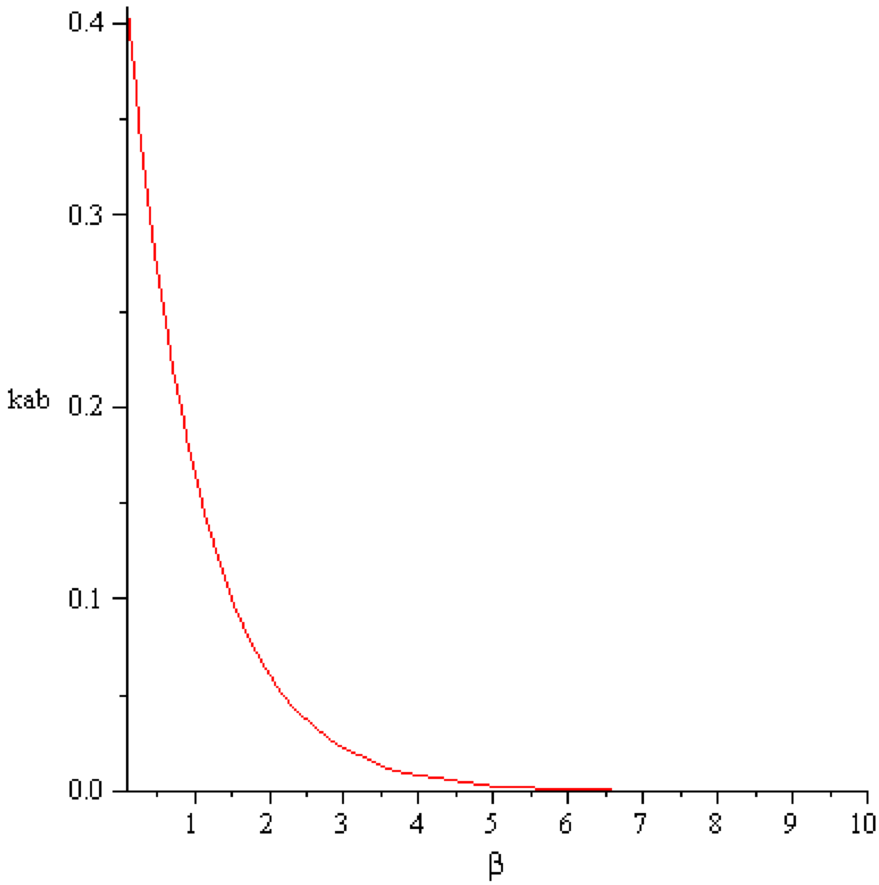
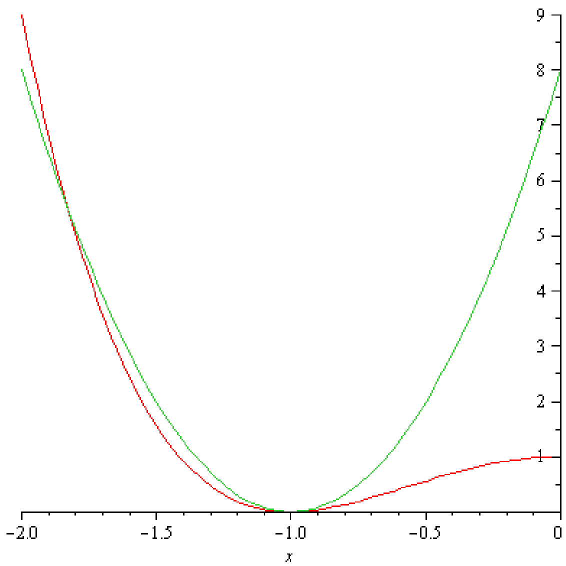
Below is a plot of the transition rate kab estimated from harmonic approximation for various values of beta (various temperatures). As expected, smaller beta (larger T) gives a larger rate constant, indicating that transitions are more likely for larger T. The curve follows a simple exponential Boltzmann type function. Note, I did not plot this function from 0.01< beta< 100 because the function changes too much over this range.



