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Systematic derivation of Generalized Langevin Equations for coarse-graining and bridge-scaling procedures

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In many branches of physics, one must often deal with processes involving a huge number of degrees of freedom. Instead of describing the dynamics of each individual of them, one rather wants to characterize the process of interest via a small set of observables that capture its main features of the process. Even if the microscopic dynamics can be resolved using Newton's equations of motion, it quickly becomes a computationally very expensive calculation to make. It is however much more convenient to come up with a self-consistent equation of motion for the 'global' observable of interest itself in order to reduce the complexity of the problem. The development of the Mori-Zwanzig formalism in the 1960's allowed to systematically derive such equations for arbitrary observables in stationary processes. This framework, derived from first principles by means of projection operator techniques, proves the structure of what is now known as the Generalized Langevin Equation, i.e. a stochastic equation of motion which a priori exhibits memory effects in the form on non-localities in time.

We propose to extend the formalism and its corollaries to a broad class of out-of-equilibrium processes. We show that the structure of the Generalized Langevin Equation is overall robust but must be adapted to account for the non-stationary dynamics [1,2]. The function that controls memory effects the stochastic term are related through a relation that can be associated to fluctuation-dissipation theorems. This formalism is very convenient to study two-time auto-correlation functions for which we can write a self-consistent differential equation as well. We finally show a new method to evaluate the memory function from numerical or experimental data [3].

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