

# Rate constants: from Sinai billiards to protein folding

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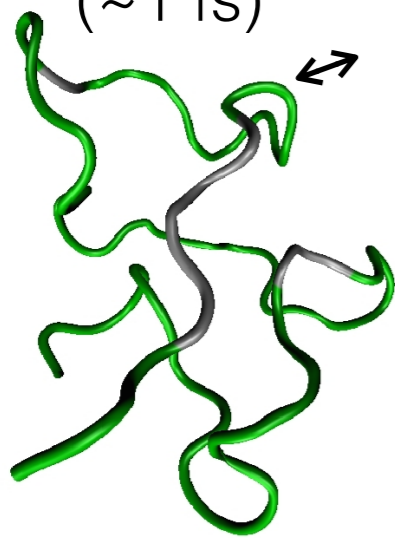
Wales group  
Department of Chemistry  
University of Cambridge

Alumni festival  
26th September 2014

# Rare events

- large separation of smallest and largest time scales

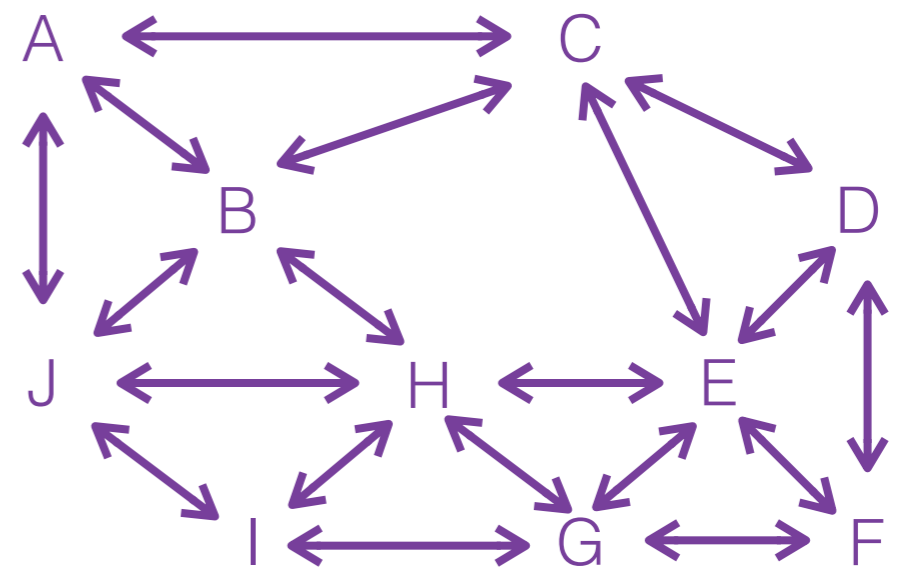
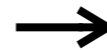
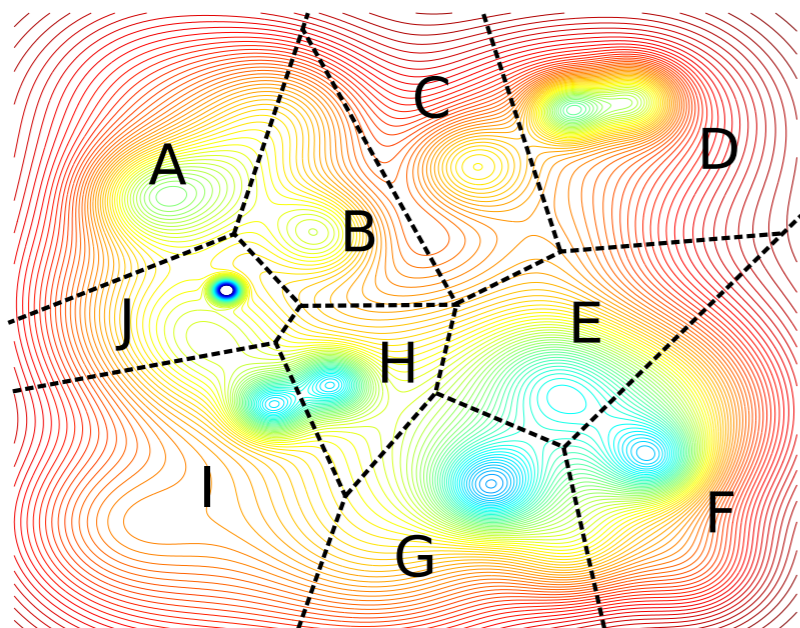
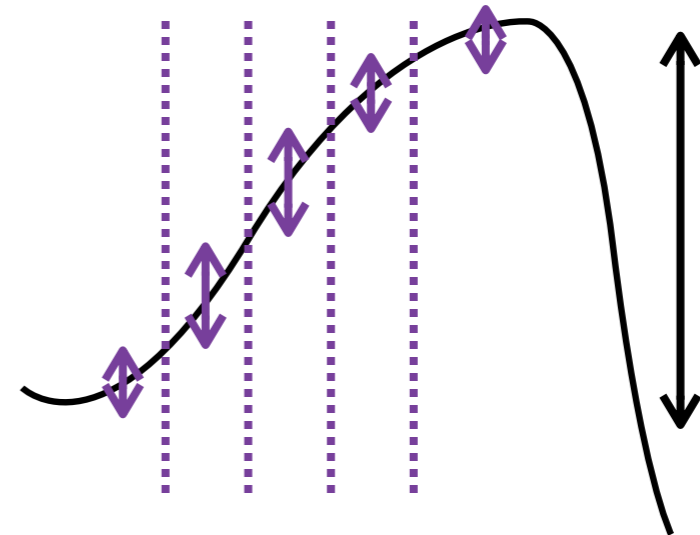
molecular vibration  
(~1 fs)



