Weekly Report

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July 13, 2018

1 One-dimensional free energy landscape

To evaluate transiton path statistics for free energy landscapes with multi intermediate barriers, following toy landscapes were constructed(Figure 1). Free energy difference between source/sink and barrier top is $5.37kT$.

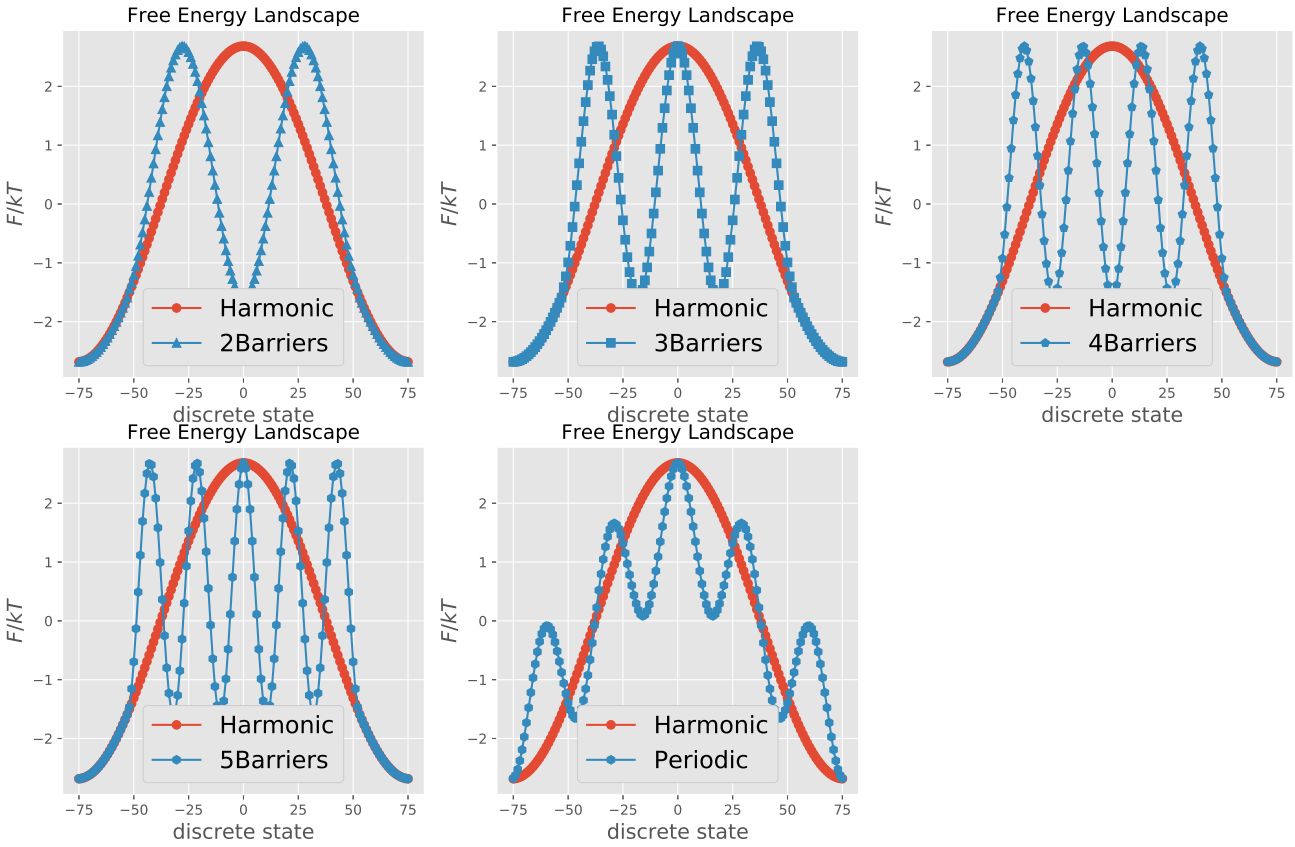

Figure 1: Model free energy landscapes.

2 Transition-path transit time distribution

Ultilizing Kinetic Monte Carlo simulation for above-mentioned 1-d discrete states model, we sampled 10000 transition-path trajectories and calculated distribution of transiton-path transit times $p(t_{AB})$ for each model landscapes.

