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Protein fluctuations and breakdown of time-scale separation in rate theories

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A long-time fluctuation correlation function with a power-law form has been observed in recent single-molecule experiments by the Xie group. By analyzing the dynamics of an elastic network model (ENM) under white noise, we show that the observed long-time memory kernel can be explained by the discrepancy between the experimentally measured coordinate (or the coordinate directly coupled to protein function) and the minimum energy path of the system. Consequently, the dynamics of the measured collective coordinate has contributions from degrees of freedoms with a broad distribution of time scales. Our study also implies that the widely used ENM Hamiltonian should be viewed as a coarse-grained model of a protein over a rugged energy landscape. Large effective drag coefficients are needed to describe protein dynamics with the ENM's.

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