folding  
(~1 ms)



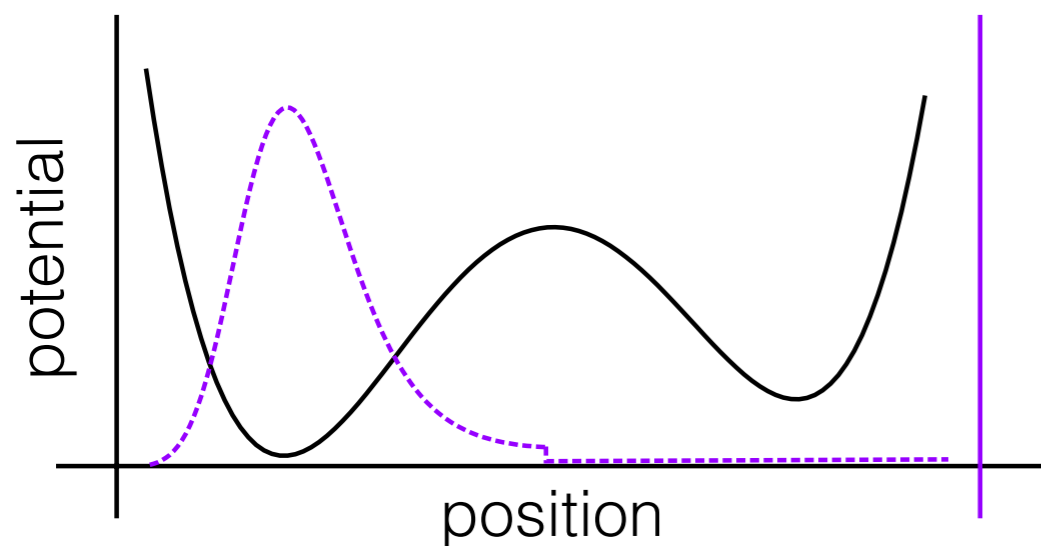
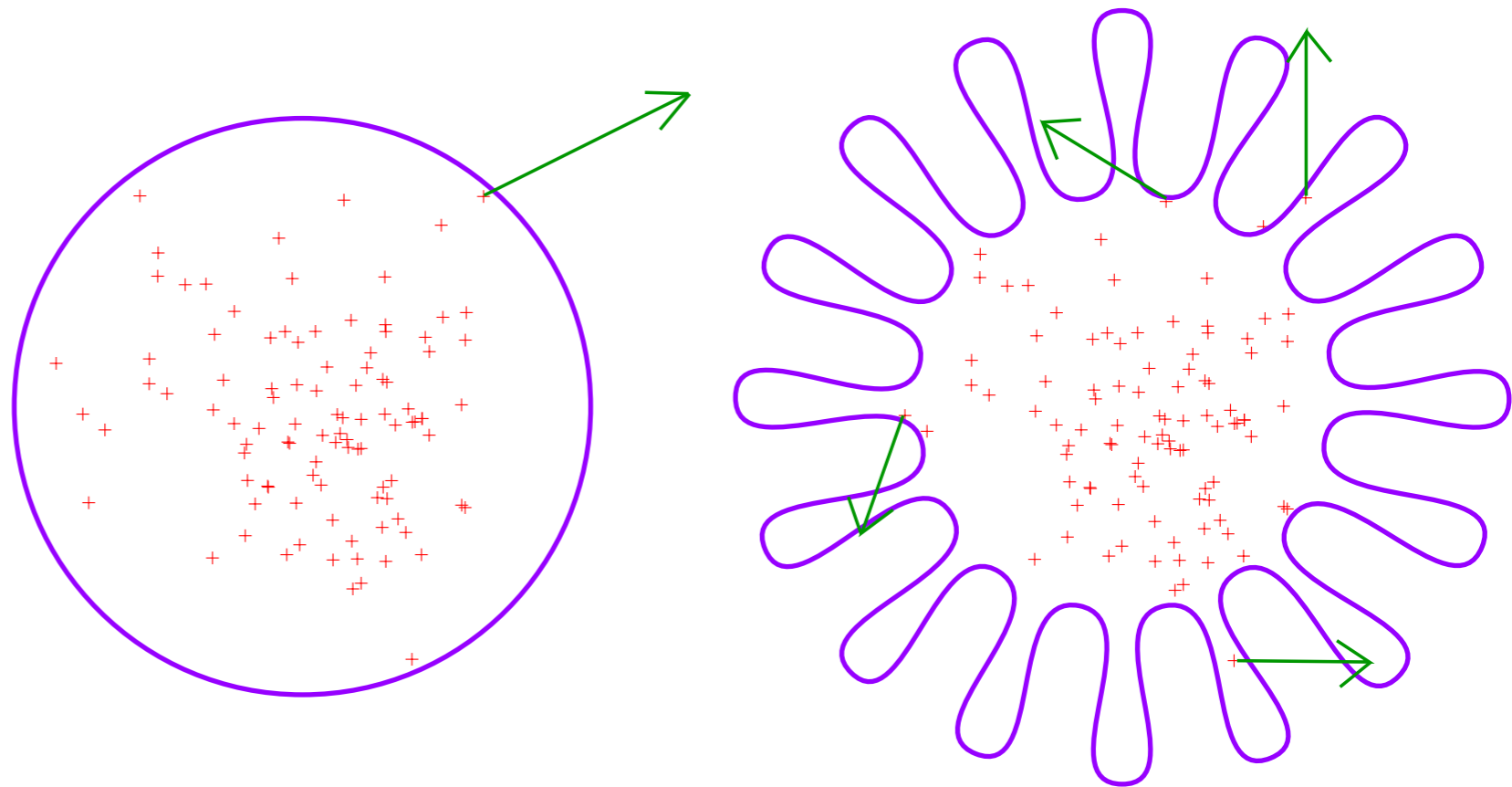
$$k_{AB} \propto \exp(-\Delta E)$$



