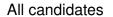
MA06326





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 Y	OU 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

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All candidates

Skoltech

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

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

$$\langle F_{rand}(t')F_{rand}(t)\rangle = \Gamma\delta(t-t')$$

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:

$$\langle F_{rand}(0)F_{rand}(t)\rangle = t^2e^{-t}$$

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

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

 U_0 is measured in energy units; $U_0 \gg k_B T$.

Total: 6 marks

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All candidates

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