CFEL SCIENCE

SEMINAR

3rd July 2019 - 1:30 p.m.

CFEL-bldg. 99, seminar room IV

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On the dynamics of reaction coordinates

Complex microscopic many-body processes are often interpreted in terms of “reaction coordinates", i.e. in terms of the evolution of a small set of coarse-grained, ensemble averaged variables. Under stationary conditions, the evolution of such coordinates is described by the generalized Langevin equation. In contrast, if the dynamics is not stationary, it is not a priori clear which form the equation of motion for an averaged observable has. We employ the formalism of time-dependent projection operator techniques to derive the equation of motion for a non-equilibrium trajectory-averaged observable as well as for its auto-correlation function. We consider, in particular, Hamiltonians and observables which depend on time explicitly as e.g. in systems under external driving.

The equation of motion which we obtain is similar in structure to the generalized Langevin equation, but it exhibits a time-dependent memory kernel as well as a fluctuating force that implicitly depends on the initial conditions of the process. We also derive a relation between this memory kernel and the autocorrelation function of the fluctuating force that has a structure similar to a fluctuation-dissipation relation. In addition, we show how the choice of the projection operator allows to relate the Taylor expansion of the memory kernel to data that is accessible in MD simulations and experiments, thus allowing to construct the equation of motion. As a numerical example, the procedure is then applied to crystal nucleation from a supercooled Lennard-Jones melt.

Host: Robin Santra – CFEL-DESY Theory Division