IISER Kolkata – Mid-Semester Examinations

CH4209- Molecular Reaction Dynamics

Total marks = 20 Duration: 1and ½ hours

Note: There are total 4 questions and each question carries 5 marks.

1. Prove that rate constant for a bi-molecular reaction is given by $k(T) = \pi d^2 \left(\frac{8k_B T}{\pi \mu} \right)^{1/2} e^{-E^*/k_B T}$, where E* is the critical relative collision energy which is required for the reaction. Other symbols have their usual meaning.

2. Effective potential for the R-coordinate, the distance between the reactants, is given by $V_{eff}(R) = -\frac{C}{R^3} + \frac{L^2}{2\mu R^2}$, where L is the orbital angular momentum and μ is the reduced mass. Assuming the reaction probability is one for kinetic energy larger than or equal to the barrier in the effective potential, find an expression for the reaction cross-section σ_R.

3. Prove that the average position of a free particle wavepacket at time t is given by $\langle x \rangle_t = \frac{\langle p \rangle t}{m} + \langle x \rangle_0$.

4. Prove that Gaussian wavepacket $\Psi(x) = N \exp(-\alpha x^2)$, where N is the normalization constant, is a minimum uncertainty wavepacket.