Path Integral Monte Carlo

a presentation by Keola Wierschem

Metropolis Monte Carlo

- based on random sampling
- an exact simulation technique
- error from approximations in atomic interactions, finite-size effects, and use of pseudo-random numbers

Sampling Technique

- start with any configuration of particles
- systematically propose and accept/reject new particle positions
- must satisfy detailed balance
- must be able to reach all possible configurations in a finite number of iterations
- an iteration occurs when a new position has been proposed and accepted/rejected for each particle in the system

Accept or Reject?

- large based on Hamiltonian of system
- large ie kinetic and potential
- large changes with temperature and forces

Path Integrals

- developed by R. P. Feynman mid-20th century
- describe quantum particles as classical "ring-polymers"
- use concept of imaginary time (inverse of temperature)
- allow one to understand the quantum effects at low temperature in terms of the better understood classical behavior at higher temperature

Path Integral Monte Carlo

- uses path integrals to reduce the temperature of interactions in standard Monte Carlo
- more paths = lower temperature
- has been used to study superfluidity, a quantum effect occuring at low temperatures

Superfluidity

- A superfluid has zero viscosity, or resistance to flow
- Helium is the observed superfluid to date
- Bulk helium becomes superfluid at about 2.17 K
- PIMC can be used to search for new superfluids
- Using computer simulation, one can study any number of systems with very little cost

