Path Integral Monte Carlo

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What is Path Integral Monte Carlo?

- A computational technique for simulating quantum systems at non-zero temperature.
- PIMC allows us to use particle interactions at some "high" temperature (where behavior is classical) to study a system at much lower temperature, where quantum fluctuations are important.
- PIMC is an exact method. In principle, no approximations are needed. In practice, particle interactions are not exact, and other approximations are made for convienence.

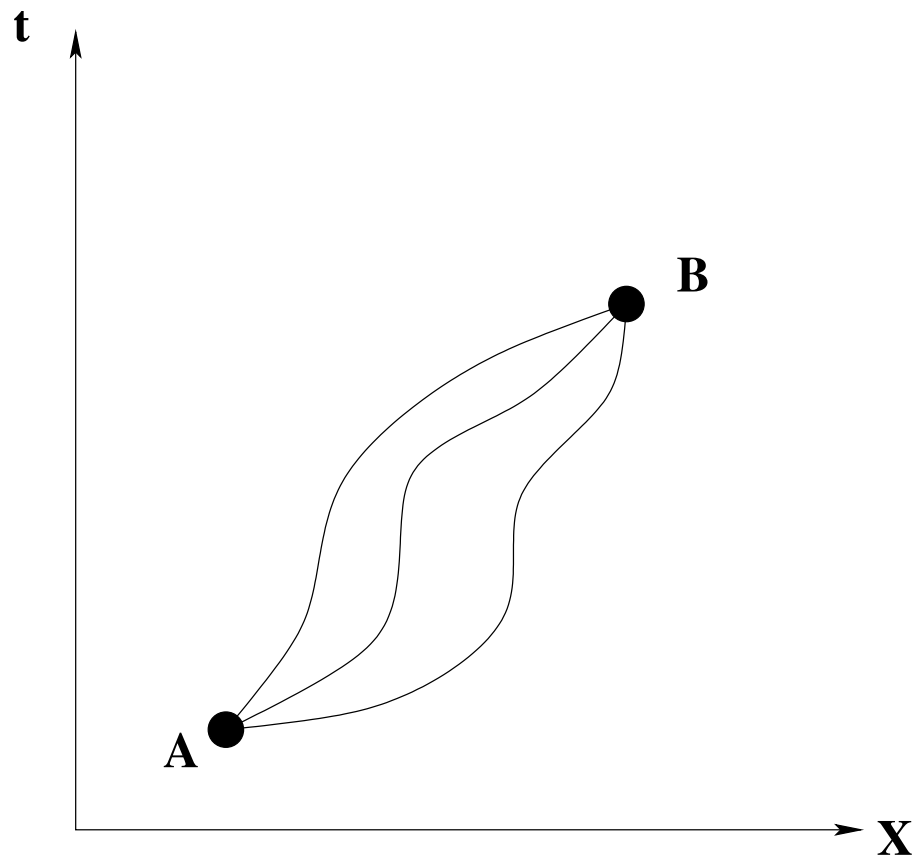
What is PIMC used for?

- In 1953, Feynman suggested the use of Path Integrals to explain superfluidity in He^4.
- Superfliudity can be understood as global permutation chains between helium atoms (indistinguishable bosons).
- In the early 1980's, the computer resources were finally available to implement a full PIMC study of liquid helium II (Ceperley & Pollock).
- In general, PIMC is used to study low temperature quantum systems consisting of weakly interacting light-weight particles.

Path Integrals and Helium

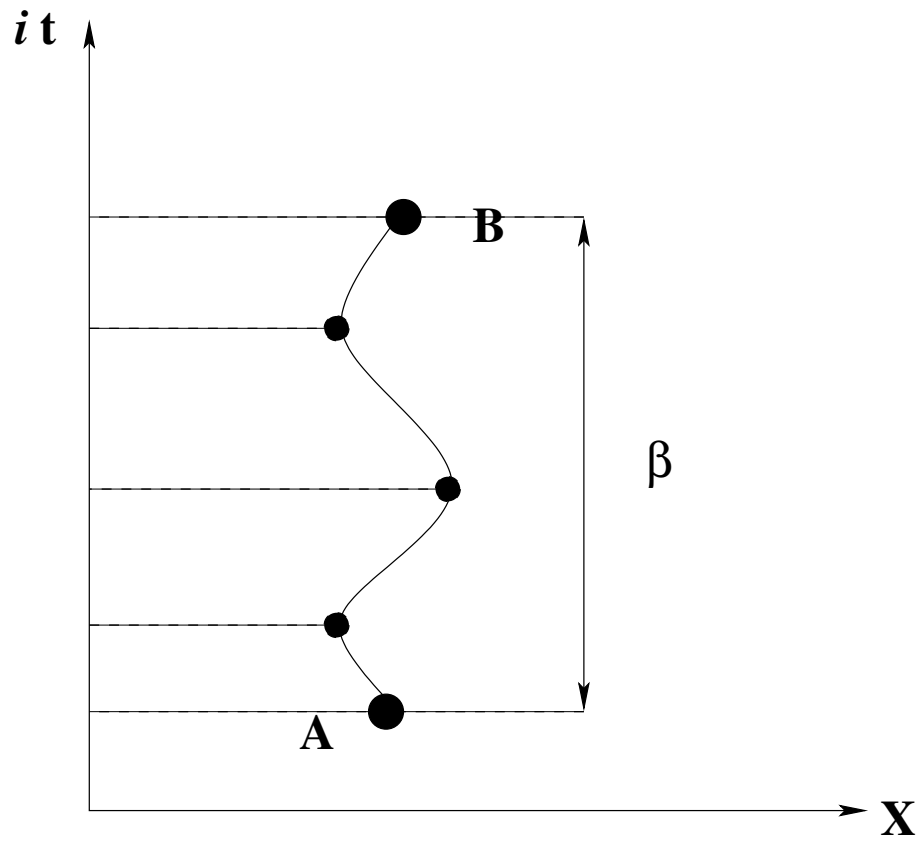
- Imaginary Time:

