Gautam Gangopadhyay

Senior Professor
CBMS
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Guidance of Students/Post-Docs/Scientists

a) Ph.D. Students

1. Premashis Kumar; Nonequilibrium thermodynamics of open nonlinear dynamical systems; Under progress

b) Post-Docs

1. Prasanta Kundu; Dynamic disorder and conformational fluctuation in reaction kinetics

Teaching

1. Autumn semester; Advanced Equilibrium Statistical Mechanics; PhD; 4 students; with 1 (Jaydeb Chakrabarty) co-teacher

Publications

a) In journals

1. Premashis Kumar and **Gautam Gangopadhyay**, *Energetic and entropic cost due to overlapping of Turing-Hopf instabilities in the presence of cross diffusion*, Physical Review E, 101, 042204, 2020
2. Prasanta Kundu, Soma Saha, and **Gautam Gangopadhyay**, *Mechanical Unfolding of Single Polyubiquitin Molecules Reveals Evidence of Dynamic Disorder*, ACS Omega, 5, 9104-9113, 2020
3. Prasanta Kundu, Soma Saha and **Gautam Gangopadhyay**, *Kinetics of escape of ssDNA molecules from -hemolysin nanopores: a dynamic disorder study*, Journal of Statistical Mechanics: Theory and Experiment, 2020, 053501, 2020
4. Sandip Saha, **Gautam Gangopadhyay** and Deb Shankar Ray, *Systematic designing of bi-rhythmic and tri-rhythmic models in families of Van der Pol and Rayleigh oscillators*, Communications in Nonlinear Science and Numerical Simulation, 85, 105234, 2020
5. Prasanta Kundu, Soma Saha and **Gautam Gangopadhyay**, *Stochastic Kinetic Approach to the Escape of DNA Hairpins from an -Hemolysin Channel*, The Journal of Physical Chemistry B, 124, 6575-6584, 2020
6. Sandip Saha, Sagar Chakraborty and **Gautam Gangopadhyay**, *Suppressing birhythmicity by parametrically modulating nonlinearity in limit cycle oscillators*, Physica D: Nonlinear Phenomena, 416, 132793, 2021
7. Prasanta Kundu, Soma Saha and **Gautam Gangopadhyay**, *An Exactly Solvable Stochastic Kinetic Theory of Single-Molecule Force Experiments*, The Journal of Physical Chemistry B, 124, 7735-7744, 2020
8. Sandip Saha, **Gautam Gangopadhyay**, Sangeeta Kumari & Ranjit Kumar Upadhyay, *Parametric Excitation and Hopf Bifurcation Analysis of a Time Delayed Nonlinear Feedback Oscillator*, International Journal of Applied and Computational Mathematics, 6, Article Number 123, 2020
9. Prasanta Kundu, Soma Saha, and **Gautam Gangopadhyay**, *Kinetics of Allosteric Inhibition of*

Single Enzyme by Product Molecules, The Journal of Physical Chemistry B, 124, 11793 – 11801, 2020

10. Krishnendu Pal, Dibakar Ghosh and **Gautam Gangopadhyay**, *Synchronization and metabolic energy consumption in stochastic Hodgkin-Huxley neurons: Patch size and drug blockers*, Neurocomputing, 422, 222 – 234, 2021

Talks / Seminars Delivered in reputed conference / institutions

1. Talk delivered on Ultrasensitivity as a Stochastic Activation Event; Mar 31, 2021; (Online); Chemistry Department, Stat Mech Gr Visva-Bharati University, Santiniketan; 4-5PM

Administrative duties

1. Member of Project and Patent Cell, SNBNCBS
2. Transparency Officer, SNBNCBS

Membership of Learned Societies

1. Indian Association for the Cultivation of Science, Kolkata
2. Indian Physical Society

Scientific collaborations with other national / international institutions (based on joint publications)

1. Dr. Soma Saha, Assistant Professor, Chemistry Department, Presidency University, Kolkata; Sl. No. 2,3,5,7; National
2. Prof. Sagar Chakraborty, Physics Department, IIT Kanpur; Sl. No. 6; National
3. Prof. D S Ray, School of Chemical Sciences, IACS, Kolkata; Sl. No. 4; National
4. Prof. Ranjit Kumar Upadhyay, Applied Mathematics, Indian School of Mines; Sl. No. 8; National
5. Prof. Dibakar Ghosh, Indian Statistical Institute, Kolkata; Sl. No. 10; National

