
CHECK YOU HAVE THE CORRECT QUESTION PAPER	
Number of Pages	3
Number of Questions	4
Instructions to Candidates	Answer all questions. All marks gained will be counted.
FOR THIS EXAM YOU ARE ALLOWED TO USE THE FOLLOWING:	
Calculators	Approved calculators may be used.
Books/Statutes provided by the University	No
Are students permitted to bring their own Books/Statutes/Notes?	Yes
Additional Stationery	No

Skoltech

1. Mathematical Background

   (a) **[1 marks]** Simplify the following expressions for the products of dyads and vectors:

$$\begin{array}{lll} \text{(i)} & \vec{a}\cdot\vec{b}\circ\vec{c} & \vec{a}\circ\vec{b}\cdot\vec{c} \\ \text{(ii)} & \vec{a}\circ\vec{b}:\vec{c}\circ\vec{d} & \\ \text{(iii)} & \text{Trace}\,(\vec{a}\circ\vec{a}) & \text{Trace}\left(\vec{a}\circ\vec{b}\right) \end{array}$$

   (b) **[1 marks]** Compute the Fourier transform of the expressions $\frac{\partial^{10} f(x)}{\partial x^{10}}$ and $f(x)cos(ax)$ (assume that $\tilde{f}(\omega)$ is known).

   (c) **[2 marks]** Compute the Laplace transform of the expression at^4+bt^2+c Compute the inverse Laplace transform of $\frac{1}{(s-b)(s^2-a^2)}$

   Total: 4 marks

2. Langevin Equation and Fokker-Planck Equation

   (a) **[1 marks]** Evolution of a particle obeys the following Langevin Equation:

$$\frac{\partial y}{\partial t} = y^6 + F_{rand}(t)$$

   where the stochastic force $F_{rand}(t)$ has the following correlation function:

$$< F_{rand}(t')F_{rand}(t) >= \Gamma\delta(t-t')$$

   write down the corresponding Fokker-Planck equation.

   (b) **[2 marks]** Evolution of a particle obeys the following generalized Langevin Equation:

$$m\frac{dv}{dt} = -\int_0^t G(t-\tau)v(\tau)d\tau + F_{rand}(t)$$

   where the stochastic force has the following correlation function:

$$< F_{rand}(0)F_{rand}(t) >= t^2e^{-t}$$

   formulate the Fluctuation Dissipation Theorem and find the Diffusion Coefficient of a particle.

   (c) **[3 marks]** Use Kramers formula to compute the mean escape time (MFPT) for the potential barrier

$$U(x) = \begin{cases} U_0(x-1/3)^2, & \text{if} \quad 0\le x\le 0.5. \\ \frac{2}{6^4}U_0 - U_0(x-2/3)^2, & \text{if} \quad 0.5\le x\le 1.. \end{cases} \tag{1}$$

   U_0 is measured in energy units; $U_0 \gg k_BT$.

   Total: 6 marks

3. Smoluchowski Equations

   (a) **[1 marks]** Write down Smuluchowski Equations for a system with aggregation only for the aggregation rate coefficients of the form, $K_{ij} = 2ij$.

   (b) **[2 marks]** Find the dependence on time of the total concentration of clusters $N = \sum_{k \geq 1} n_k$ for the mono-disperse initial conditions, $n_k = \delta_{k,1}$. Provide a physical interpretation of the time behavior of $N(t)$.

   (c) **[2 marks]** Using generation function solve Smoluchowski Equations for $K_{ij} = 2$.

Total: 5 marks

4. Chapman-Enskog approach to the Boltzmann equation

   (a) **[1 marks]** Describe the main four steps of the Chapman-Enskog approach. What are the two main assumptions of this method?

   (b) **[1 marks]** What is the zero-order solution of the Chapman-Enskog scheme?

   (c) **[3 marks]** Using the BGK model for the Boltzmann equation with the relaxation time $\tau = \tau_0 (V/v_T)^{2b}$ compute the shear viscosity coefficient η.
   Hint: use the integrals,
$$\int_0^\infty x^n e^{-ax^2} = \frac{\Gamma\left(\frac{n+1}{2}\right)}{2a^{(n+1)/2}}$$
   .

Total: 5 marks