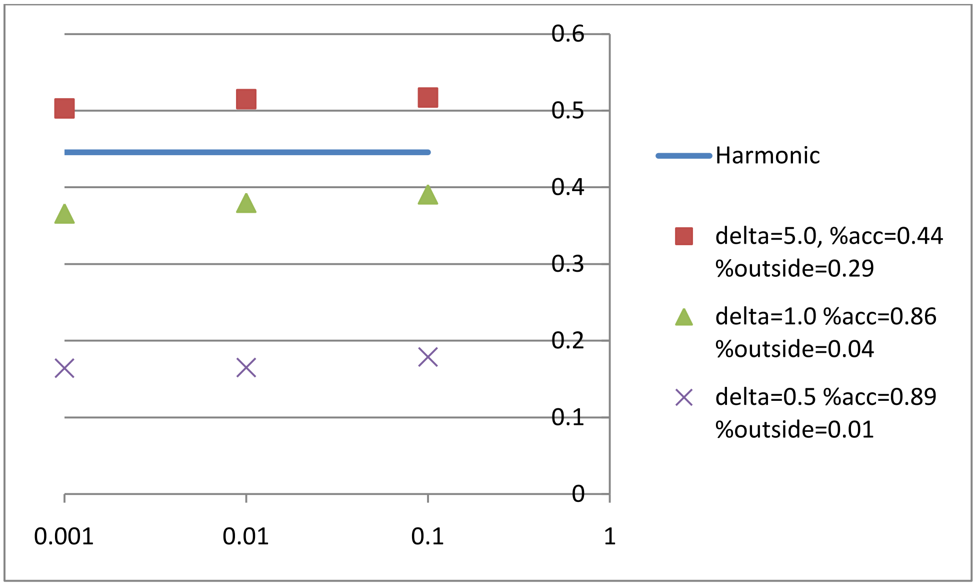
Curvature constant k = 8.0

Below is a plot of the harmonic potential approximation (with k=8.0 from the exact potential). One can see that near the local maximum at U(x=0)=1.0 the harmonic potential overestimates the energy required for a particle to reach x=0.



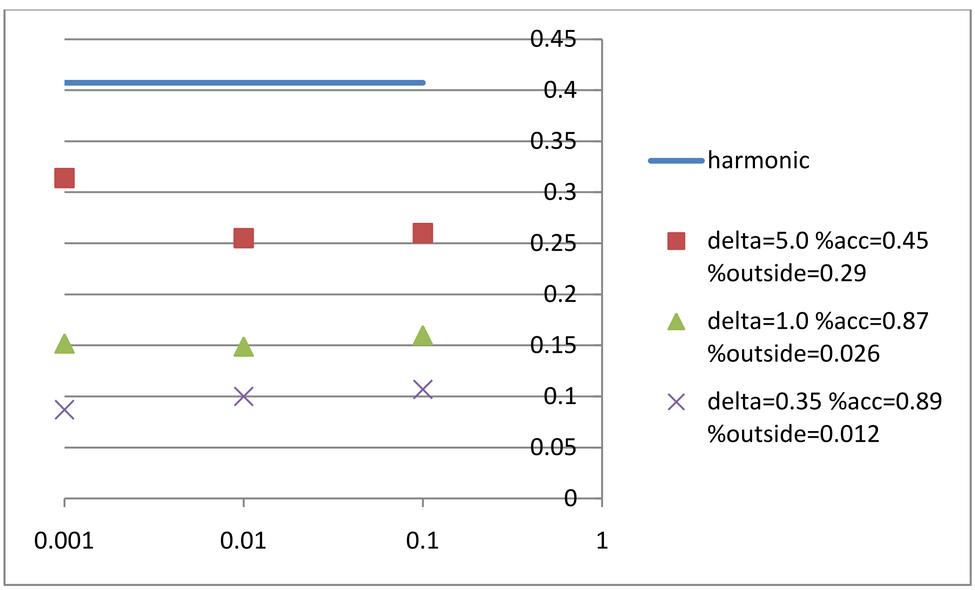
Below is a plot of the rate constant Kab estaimed from various MC runs compared with the harmonic approximation. Listed for each data series is a different choice of the MC step size delta. The plot is the value of Kab as a function of the bin size epsilon. For each value of delta a percent accept is reported, which is the percentage of accepted moves compared to the total number of moves which are either accepted or rejected, but not because x_trial>xstar+epsilon/2. Also reported is the "%outside", which is percent of total trial moves which have x_trial>xstar+epsilon/2. One would think (intuitively) that this "%outside" should be small. However, I don't see any clear trends for any of these calcuatlions. If one uses the metric %acc~0.5, then that gives one answer for Kab which seems converged for the choice of epsilon. However, other of delta give completely different values for Kab, which also seems to be converged for various values of epsilon. Also, the harmonic approximation (in this case) should be underestimating the value of the rate constant since it overestimates the value of the energy U(x) both at xstar U_{exact}(xstar)=1.0 and U_H(xstar)=8*(0.0+1)^2 =8. One would expect this difference in the energy to be negligible when kbT>>U_{exact}-U_H. One would also expect that the harmonic approximation should always underestimate the value of Kab in the case where it overestimates the value of the energy at xstar and around xstar.

