A Generalized Langevin Equation Approach for Barrier Crossing Dynamics in Conformational Transitions of Proteins

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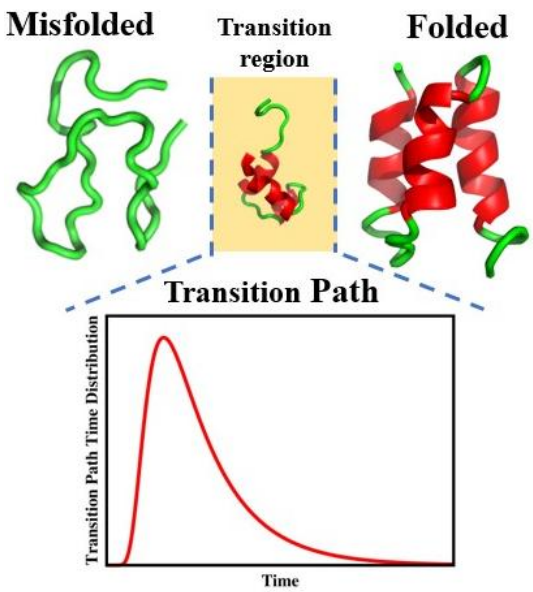
Barrier crossing dynamics in conformational transitions of proteins are investigated in the framework of the inertial generalized Langevin equation with an exponential memory kernel in a parabolic potential [1]. This approach yields an exact analytical expression for the time dependent Grote–Hynes rate and the transmission coefficient, which typically determines the kinetics of such transitions. The complete transition path time distribution (TPTD) and the mean transition path time (MTPT) are evaluated as a function of the frictional coefficient and barrier curvature. The results of TPTD show an excellent agreement with the experimental results of TPTD for the PrP prion protein and theoretical results in the high friction limit [2, 3], while they exhibit a considerable deviation from the results of theory at the intermediate and low friction limits. The inertial terms significantly affect the short time dynamics of such transitions [4]. The results of the TPTD and MTPT are discussed at low and high frictional limits with varying curvatures of the potential barrier [1, 5]. The TPTD decreases with an increase in the barrier curvature at the high friction limit and exhibits an exponential decay at long times [1]. The MTPT decreases with an increase in the curvature of the barrier.



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