

## 24-623 2010 HW#6

Assigned: March 29, 2010.

Due: April 21, 2010 at the beginning of class. Please use the Blackboard discussion board to ask questions of the instructor or the other students.

In this homework, you will use transition state theory and Monte Carlo simulation to further study the properties of the single oscillator with potential energy  $U(x) = x^4 - 2x^2 + 1$  (seen previously in HW#2 and HW#4). Define state A as the left well and state B as the right well.

1. (5 points) Estimate  $k_{A \rightarrow B}^{TST}$  from the harmonic theory expression developed in class. Plot  $k_{A \rightarrow B}^{TST}$  as a function of  $\beta$  for  $0.01 < \beta < 100$ .
2. (20 points) Using the method described in class, use Metropolis *NVT* Monte Carlo simulations to predict  $k_{A \rightarrow B}^{TST}$  for  $\beta = 0.01, 0.1, 1, 10$ , and  $100$ . Plot these points with the results of part (a). Explain how you ran your simulations (number of steps, step size, etc.).
3. (5 points) Comment on how your two predictions for  $k_{A \rightarrow B}^{TST}$  compare to each other and on their overall physical significance.