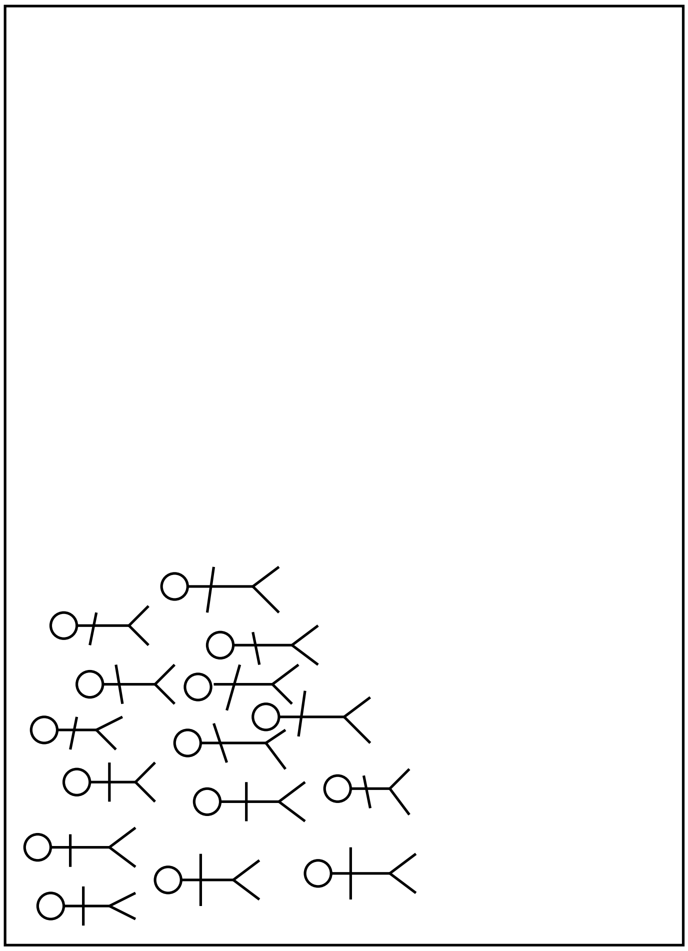

Figure 1: Initial configuration of humans

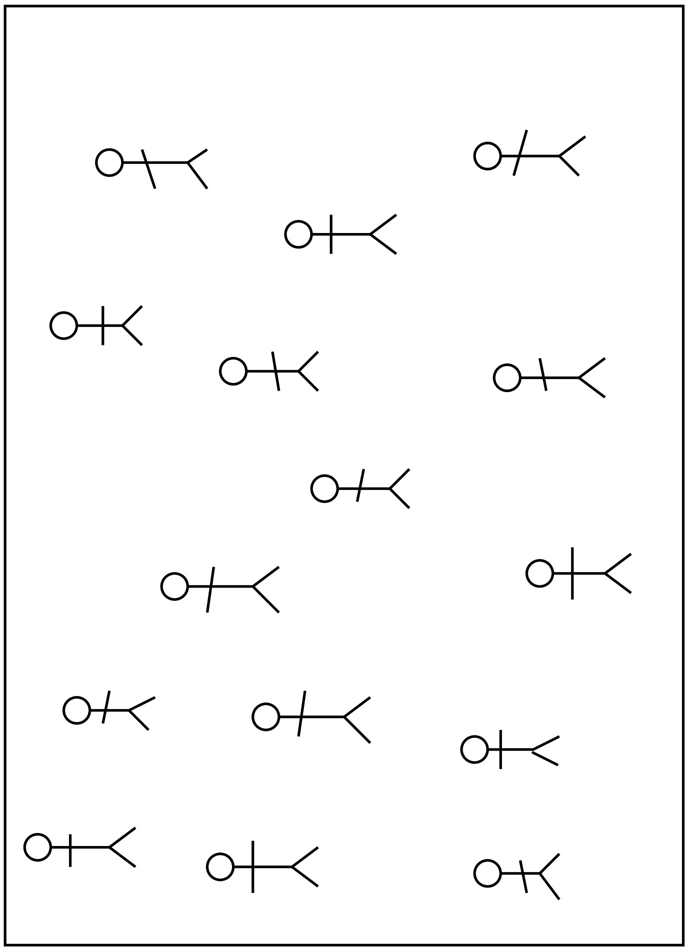

Figure 2: Relaxed configuration of humans

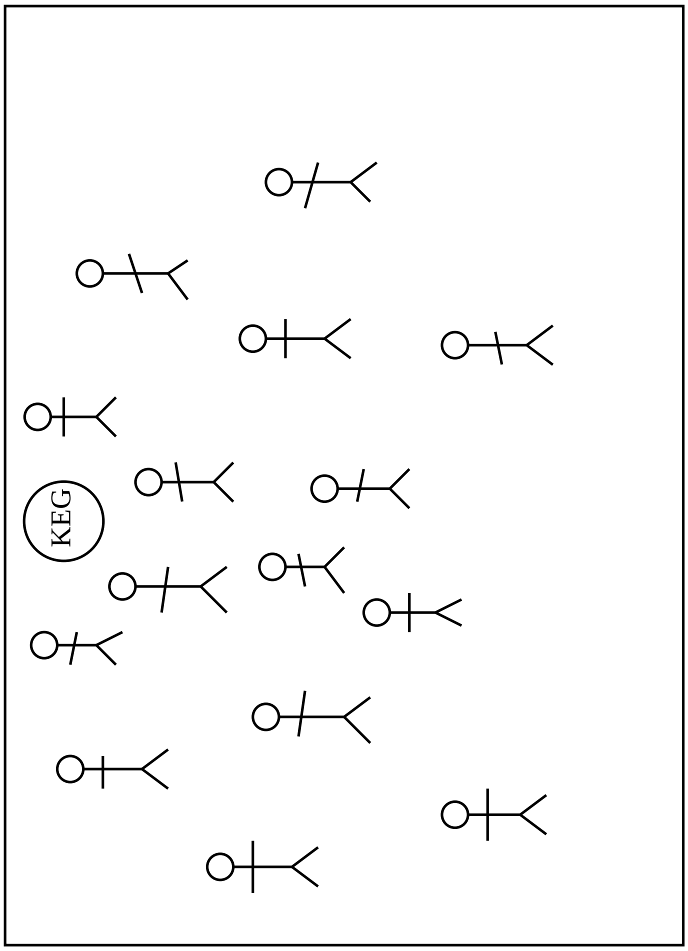

Figure 3: Relaxed configuration of humans adjusted by KEG

Summary

- Monte Carlo is a powerful technique based on random sampling
- Path integrals, when applied to MC, allow one to simulate the quantum effects of particles that occur at low temperatures

