Path Integrals

- First formulated by R. P. Feynman
- Introduces concept of "imaginary time", $\tau = \frac{1}{k_B T}$

The Density Matrix, ρ

- "All static properties and, in principle, dynamic properties of a many-body system in thermal equilibrium are obtainable from the density matrix."[1]
- $H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} v(\mid r_i - r_j \mid)$
- $\rho(R, R'; \beta) = \langle R \mid e^{-\beta H} \mid R' \rangle$
- $e^{-\beta H} = (e^{-\frac{\beta}{m}H})^m$
- $\rho(R, R'; \beta) =$
  $\int ... \int \rho(R, R_1; \frac{\beta}{m})\rho(R_1, R_2; \frac{\beta}{m})...\rho(R_{m-1}, R_m; \frac{\beta}{m})\rho(R_m, R'; \frac{\beta}{m})dR_1 dR_2...dR_m$
- $\rho(R, R'; \beta) = \langle R_0 \mid e^{-\frac{\beta}{m}H} \mid R_1 \rangle ... \langle R_{m-1} \mid e^{-\frac{\beta}{m}H} \mid R_m \rangle$

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[1] D. M. Ceperley and E. L. Pollock, in Monte Carlo Methods in Theoretical Physics, 35 (1992).

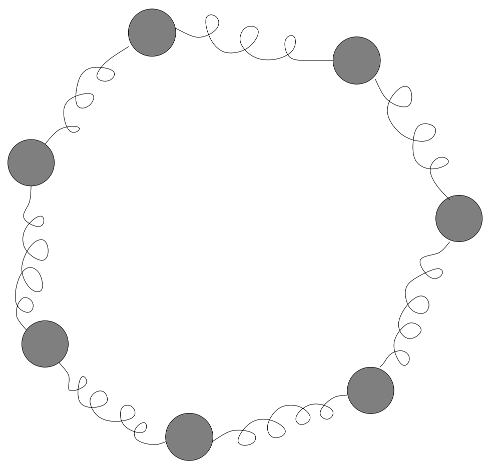
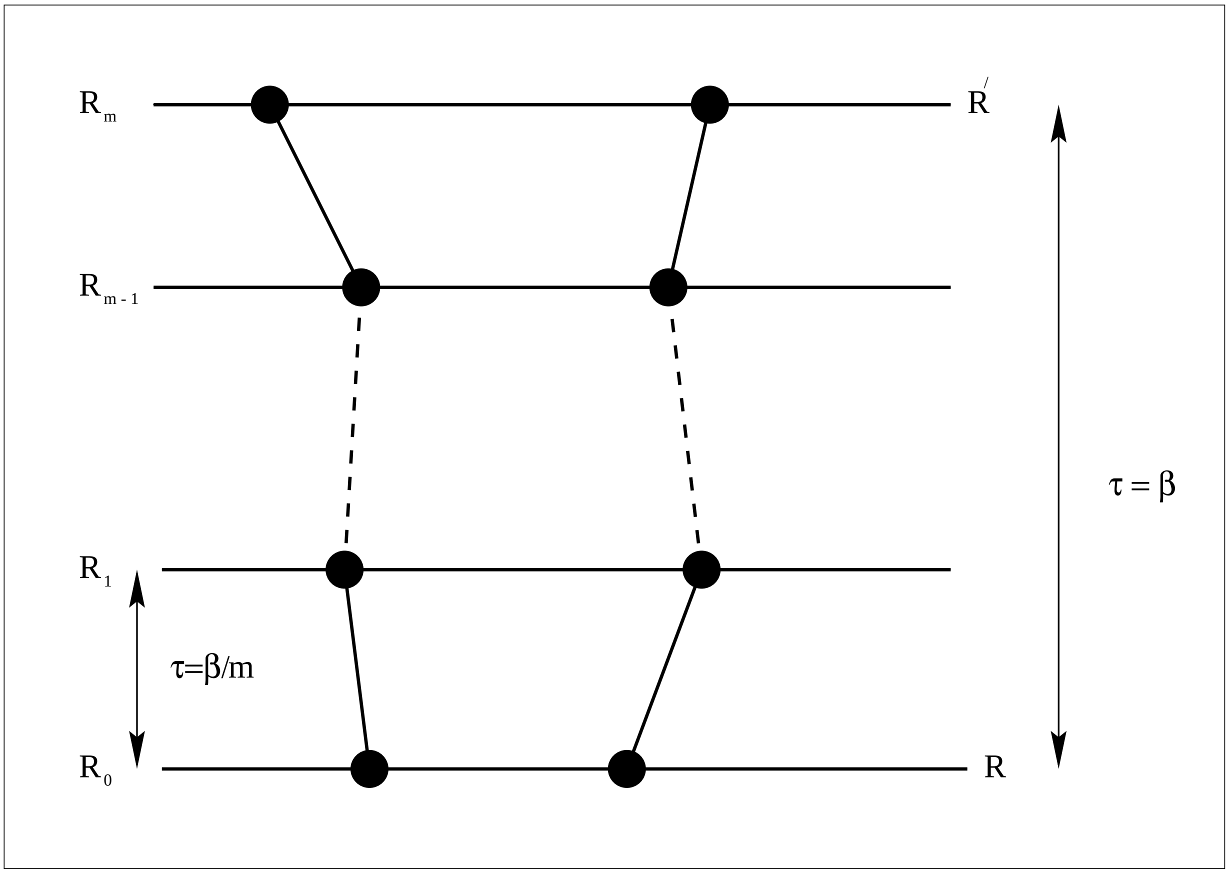


