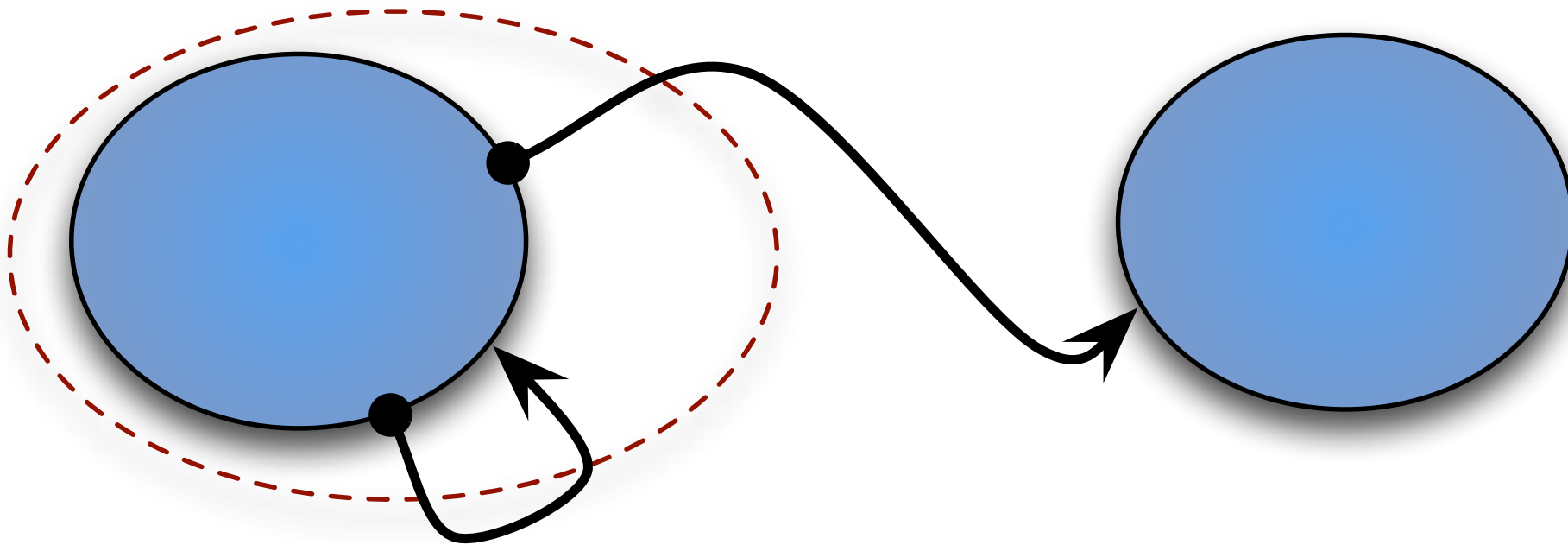


Path ensembles

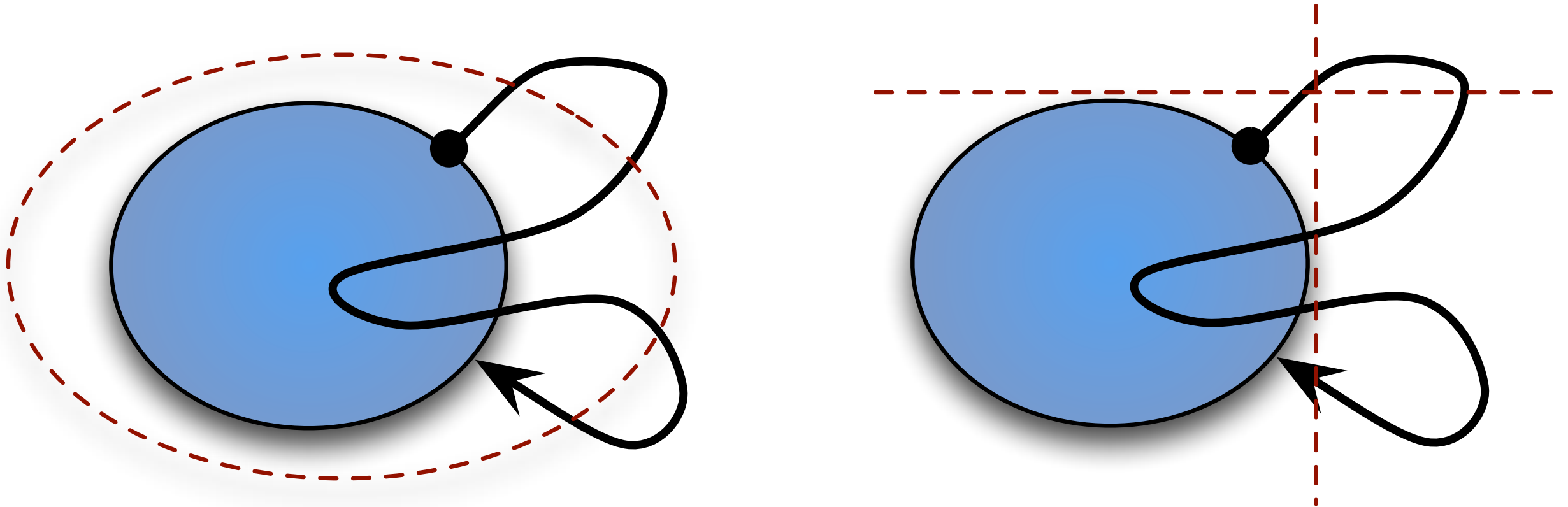


Transition interface sampling:

Use many interfaces to enhance rate calculation

$$k_{AB} = \langle \phi_A \rangle \prod_{i=0}^N P(\lambda_{i+1} | \lambda_i)$$

Path ensembles



Minus ensemble, multiple interface set minus ensemble:

Useful for increasing decorrelation in TIS;
flux calculation for TIS