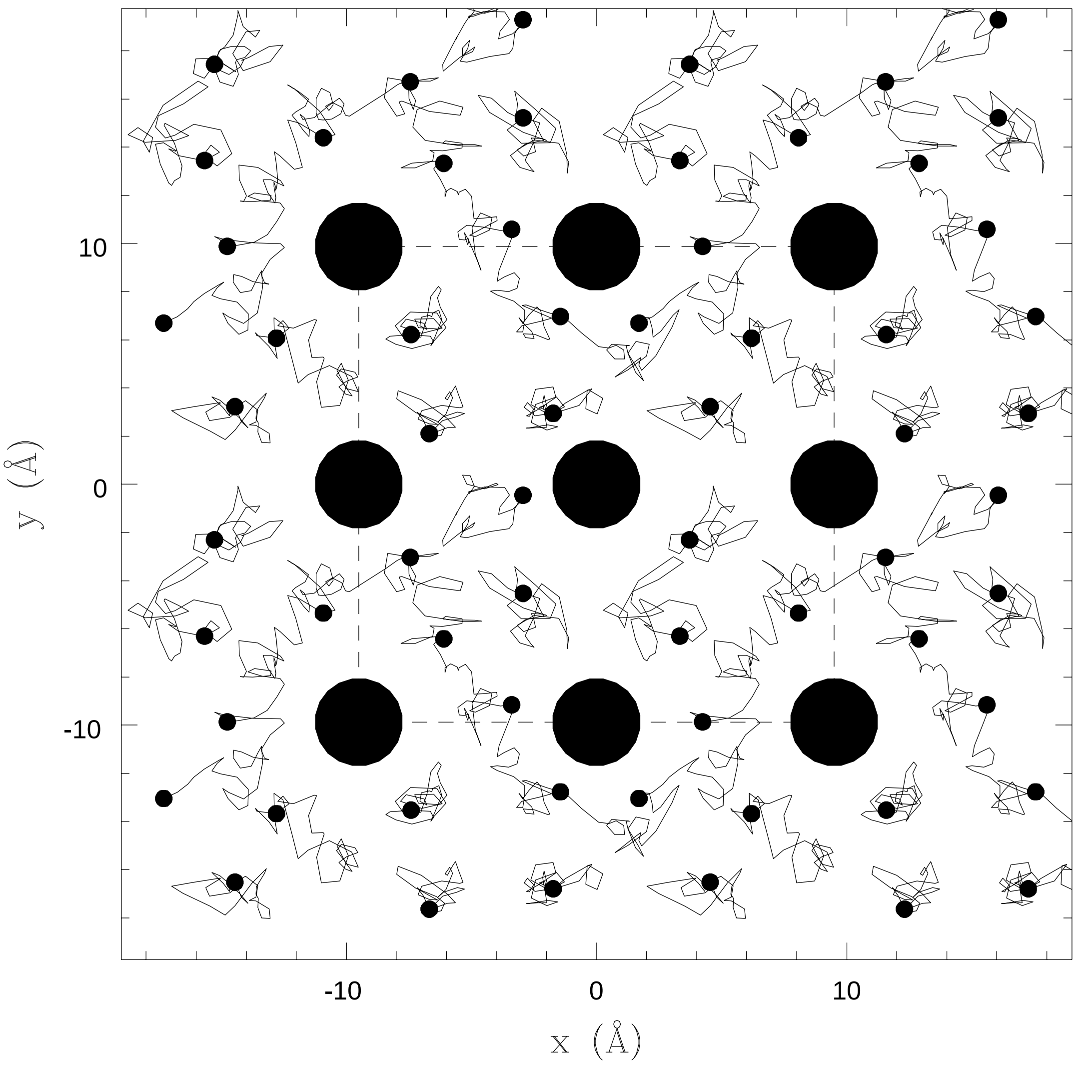

Figure 4: from Ceperly and Gordillo: superfluid hydrogen on silver doped with alkali metal