Figure 1: Sketch of a ”Ring Polymer”

Monte Carlo

- Based on random numbers
- New particle positions are proposed
- New positions can be chosen randomly or with some specific distribution, as long as each particle can move to any point in configuration space with a finite number of moves
- Probability of new positions are calculated in a systematic manner
- Random number drawn to determine if move occurs
- Process is repeated until relaxes



R
m
R
m - 1
R
1
R
0
R
/
R
τ=β/m
τ = β

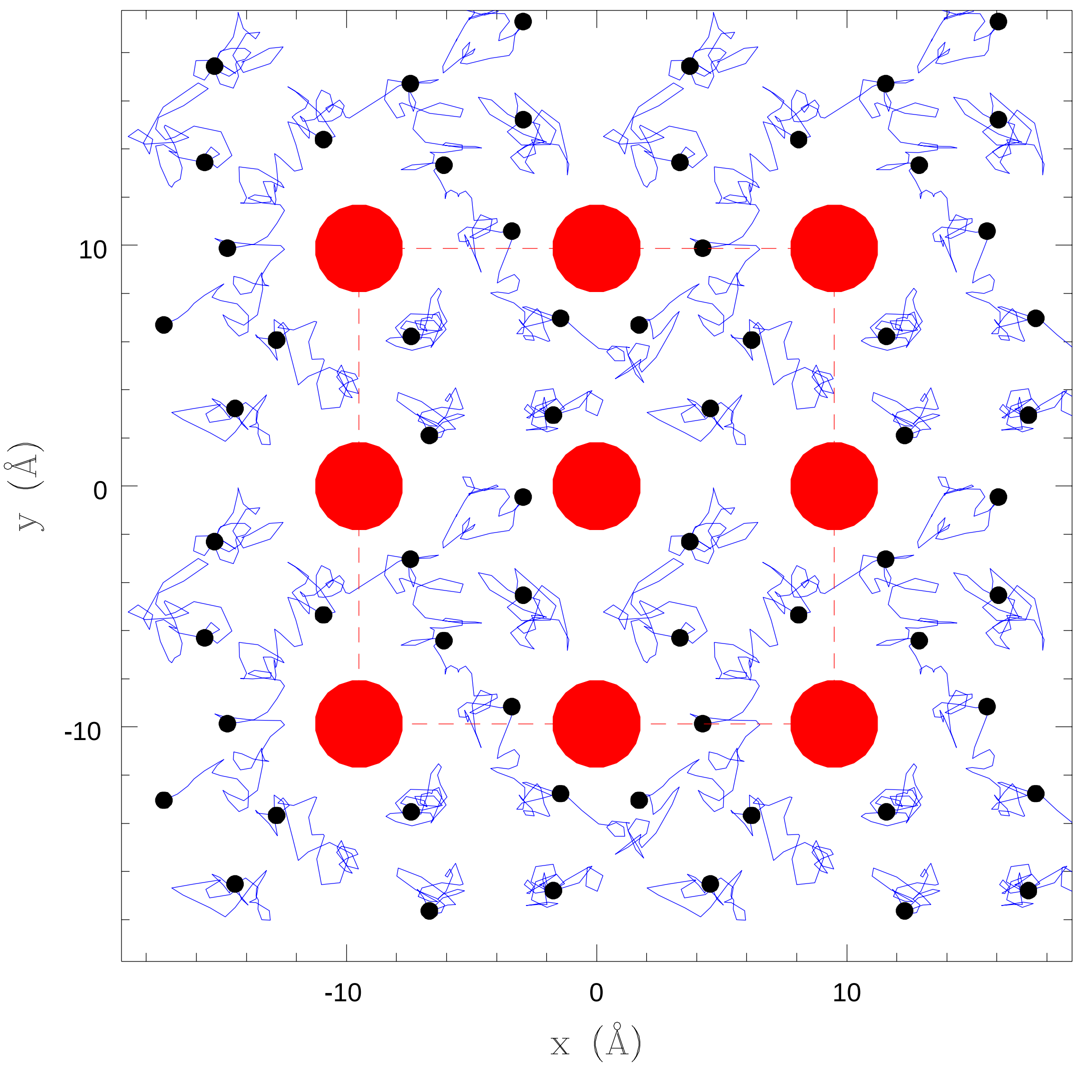


Figure 2: PIMC simulation