Beta=0.01

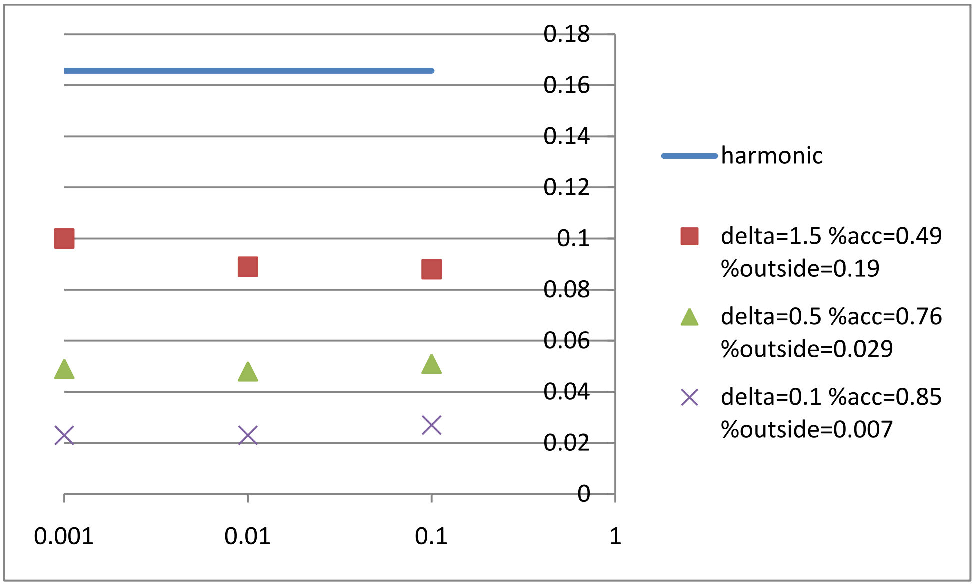


If we look at larger values of beta, the calculated Kab from MC is actually lower than the harmonic approximation, and is again dependent on the choice of delta:

