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Investigating the dynamics of biopolymers using field theory and path integrals

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Biopolymers (such as proteins or nucleid acids) are prototypical examples of complex open systems. Indeed, in these systems, the interplay between strong correlations and large thermal fluctuations gives raise to non-perturbative phenomena such as frustration, meta-stability and cooperativity which are typical of complex systems.

Large scale computer simulations of their classical structural dynamics and their quantum electronic structure could in principle provide a poweful and theoretically sound framework for theoretical investigations. Unfortunately, these methods are limited by their intrinsic complexity of the systems and by the co-existence of multiple widely separated time-scales. As a result, a gap of many orders of magnitude exists beteween the time scales which can be presently simulated by molecular dynamics and those which are relevant for biological applications.

In this talk I will show how theoretical physics techniques originally developed in the context of high-energy and nuclear physics such as path integrals and renormalization group can be used to develop computational approaches which enable to perform simulations which are inaccessible to standard molecular dynamics. In particular, I will discuss an approach which enables to investigate in a unified manner both biologically relevant conformational transitions (such as protein folding) and the transport and decoherence of optically excited electronic excitations.

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