# A study of Fluctuations and Transport in Non-equilibrium systems

by

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# *Certificate:*

This is to certify that the thesis entitled **A study of Fluctuations and Transport in Non-equilibrium systems** submitted by **Mr. Rahul Marathe** for the award of the degree of Doctor of Philosophy of Jawaharlal Nehru University is his original work. This has not been published or submitted to any other University for any other Degree or Diploma.

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I hereby declare that the work reported in this thesis is entirely original. This thesis is composed independently by me at Raman Research Institute under the supervision of Prof. Abhishek Dhar. I further declare that the subject matter presented in this thesis has not previously formed the basis for the award of any degree, diploma, membership, associateship, fellowship or any other similar title of any university or institution.

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# Preface

There are very few general results in statistical physics which are valid for systems far from equilibrium. Among these are the non-equilibrium fluctuation theorems which put conditions on the probability distribution of entropy production in non-equilibrium systems. Another is the Jarzynski equality, which relates the non-equilibrium work done on a system to equilibrium free energy differences. Unlike linear response theory, these relations are valid for systems arbitrarily far away from equilibrium. These relations are exact no matter how far the system is driven out of equilibrium and are independent of the rate and strength of perturbation. In the first part of the thesis we look at some examples of non-equilibrium processes in the context of these new results.

A class of far from equilibrium systems are the so called ratchet models and microscopic models of pumps and engines. These models exhibit net directed transport of particles in the system in the presence of noise and driving and in the absence of any applied external bias. The first such construct of a miniature molecular engine was by Feynman. This is the Feynman ratchet and pawl engine, ( discussed in *Feynman lectures on Physics* ), which was first proposed as a microscopic mechanical model to explain the problem in constructing a Maxwell's demon. Similar models, based on the same principle, have recently been studied to understand the working of molecular motors and pumps in biological systems. These molecular motors ( e.g. kinesin ) move uni-directionally on the microtubules inside biological cells. Also, molecular pumps, like sodium or potassium pumps, maintain active transport across membranes against a concentration gradient. These motors and pumps are in a very noise environment but still they exhibit net uni-directional motion. The second part of the thesis includes studies on some new models of heat/particle pumps and engines.

In chapter 2 of the thesis we look at the validity of different fluctuation theorems for a simple system of a single Ising spin in contact with a heat bath and driven by an external time dependent magnetic field. We explicitly compute the distribution of the work done in driving the spin over a fixed time interval. The time evolution of the spin is modelled using Glauber dynamics. Monte-Carlo simulations are performed to find the work distributions at different driving rates. We find that in general the work-distributions are broad with a significant probability for processes with negative dissipated work. The special cases of slow and fast driving rates are studied analytically.

In chapter 3 we look at some simple models of heat pumps. Motivated by recent studies on models of quantum particle and heat pumps, we study similar classical models and examine the possibility of heat pumping. Unlike many of the usual ratchet models of molecular engines, the models we study here do not have particle transport. We consider a two-spin system and a coupled oscillator system which exchange heat with multiple heat reservoirs and which are acted upon by periodic forces. The simplicity of our models allows accurate numerical and exact solutions and unambiguous interpretation of results. We demonstrate that while both our models seem to be built on similar principles, one is able to function as a heat pump ( and also as an engine ) while the other is not.

In chapter 4 we look at a model of a particle pump. We study a symmetric exclusion process in which the hopping rates at two ( or more) chosen sites vary periodically in time and have a relative phase difference. This mimics a colloidal suspension subjected to external space and time dependent modulation of the diffusion constant. The two special sites act as a classical pump by generating an oscillatory current with a nonzero $\mathcal{DC}$ value whose direction depends on the applied phase difference. We analyze various features of this model through simulations and obtain an expression for the $\mathcal{DC}$ current via a novel perturbative treatment.

This work is done in collaboration with my thesis supervisor Prof. Abhishek Dhar and with Prof. Arun Jayannvar, Institute of Physics, Bhubaneshwar, Dr. Kavita Jain, JNCASR, Bangalore and Dr. Abhishek Chaudhury, Raman Research Institute, Bangalore.

## Publications


- Work distribution functions for hysteresis loops in a single-spin system, Rahul Marathe and Abhishek Dhar, Phys. Rev. E **72**, 066112 (2005).

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