

On the Reconstruction of Bistable Poisson State Using Periodic Measurement

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Reversible molecular dynamics has been the subject of significant scientific interest. Energy barriers that dictate the transition rate in molecular dynamics can be determined by detecting thermal activated motions of molecules. In particular, in the case of molecular processes with low transition rates, the residence time in each state can be directly measured. Recently the residence times of metastable molecular states have been measured using scanning tunneling microscopy with an atomic resolution. In these studies, energy barriers have been obtained by detecting variation in tunneling current or utilizing real-time continual imaging methods. We will show that these methods have all intrinsic errors. We performed numerical error analysis of the residence time in bistable Poisson states found in the data measured by an analog-to-digital converter type of periodic detection schemes. Monte carlo simulations show that the time-averaging method produces consistently better results than ones using conventional exponential fits. We will demonstrate these error factors by comparing real tunneling current data to data obtained by real-time continual imaging methods interspersed by atom-tracking.