lj-example.cpp

This program replicates the LJ7 cluster calculation in the Hairer and Weare paper introducing the method (though see the correction). This example shows how the new TDMC method can be applied to an enhanced sampling problem that DMC could not be.

The first section of variable definitions sets the temperature γ (physicists' kT), TDMC walker birth-death function strength λ, and dynamical time step ϵ; the number of replicates to run is set just after these parameters. These are hardcoded parameters because the program is simple to compile and running many replicates benefits substantially from compiler optimizations. As an alternative to tediously editing for each run by hand, the script run-lj-example.sh is designed to create a copy with chosen parameters, compile that, and run. It is written using Clang and Perl but can easily be edited to use any other C++11-compatible compiler or Perl alternative.

The LJ7 cluster rearrangement studied in this example is a rare event system that obeys large deviations theory at low temperatures, so the probability of a cluster rearrangement in a fixed time should show an Arrhenius rate law at low temperatures. Figure 1 confirms that the probabilities of two types of cluster rearrangement transitions do appear to follow the expected law as $\gamma \to 0$.

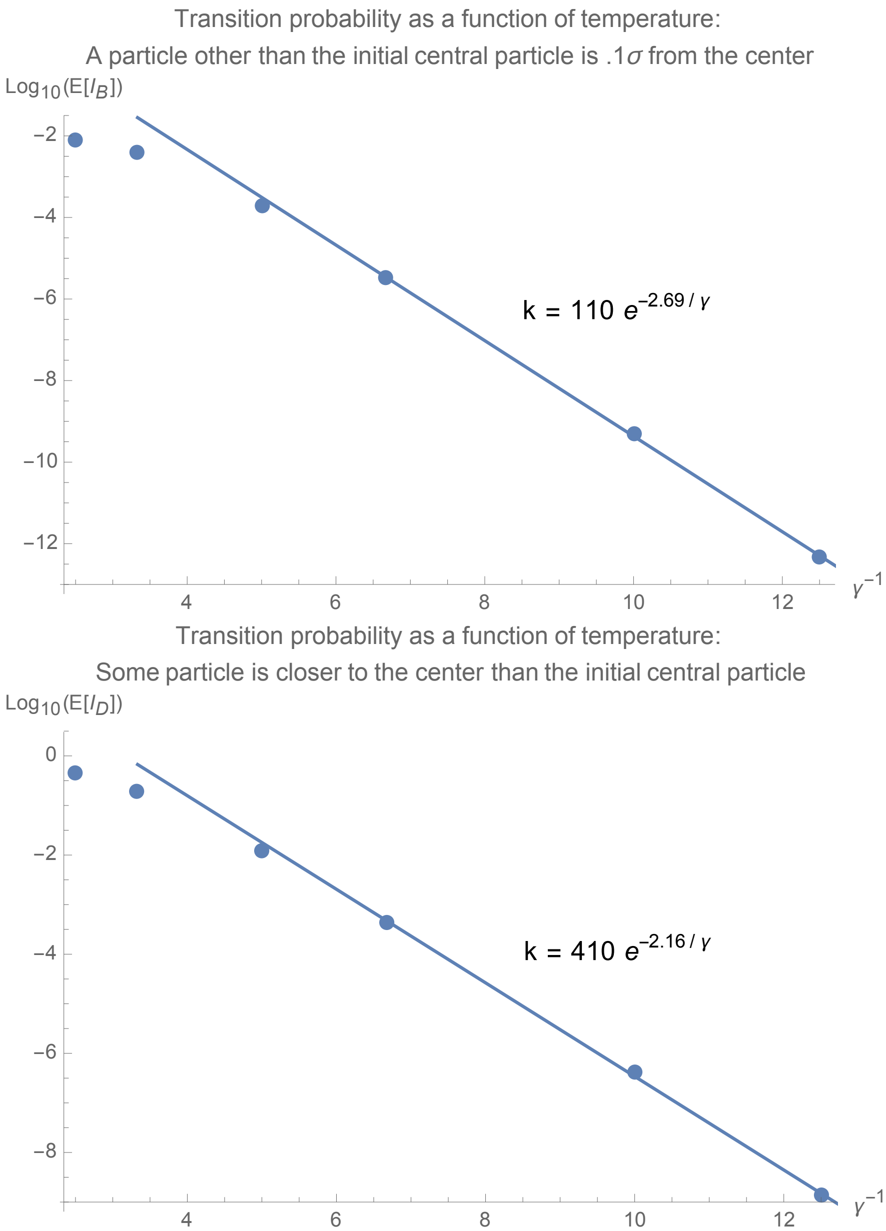

Figure 1: Probabilities of two types of rearrangements in an LJ7 cluster after 2 LJ time units as a function of inverse temperature γ, with superimposed Arrhenius rate laws fit to the low temperature regime ($\gamma^{-1} > 4$).