Politecnico di Torino

MATHEMATICAL SCIENCES

AMMIN/DISMA - Response theory, fluctuation theorems and phase transitions

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Context of the research activity	A statistical mechanical theory of equilibrium states is available, and is complemented by a theory of response to small perturbations of such equilibrium states. far from phase transitions. For systems of mildly away from equilibrium, linear laws such as the Fick, Ohm and Fourier laws apply. However, a general theory of response to perturbations that may may be large or involve phase transitions has only recently began to be considered. The project will aim at developing and applying such novel response theories.

	The study of out-of-equilibrium systems, starting from the microscopic constituents of matter, is notoriously more challenging than the case of systems in equilibrium. At equilibrium, the probability distributions of the systems microscopic constituents, expressed in the degrees of freedom relevant to the dynamics, is often a multivariate Gaussian. This significantly simplifies the mathematical treatment, even though exact treatments, even for simple models like the three-dimensional Ising model, remain elusive to this day. However, in this case, the limitations appear as a mere manifestation of computational complexity. The situation in the case of non-equilibrium is quite different: rigorous results are limited, and often the behavior of systems, and the models that describe them, depend on the protocols used to create the non-equilibrium situations of interest. An important chapter in the theoretical study of these phenomena concerns the possibility of "exploiting" knowledge of a system's equilibrium properties to deduce its non-equilibrium behavior. Two examples include the theory of linear response, with the associated fluctuation dissipation relations, and certain formulations of fundamental principles closely tied to fluctuation theorems, such as the Jarzynski and other equalities. Generally speaking, under certain assumptions about the protocols used to take a system out of equilibrium, it is possible to recognize the imprint of equilibrium probability distributions even if the forced system strongly departs from equilibrium.

Objectives	However, applying these paradigms in practice is not always possible or successful. For instance, to reproduce the predictions implied by the Jarzynski equality, one would, in theory, need to sample (as the initial condition for each repetition of the same experiment) a significant number of microstates corresponding to the initial macroscopic equilibrium ensemble. As the equilibrium distribution is exponential in microscopic variables, it may thus require such a vast number of repetitions, often beyond our reach. In modeling, the problem can at times be circumvented, but only if exactly solvable models are known, as even numerical simulations may not provide sufficient resources to meaningfully sample rare events necessary for reconstructing the equality. Moreover, such a full statistical exploration may in fact not correspond to the reality of the experiments at hand. Other modern theories of macroscopic or microscopic non-equilibrium fluctuations incur in similar problems. A recent interesting development has tackled the problem of studying exactly solvable models by imposing a truncation that excludes microstates with low probabilities from the probability measure. Comparisons of the results obtained with exact (non-truncated) solutions have revealed intriguing results. Among these, to mention one example, is the ability to recognize phase transitions that would occur during transformations caused by external forcing. Interestingly, this could happen even in systems of not very large size, where equilibrium phase transitions, formally, require the mathematical limit of infinite size. This represents an important and novel step toward characterizing out-of-equilibrium systems based on knowledge of equilibrium states. This, and the exact response theory under development open up broad areas for new studies. The present project proposes to investigate how similar phenomena may be linked to percolation models, for example on lattices or graphs. Among percolation models, cases like bootstrap percolation (on regular lattices) or k-core percolation (on graphs) provide complex study systems where different types of phase transitions are observed, such as first-order, second-order, hybrid types, and non-equilibrium phase transitions. The idea of verifying for which types of transitions the same phenomenon can be observed is deemed interesting and worthy of further investigation—namely, recognizing the trace of phase transitions in the properties of systems subjected to out-of-equilibrium protocols, under the effect of a truncation of the equilibrium probability measure, or of the exact response of suitable observables. Far from being merely mathematical artifices, the finite sizes and truncated distributions often better represent real experiments performed at small scales or over short times. In these case, it is not only impossible but often misleading the use of of statistics strictly referring to infinite systems. Models to be considered will include one-dimensional systems, exactly solvable at equilibrium, described either by stochastic processes or deterministic dynamics, depending on the application of interest.

Skills and competencies for the development of the activity	Mathematical, physical and computational background of Mathematics, Physics, Chemistry, Engineering programs.