Areas of Research

Theoretical Chemical Physics

1. Exploration of the energetic and entropic cost in nonlinear open system:

   A systematic introduction to nonequilibrium thermodynamics of dynamical instabilities are considered for an open nonlinear system beyond conventional Turing pattern in presence of cross diffusion. An altered condition of Turing instability in presence of cross diffusion is best reflected through a critical control parameter and wave number containing both the self- and cross-diffusion coefficients. Our main focus is on entropic and energetic cost of Turing-Hopf interplay in stationary pattern formation. Depending on the relative dispositions of Turing-Hopf codimensional instabilities from the reaction-diffusion equation it clarifies two aspects: energy cost of pattern formation, especially how Hopf instability can be utilized to dictate a stationary concentration profile, and the possibility of revealing nonequilibrium phase transition. In the Brusselator model, to understand these phenomena, we have analyzed through the relevant complex Ginzberg-Landau equation using multiscale Krylov-Bogolyubov averaging method. Due to Hopf instability it is observed that the cross-diffusion parameters can be a source of huge change in free-energy and concentration profiles.

2. Multiscale dynamics in open Chemical and Biological Systems:

   The self-sustained chemical oscillations are also regularly observed in biological world to maintain a cyclic steady state e.g., cell division[, circadian oscillation, calcium oscillations and other bio-systems. Our aim in this project is to look into the physical and mathematical properties of weakly nonlinear systems containing periodic orbits by adopting various methods of multiscale perturbation analysis to cover single to multi-limit cycles which can arise in various practical situations. We have presented an unified scheme to express a class of system of equations in two variables intoa Liénard - Levinson - Smith(LLS) oscillator form. We have derived the condition for

limit cycle for arbitrary polynomial functions of damping and restoring force. A method is devised to determine the maximum number of limit cycles admissible for a LLS oscillator. Based on this approach we proposed a scheme for systematic designing of generalised Rayleigh andVan der Pol families of oscillators with a desired number of multiple limit cycles.

3. A single molecule approach to deal with the dynamic disorder in various chemical and biological processes:

   The decay of the nonexponential kinetics at the microsecond timescale, points to the relevance of having possible influence of dynamic disorder on the reaction kinetics. To rationalize the experimental results by a microscopic model in which the dynamics of protein is described in terms of the anomalous diffusion of a Brownian particle in a harmonic potential well under the action of fractional Gaussian noise. Starting from a non-Markovian diffusion equation supplemented with an exponential sink term accounts for the electron transfer reaction between the donor and acceptor groups, we calculate the survival probability from the solution of the corresponding diffusion–reaction equation to quantify the average activation energy for the conformational dynamics suggesting an alternative interpretation for the observed non-exponential ET kinetics associated with dynamic disorder rather than a static heterogeneity.

Plan of Future Work Including Project

1. Energetic and entropic cost in nonequilibrium steady state A systematic introduction to nonequilibrium thermodynamics of dynamical instabilities can be considered for an open nonlinear system beyond conventional Turing pattern. Our main focus is on entropic and energetic cost of stationary pattern formation which can clarify: energy cost of pattern formation, and the possibility of revealing nonequilibrium phase transition. In this context, complex Ginzberg- Landau equation can be utilized to see how the different nonlinear phenomena play their roles in stationary pattern, for example, Hopf instability and the cross-diffusion parameters etc in controlling the free-energy and concentration profiles. In similar spirit, the role of energetic discrimination is of utmost importance for the reaction network of high specificity when the rate is arbitrarily low, which can be implemented for improving ac- curacy through a proofreading network for error-dissipation trade-off regime and beyond. The nonequilibrium steady state theory can be incorporated with a recently developed thermody- namic framework to obtain the error basin, dissipation, and energetics of kinetic proofreading with energetic discrimination in binding and unbinding processes. It can be advantageous in maintaining and enhancing the specificity with externally controllable concentration parameters.