

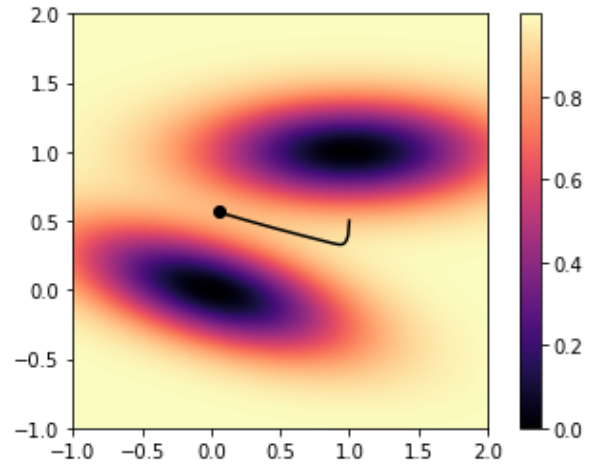
**Methods of Computational Physics**  
**WiSe 19/20**  
**Sheet 3: Rare Events**  
**Ayush Paliwal**  
**Matriculation Number: 21915793**

**Transitions between two minima**

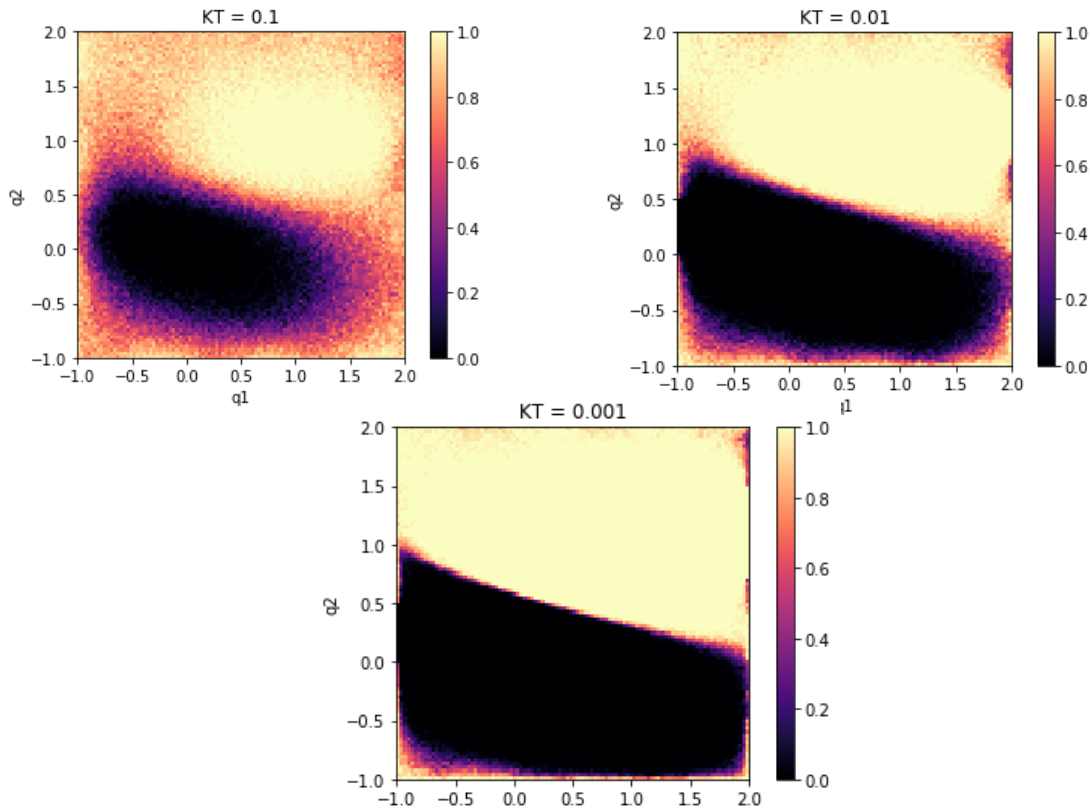
**a) Saddle Point - Henkelman's Dimer method**

$q_1=0.0499804$  (along horizontal)

$q_2=0.563678$  (along vertical)



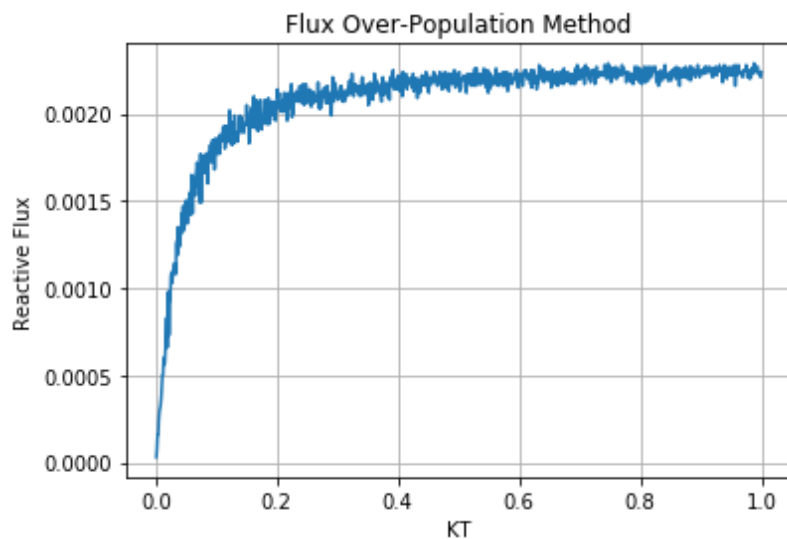
**b) With decrease in temperature, **committor probability** decreases for particles starting from regions nearing sink A and reaching to sink B. The colour bar depicts the committor probability.**



Committor probability  $q_+(q) = 0.5$  can be seen from colour-bar corresponding to 0.5, it comes out to be a line.

c) **Flux Over - Population Method**

With increase temperature more particles are able to jump from A to B. The increase is exponential in the beginning, settling down to a stagnant behaviour over  $KT=0.4$ .



d) **Minimum energy path via the string method** (Black dot shows the saddle point)

