

The transition path time distribution - protein folding, quantum mechanics, tunneling times and uncertainty

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Recent experimental measurements of the transition path time distributions of proteins present theory with challenges. They lead to barrier heights which are much lower than the free energies of activation of the observed transitions. Secondly, can one use the transition path time distribution to obtain insight into some of the intriguing questions of quantum mechanics, such as how long does it take to tunnel? In this talk, I introduce the paradigm of a transition path barrier height for the protein folding problem, and show that it should be smaller than the activation energy, resolving the low barrier

height puzzle. The transition path distribution for a parabolic barrier is derived for arbitrary memory friction. In the second phase of this talk, the quantum mechanical transition path time probability distribution will be discussed. Standard approaches to tunneling times are replaced by considering time correlation functions. The formalism is used to study the quantum dynamics of thermal position correlation functions. Highlights are the proof of a vanishing mean tunneling time at the parabolic barrier crossover temperature and that increasing the length of the path traversed decreases the mean transition time. The mean transition path time is used to define a coarse-grained momentum for passage from one side of the barrier to the other. The product of the uncertainty in this momentum with the uncertainty in the location of the particle is shown under certain conditions to be smaller than the $\hbar/2$ formal uncertainty limit.

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