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Looping and direct transit in Brownian particle escape from force-biased and entropic traps

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Recent experiments with single biological nanopores, as well as single-molecule fluorescence spectroscopy and pulling studies of protein and nucleic acid folding raised a number of questions that stimulated theoretical and computational studies of the barrier crossing dynamics. We focus on trajectories of Brownian particles that escape from traps either in the presence of an external force or an entropy potential of a cone. To gain new insights into the escape dynamics, we divide the trajectories into two segments: a looping segment, when a particle unsuccessfully tries to escape returning to the trap bottom, and a direct-transit segment, when it finally escapes moving without returning to the bottom. Analytical expressions are derived for the Laplace transforms of the probability densities of the durations of the two segments. These expressions are used to find the mean looping and direct-transit times as functions of the external force or entropy potential. It turns out that the force/potential dependences of the two mean times are qualitatively different. The mean looping time monotonically increases with the force pushing the particle to the trap bottom or with the increasing entropic barrier at the exit. In contrast to this intuitively appealing result, the mean direct-transit time shows rather counterintuitive behavior: it is reduced by force application independently of whether the force pushes the particles to the trap bottom or to the trap exit and it turns out to be insensitive to the entropy potential.

Primary author(s) : BEZRUKOV, Sergey (National Institutes of Health, Bethesda, MD 20892, USA)

Co-author(s) : BEREZHKOVSKII, Alexander (National Institutes of Health, Bethesda, MD 20892, USA); DAGDUG, Leonardo (National Institutes of Health, Bethesda, MD 20892, USA and Universidad Autonoma Metropolitana-Iztapalapa, 09340 Mexico City, Mexico)

Presenter(s) : BEZRUKOV, Sergey (National Institutes of Health, Bethesda, MD 20892, USA)

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