Beta=0.1

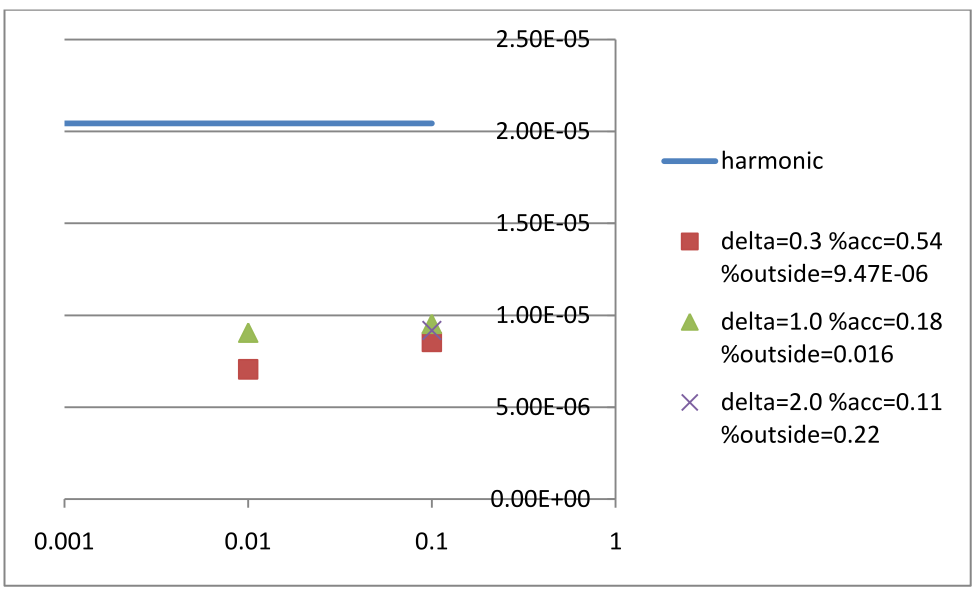


Beta=1.0



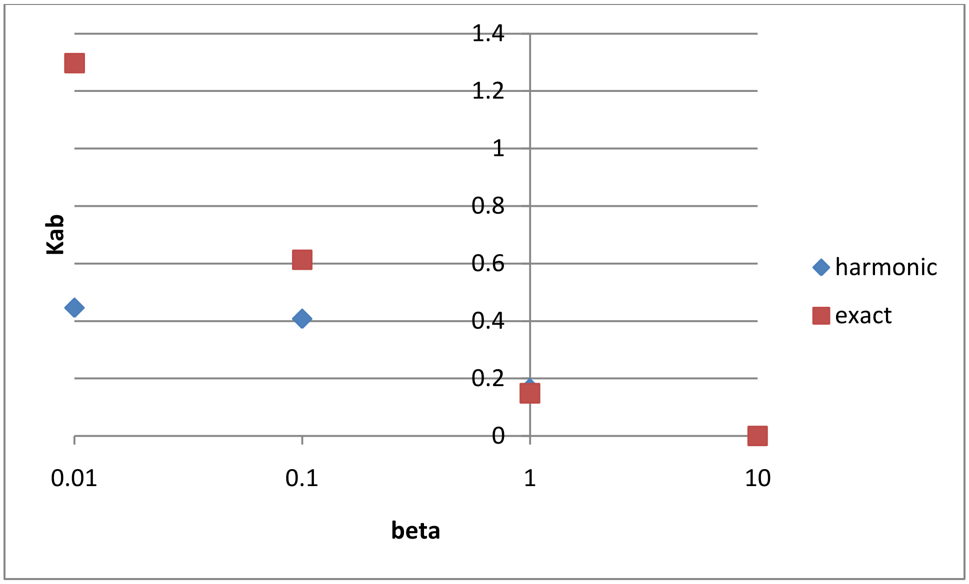
By the time you get to beta=10.0, you have to use 10E08 number of trial moves, and even then you can only get statistically significant results (numbin~100) by using epsilon>/0.01:

Beta=10.0

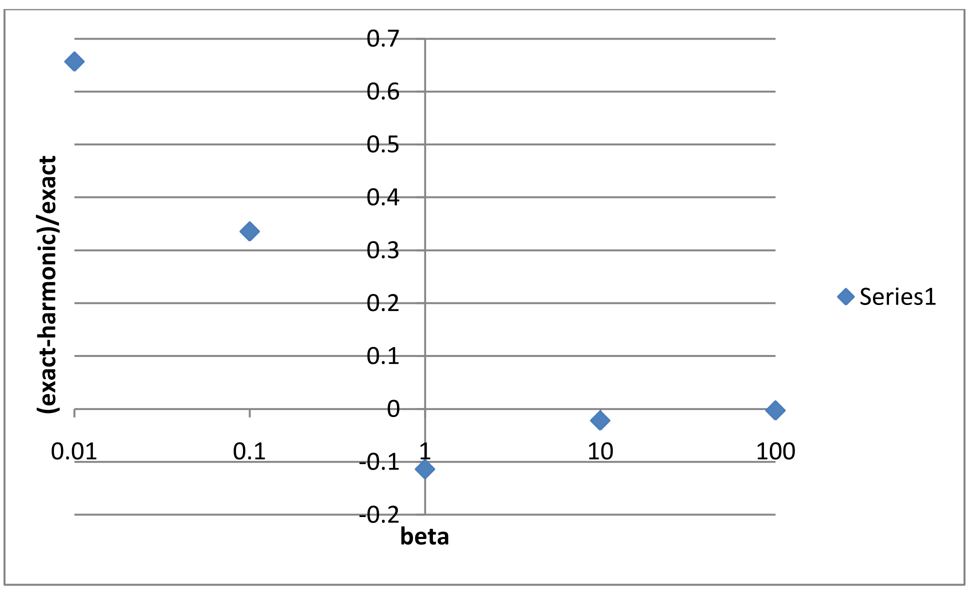


These results seem a little bit better converged with respect to both delta and epsilon. For the case beta=100.0, I never observe any points falling into a bin of size epsilon=0.1. The harmonic approximation at beta=100.0 is Kab=1.67E-44.

Below is a plot of the comparison of Kab to the harmonic approximation and also computing Kab numerically using the exact potential U(x) and simson's rule:



One sees that the harmonic approximation underestimates Kab, but that the two Kab converge for large beta. This is somewhat unintuitive for me. Below is a plot of the relative difference between harmonic and exact, (exact-harmonic)/exact, which shows the same behavior:



One sees at a value of beta that the harmonic approximation actually overestimates Kab, which again is quite unintuitive.