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Aspects of non-equilibrium in classical and quantum systems: Slow relaxation and glasses, dynamical large deviations, quantum non-ergodicity, and open quantum dynamics*

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HIGHLIGHTS

- Basic concepts on slow relaxation and non-ergodicity in both classical and quantum systems are introduced.
- Kinetically constrained models are described as simple models for slow dynamics.
- Large deviations methods applied to non-equilibrium dynamics, both in classical systems and in open quantum systems, are presented.

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ABSTRACT

In these four lectures I describe basic ideas and methods applicable to both classical and quantum systems displaying slow relaxation and non-equilibrium dynamics. The first half of these notes considers classical systems, and the second half, quantum systems. In Lecture 1, I briefly review the glass transition problem as a paradigm of slow relaxation and dynamical arrest in classical many-body systems. I discuss theoretical perspectives on how to think about glasses, and in particular how to model them in terms of kinetically constrained dynamics. In Lecture 2, I describe how via large deviation methods it is possible to define a statistical mechanics of trajectories which reveals the dynamical phase structure of systems with complex relaxation such as glasses. Lecture 3 is about closed (i.e. isolated) many-body quantum systems. I review thermalisation and many-body localisation, and consider the possibility of slow thermalisation and quantum non-ergodicity in the absence of disorder, thus connecting with some of the ideas of the first lecture. Lecture 4 is about open quantum systems, that is, quantum systems interacting with an environment. I review the description of open quantum dynamics within the Markovian approximation in terms of quantum master equations and stochastic quantum trajectories, and explain how to extend the dynamical large deviation method to study the statistical properties of ensembles of quantum jump trajectories. My overall aim is to draw analogies between classical and quantum non-equilibrium and find connections in the way we think about problems in these areas.

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Introduction

The purpose of these lecture notes is to introduce some general and simple ideas about slow relaxation and nonequilibrium dynamics in many-body systems, both classical and quantum. The aim is not to be comprehensive, but rather to describe particular ways in which to address certain interesting questions in non-equilibrium, and to highlight potential connections between problems in areas that may appear very different. The first part of these notes deals with classical systems. Lecture 1 is about the glass transition problem, an important and yet not fully understood general problem in condensed matter science, and also a paradigm of slow and complex relaxation more generally. I describe basic questions that emerge from the phenomenology of glass forming systems such as supercooled liquids, and briefly discuss basic theoretical perspectives. Most of the focus is on a general modelling of glasses in terms of systems with constraints in their dynamics, an approach that has wider applicability, as discussed later in the notes. A key insight that emerges from these considerations is that the interesting behaviour in many systems with cooperative dynamics is to be encountered in properties of the trajectories of the dynamics rather than in configurations, highlighting the need for a statistical mechanics approach to study trajectory ensembles. Lecture 2 describes how such approach can be constructed with dynamical large deviation methods. Such an approach leads to thinking about dynamics in a thermodynamic-like fashion, for example by revealing the existence of dynamical phases – and phase transitions between them – that underlie observed fluctuation behaviour in the evolution of systems with cooperative and collective dynamics.

The second part of these notes is about non-equilibrium in quantum systems. Lecture 3 discusses dynamics in isolated quantum many-body systems, where despite unitary evolution, there is both equilibration and thermalisation. I furthermore describe many-body localisation in disordered systems as a novel paradigm for quantum non-ergodicity. I also consider similarities and differences between many-body localisation and slowdown and arrest in classical glasses, contrasting mechanisms based on disorder to those based on dynamical constraints. Lecture 4 is about open quantum systems. I discuss how the dynamics of quantum systems that interact with an environment can be described in an approximate Markovian way, considering similarities and differences with classical stochastic systems. I also explain how to extend large deviation methods to the open quantum case in order to study properties of quantum jump trajectories using similar ideas to those employed in classical non-equilibrium.

There are many excellent reviews on several of the topics covered in these notes. For the glass transition problem these include Refs. [1-7]; for kinetically constrained models, Refs. [8,9]; for large deviations, Refs. [10-12]. In the case of quantum systems, comprehensive recent reviews on thermalisation and many-body localisation include Refs. [13-15]; and on open quantum systems, Refs. [16-19]. The selection of topics, many of the examples shown, and the overall approach to the problems discussed here is also based on my own work in these areas.

1. Slow relaxation in classical systems

1.1. Phenomenology of the glass transition

In the physical sciences glasses are the paradigm of non-equilibrium matter: when too cold or too dense fluids cease to flow, forming the amorphous solid-like material we call glass. This solidification occurs in the absence of any apparent structural ordering, in contrast to more conventional condensed matter. Dynamical arrest like that of glasses is ubiquitous in nature. It occurs in a vast range of systems spanning microscopic to macroscopic scales. Despite its practical importance, a fundamental understanding of the glass transition is still lacking, making it one of the outstanding problems of condensed-matter science. For reviews see [1–5].

Fig. 1 illustrates the glass transition problem. The central physical ingredient necessary for glassy slowing down is that of excluded volume interactions at high densities. Under such conditions motion is severely restricted through steric constraints, cf. Fig. 1(a), and particles can only move if the neighbouring particles that are blocking their path move before. The higher the density the more collective motion becomes. Cooperative relaxation leads to separation of timescales, where short scale motion (e.g. harmonic and anharmonic vibrations) is fast but the larger scale motion required for structural relaxation is slow. This becomes manifest in time correlations displaying metastability and decaying stretched exponential manner in time, indicative of a wide distribution of relaxation timescales, cf. Fig. 1(b). The typical relaxation time of supercooled liquids (inferred either from dielectric relaxation or from their viscosity) grows dramatically with decreasing temperature, a phenomenon which is quasi-universal, cf. Fig. 1(c). By convention, when relaxation time becomes 100 s (corresponding to a viscosity of fifteen orders of magnitude higher than that of a normal liquid), a liquid cannot be experimentally distinguished from a solid and such materials undergo a so-called experimental glass transition, corresponding to a falling out-of-equilibrium into the solid amorphous glass.

A hallmark of dynamics close to the glass transition is dynamical heterogeneity, illustrated in Fig. 1(d) which shows the spatial pattern of relaxation in a two-dimensional supercooled Lennard-Jones mixture. The slower the relaxation the more relaxation fluctuates in time and space: dynamics of systems close to the glass transition is fluctuation dominated and far from mean-field. It is important to note that the generic physics of the glass transition occurs in classical many-body systems in the absence of disorder, making them different from disordered systems such as spin-glasses.

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