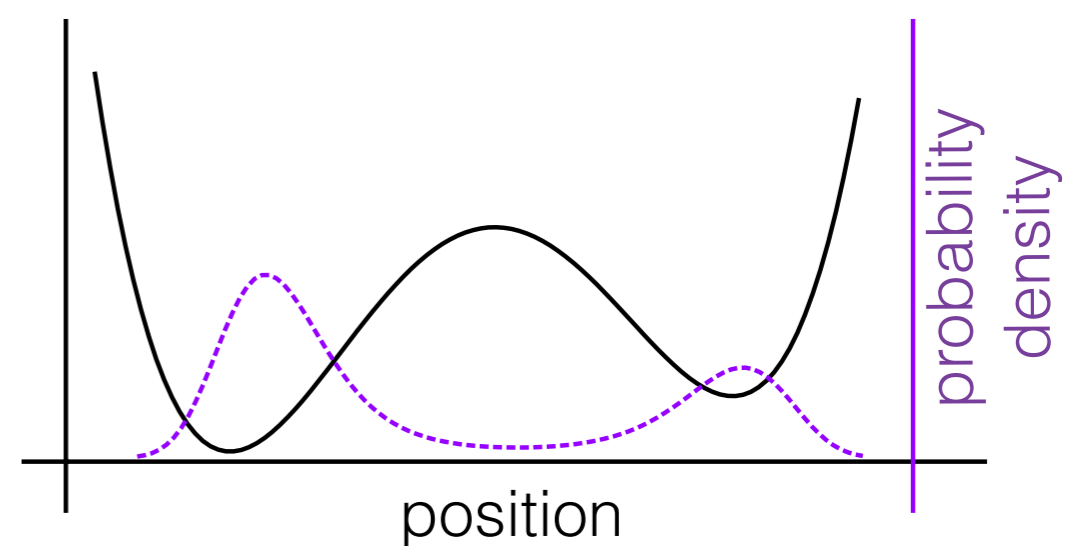
# Transition state theory

$$k_{AB}^{\text{TST}} = \frac{\text{eq. flux}}{\text{eq. population}}$$

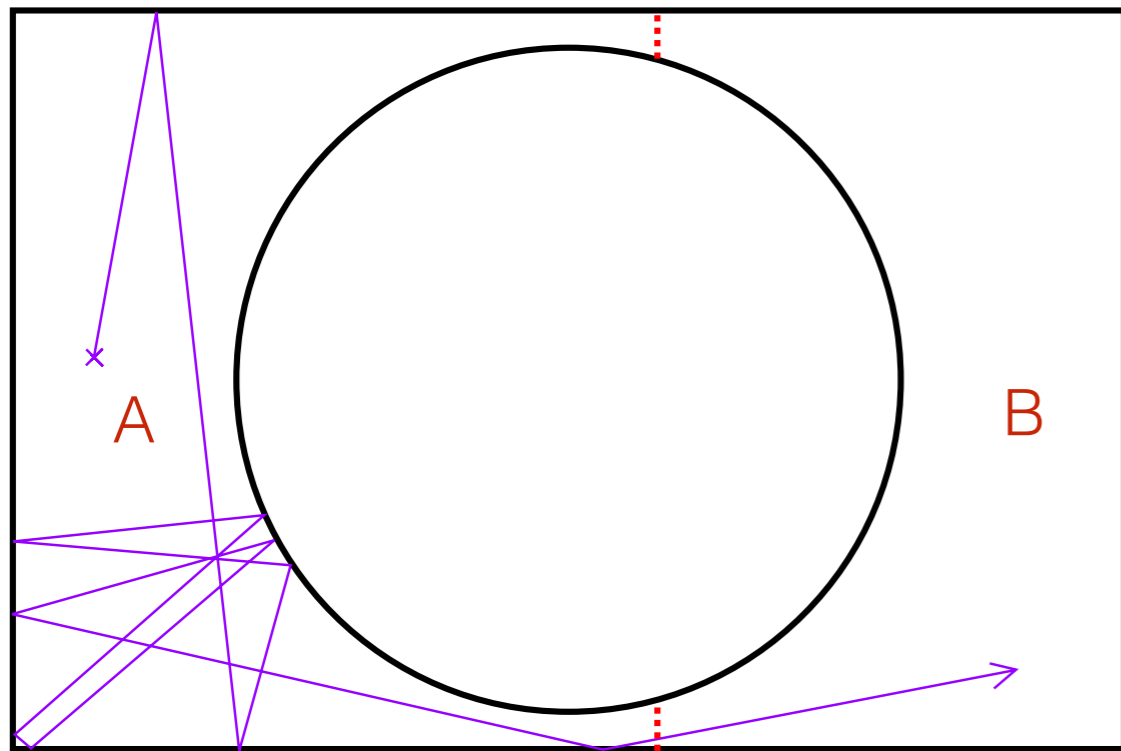
- cell-to-cell rate constant in DRPS is based on relaxation:



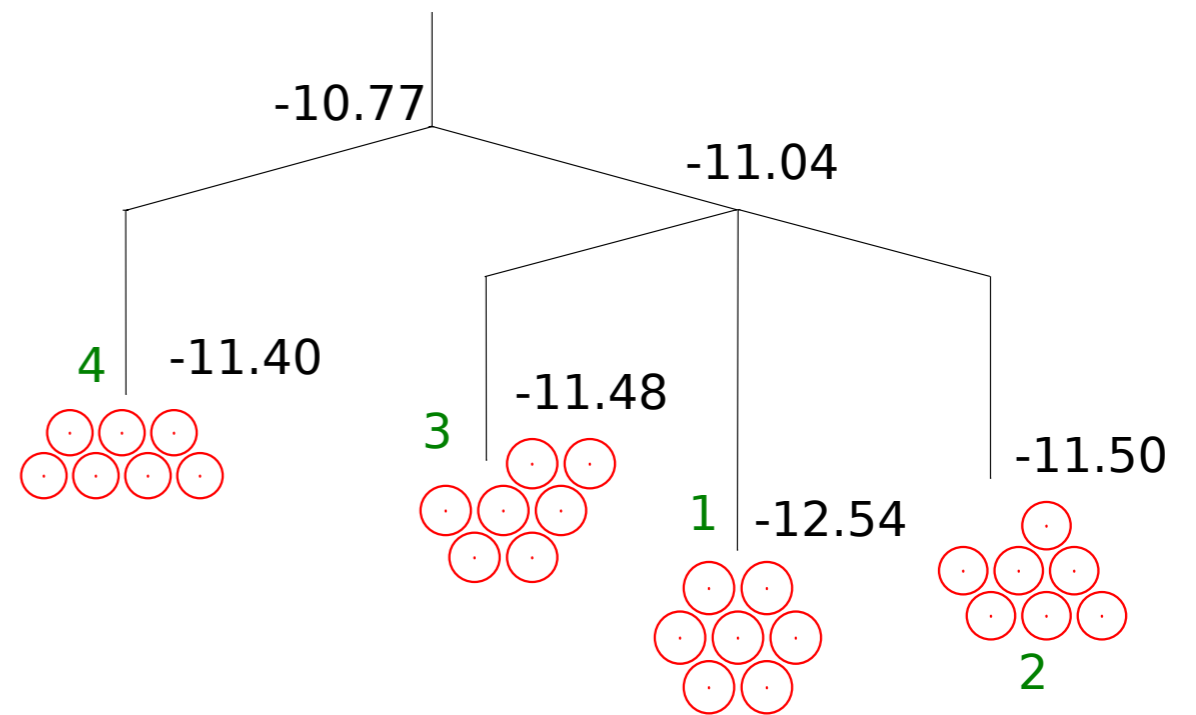
relaxation



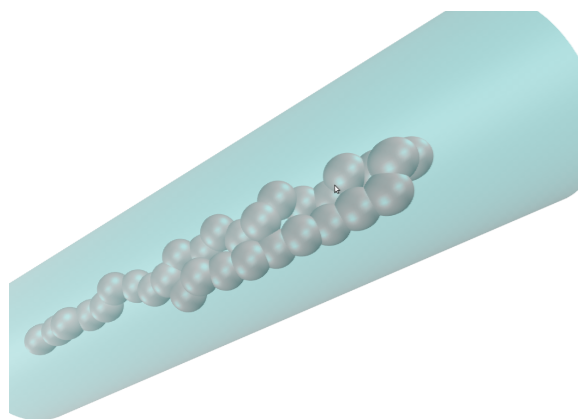
# From Sinai billiards to folding



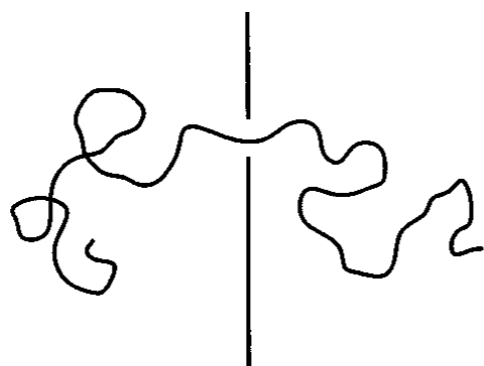
Sinai billiards