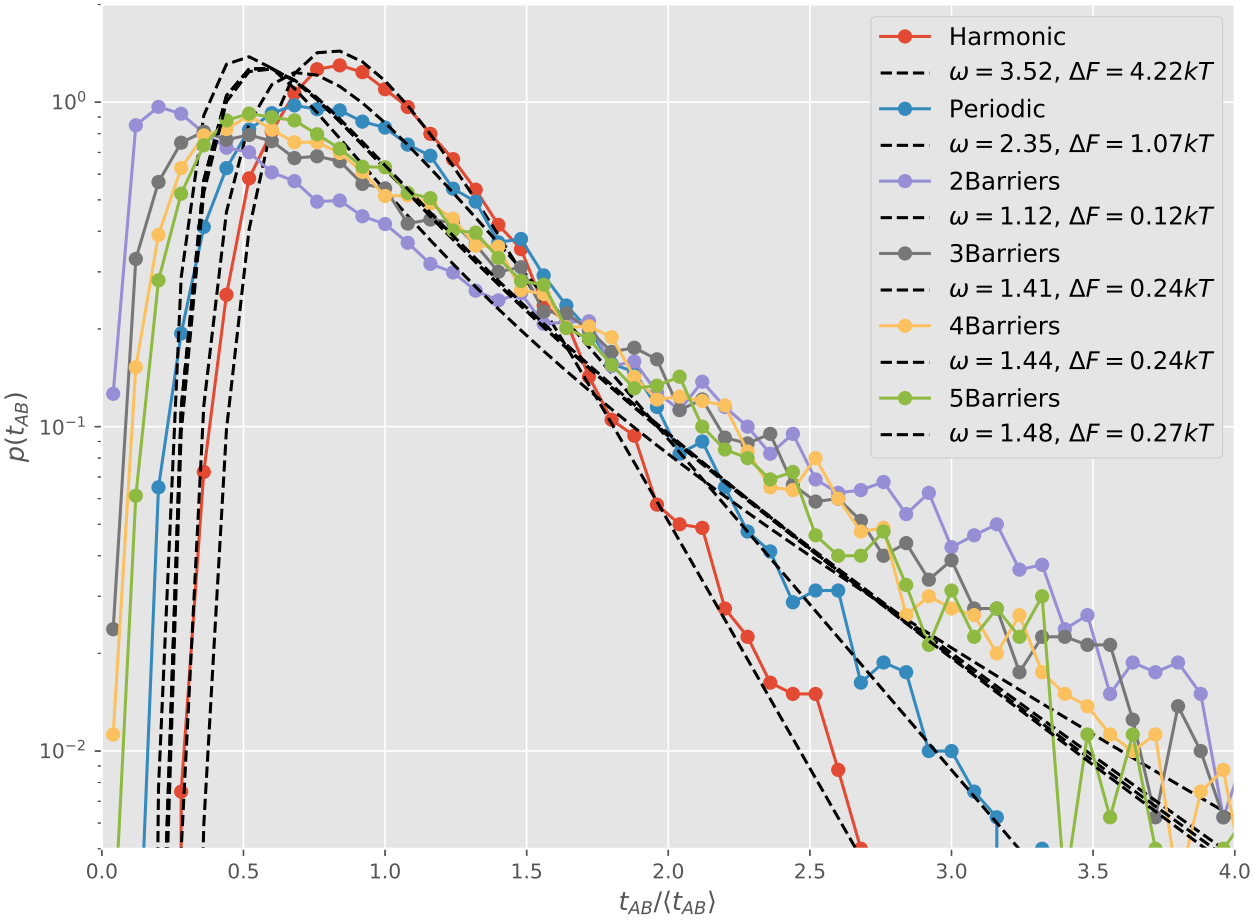

Figure 2: Transition-path transit time distribution

For each transit time distribution, the apparent force constant of the barrier ω was determined by fitting the decay constant ω^{-1} of the asymptotic exponential tail($p(t_{AB} > 1.5)$); barrier height ΔF was then determined by fitting theoretial expression of $p(t_{AB})$ to simulation distribution of transit times. We demonstrated that even for the harmonic landscape, deviation from theoretial expression for parabolic barrier crossing is non-negligible; for multi-harmonic barriers model, significant deviation from theoretical distribution was observed,resulting in much smaller and relatively unphysical fitting result for barrier height ΔF.