$$e^{-\frac{i}{\hbar}t\hat{H}} \text{ vs. } e^{-\beta\hat{H}}$$



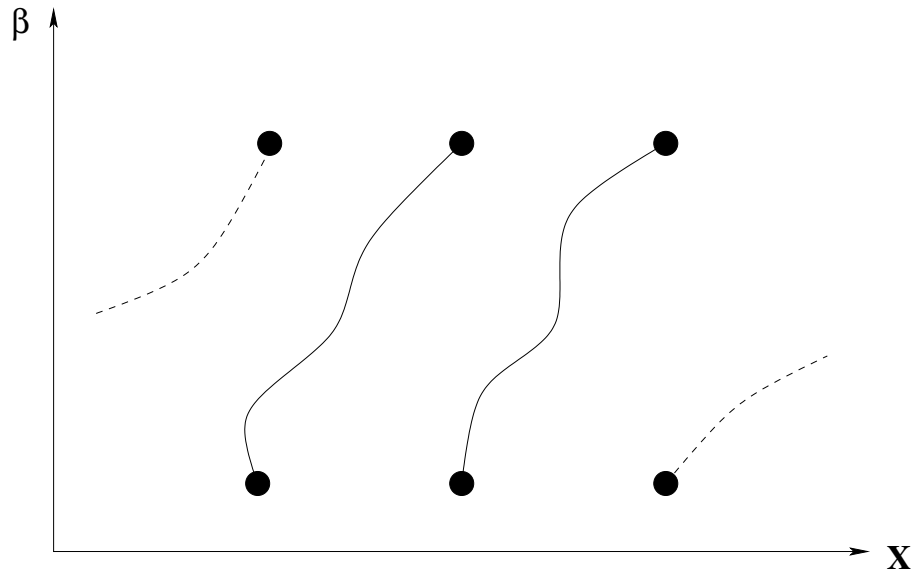
Path Integrals and Helium

- In statistical mechanics, the partition function is diagonal, so a particle must end up where it began after β.



Path Integrals and Helium

- For a system of bosons, the end position can be any permutation of the one a "time" β earlier.



Metropolis Monte Carlo

- Starting from an initial configuration, propose new particle positions and accept them with probability:

$$P_{a \to a'} = min[1, \frac{e^{-\beta E_{a'}}}{e^{-\beta E_a}}]$$

- The system will approach the Boltzmann (Gibbs) ensemble, and equilibrium properties of the system may be obtained.

Quantum Statistical Mechanics and PIMC

- Need to know the density matrix, $e^{-\beta\hat{H}}$.
- Note that $e^{-\beta\hat{H}} = e^{-\frac{\beta}{2}\hat{H}}e^{-\frac{\beta}{2}\hat{H}} = [e^{-\frac{\beta}{M}\hat{H}}]^M$
- By connecting M ensembles through path integrals, the resulting system is identical to a single ensemble, but at a temperature reduced by a factor of M.
- Because the ensemble at imaginary time steps 1 and M+1 must be the same (the partition function is diagonal), this system corresponds to a classical system of ring-polymers.

The Primitive Approximation in PIMC

- Split the density matrix into kinetic and potential terms (to first order in τ): $e^{-\tau\hat{H}} = e^{-\tau\hat{T}}e^{-\tau\hat{V}}$
- $M\tau = \beta$
- Approximation is exact in the limit that $M \to \infty$.
- After applying path integrals and quantum mechanics, we get the following:

$$e^{-\tau\hat{H}} \longrightarrow e^{-\frac{\Delta\vec{R}^2}{4\lambda\tau}} e^{-\tau V(\vec{R})}$$

- This becomes our new Boltzmann factor in the Metropolis routine, as well as our basis for energy calculations.