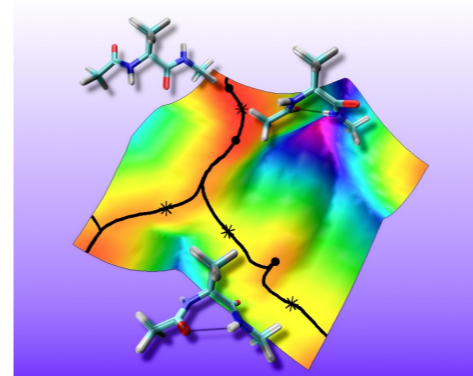
Cluster rearrangement



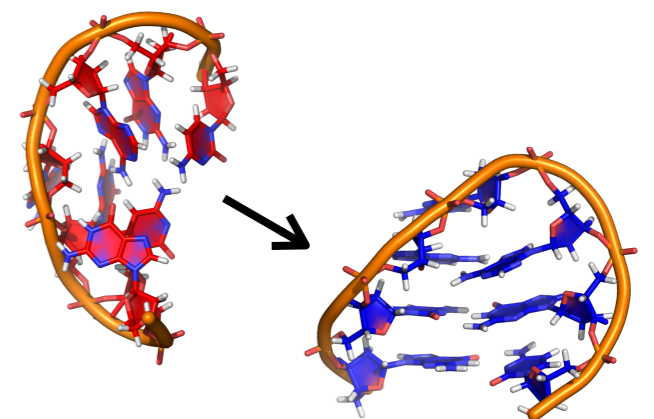
polymer reversal



polymer translocation



peptide dynamics



biomolecular folding

QUESTIONS?