PHY 690 Y: Thermal Physics at Nano-scale

Instructor-in-charge: Prof. Debashish Chowdhury

1. Course Objectives:

   Classical thermodynamics was developed for macroscopically large systems. Equilibrium statistical mechanics, as developed by Maxwell, Boltzmann and Gibbs, could not only provide microscopic justification of the laws of thermodynamics but also account for fluctuations in finite systems. However, for systems as small as a few nano-meters, a fundamental question arises: how do the laws of thermal physics for such systems deviate from those for macroscopic (practically infinite) systems so that in the infinite-size limit the laws of macroscopic thermodynamics are recovered? How are energy transduction by nano-engines and information processing by nano-computers constrained by the fundamental laws of thermal physics at the nano-scale? Research works addressing such questions are expanding the frontier of thermal physics that is often referred to as "Stochastic Thermodynamics". Students will get an exposure to this rapidly expanding frontier in this course.

2. Prerequisites: Thermal Physics / Thermodynamics at the UG level.

3. Course Contents:
   1. Brief overview of Thermal Physics at Macro-scale:
      Laws of thermodynamics; fundamental relations
      and equations of state;
      Energy transduction by heat engines.
      Rules of calculation of equilibrium Statistical Physics
      from Jaynes maximum entropy principle;
      Fluctuations and relation with response functions.
      Hill's nano-thermodynamics. (3 Lectures)
   2. Free energy landscape: meta-stable and un-stable states:
      Langevin equation and Fokker-Planck equation; Diffusion;
      Kramers theory of activated barrier crossing-
      Application to relaxation of magnetic nano-particles
      Becker-Doring theory of nucleation. (9 Lectures)
   3. Discrete state space: non-equilibrium steady states:
      Master equation- Random Walk as an example;
      Gillespie algorithm for numerical solution;
      Non-graphical solution in NESS by matrix inversion;
      Graph theoretic solution in NESS; Detailed balance;
      Applications to NESS of ASEP. (9 Lectures)
   4. Stochastic mechanics:
      Elasticity of single molecules, entropic springs;
      Thermodynamics and kinetics of mechanical rupture
      of bonds, Slip- versus catch-bonds. (6 Lectures)
   5. Stochastic thermodynamics: fluctuation-dissipation
      Fluctuation theorems, Jarzynski and Crooks identities;

Dissipation, entropy production in irreversible processes;
From ensemble thermodynamics to trajectory thermodynamics;
Energy Transduction: Enzymes and chemo-chemical
nano-machines; Energy transduction and information
processing by nano-motors. (15 Lectures)

4. Lecture & Venue: As announced by OARS.
5. E-mail id of instructor: debch@iitk.ac.in
6. Evaluation Components & Policies:

   End-semester Examination (weightage: 55%).
   Mid-semester Examination (weightage: 35%)
   Quizzes (combined weightage: 10%)

7. Course Policies: Attendance is compulsory.

8. Textbook and References:

   1. D.E. Makarov, "*Single Molecule Science: Physical Principles and Models*, (CRC Press, 2015).
   2. D.J. Evans, D.J. Searles and S.R. Williams, "*Fundamentals of Classical Statistical Thermodynamics: Dissipation, Relaxation and Fluctuation Theorems*" (Wiley-VCH, 2016).
   3. L.A. Blumenfeld and A.N. Tikhonov, "*Biophysical Thermodynamics of Intracellular Processes: Molecular Machines of the Living Cell*" (Springer, 1994).
   4. T.L. Hill, "*Free Energy Transduction and Biochemical Cycle Kinetics*" (Springer, 1989).
   5. T.L. Hill, "*Free Energy Transduction in Biology*" (Springer, 1977).
   6. K. Sekimoto, "*Stochastic Energetics*", (Springer, 2010).
   7. U. Seifert, "*Stochastic thermodynamics, fluctuation theorems and molecular machines*", Reports on Progress in Physics, 75, 126001 (2012).