The Center for Nanophase Materials Sciences
presents
A Nanomaterials Theory Institute Mini-Symposium
April 22-24, 2008

Nonlinear Response Theory and the Fluctuation Theorems

A series of three lectures presented by

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***Background**. The fluctuation theorems derived by Denis Evans and co-workers are the first rigorous characterizations of deviations from equilibrium in systems subject to arbitrary external fields. They predict the precise mathematical relationship between the probability of negative entropy producing states (i.e., violations of the second law of thermodynamics), the probability of positive entropy producing states (i.e., consistent with the second law of thermodynamics), and the state and size of the system. The predictions of the fluctuation theorems have been validated by experiments in classical (optical tweezers) and quantum systems. This is an example of a phenomena initially discovered computationally (in non-equilibrium simulations), that led to theoretical development (non-linear response theory and the theorems themselves), finally validated by experiment. Denis Evans will be visiting the Nanomaterials Theory Institute in the Center for Nanophase Materials Sciences April 22-25 and will be presenting three lectures on the fluctuation theorems. Anyone from the ORNL community is welcome to attend.*

Lecture I: Computer Simulation, Chaos, Lyapunov Exponents and Transport Coefficients

Tuesday, April 22 at 10:00 am in room L183, building 8610

Abstract

We very briefly describe the historical development of non-equilibrium statistical mechanics and computer simulation. We describe how algorithms were developed and how they were proved to be correct. We also describe the impact that the mathematical study of chaos has had on non-equilibrium statistical mechanics. We briefly describe new mathematical relationships between transport processes, the Second Law of Thermodynamics and chaotic measures.

Lecture II: The Fluctuation & Dissipation Theorems, Theory & Experiment

Wednesday, April 23 at 1 pm in room L183, building 8610

Abstract

Recently there has been considerable theoretical and experimental interest in the so-called Fluctuation Theorem. These Theorems show how time reversible microscopic dynamics leads to irreversible macroscopic behavior as either the system size or the observation time increases. In the lecture we discuss the Evans-Searles Fluctuation Theorems and we go on to show that the argument of the Evans-Searles Fluctuation Theorem, the dissipation function, also plays a central role in nonlinear response theory. Exact expressions for the nonlinear response of a classical N-body system to a nonequilibrium process, are derived in terms of the Evans-Searles dissipation function. These expressions should be verifiable in the laboratory. When linearized, these expressions reduce to the well-known Green-Kubo expressions for the linear response.

Lecture III: NonEquilibrium Free Energy Theorems including the Crooks Fluctuation Theorem and the Jarzynski Equality

Thursday, April 24 at 8:30 am in room L183, building 8610

Abstract

The Jarzynski Equality and the Crooks Fluctuation theorem provide means to compute the change in a system's free energy from non-equilibrium pathways. These theories consider processes where the system is driven out of equilibrium by a mechanical external agent while remaining in contact with a thermal reservoir at a fixed temperature. We discuss these theorems and give generalizations to handle processes driven by any type of external agent, be it thermal or mechanical. We also discuss the close linkages between these relations and the Evans-Searles Fluctuation Theorem.

Refreshments will be served at the beginning of each lecture.
Enquiries should be directed to Thomas Schulthess or Peter Cummings.

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