We also calculated the probability density $P(TP|x)$ that an arbitrary trajectory crossing state x is a transiton path trajectory;

3 Finite time displacement distribution

In order to examine when the one-dimensional coordinate projection could be recognized as effective reaction coordinate, we then examine the probability distribution of committors for transition path trajectories $p(q|TP)$, for which a single peak of probability $p(q|TP)$ have been ultilized as a indicator for 'good' reaction coordinates. Firstly, We found that for harmonic toy model, the shape of $p(q|TP)$ is very sensitive to the definition of source/sink region. For illustration, $p(q|TP)$ for two different selection of source/sink regions was compared: in the first case, only two free energy minimum was indentified as source or sink**(S1)**; in the second case, only the barrier top was defined as the transition path, while other two region of the free energy landscape was calssified as source/sink**(S2)**.

local linked

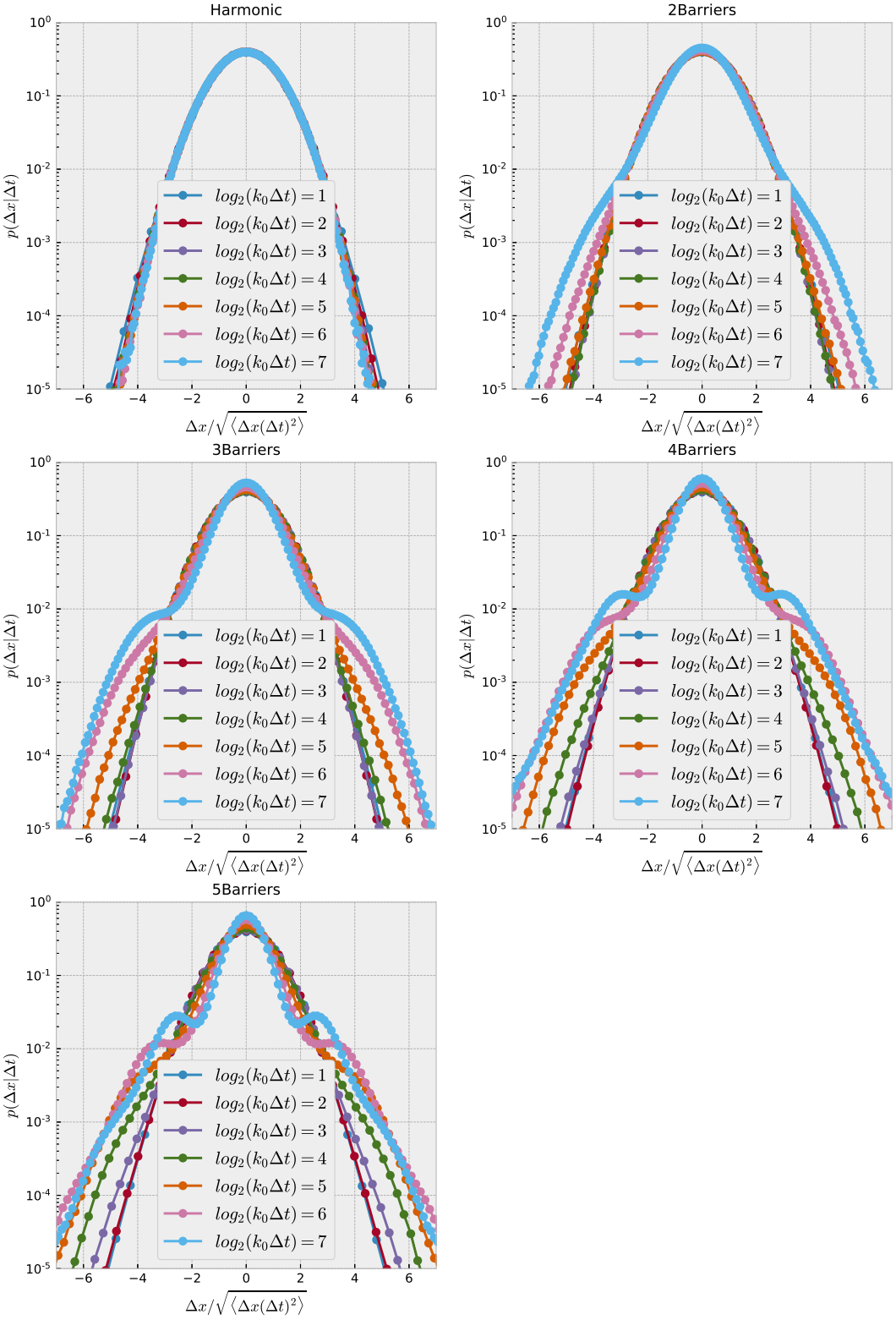

Figure 3: Distribution of finite time displacements.