Worm Algorithm PIMC Application to Liquid and Solid $^4$He

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Outline of the talk

**Theoretical problem:** investigation of superfluid behavior of matter in unusual settings

- Bulk solid $^4$He or $H_2$
- Interfaces, grain boundaries etc.
- Quantum clusters
- Adsorbed films

**Path Integral Monte Carlo:** powerful numerical tool to study Bose systems (D. Ceperley, RMP 67, 279, 1995)

- Accurate - No adjustable parameter - no trial wave function
- Microscopic Hamiltonian - only input is the potential
- Allows direct computation of $\rho_s(T)$ and $n_0(T)$
- **Problem:** finite-size effects ("large" system sizes needed)
Outline (cont’d)

**Worm Algorithm:** overcomes size limitation of existing PIMC technology ($\rho_s(T)$ hard to compute for $N \geq 100$)

**Grand Canonical:** allows simultaneous calculation of structural, energetic properties, as well as **dynamic** (imaginary-time) correlations (e.g., Matsubara Green function)

Affords **considerable** efficiency gain in the calculation of $\rho_s(T)$ - $N$ can be as large as **several thousands** (accurate determination of $T_c$ possible)

**Illustrative applications:** superfluid transition in liquid $^4$He in 2 and 3 dimensions

**Application to commensurate solid $^4$He**
Path Integral Monte Carlo

Thermal averages of physical operators at finite $T=1/\beta$
\[ \langle \hat{O} \rangle = \text{Tr}(\hat{O}\rho) = \int dR \; O(R) \; \rho(R,R,\beta) \]

\( \rho(R,R,\beta) \) many-body density matrix (unknown in general)

Feynman’s recipe:
\[ \rho(R,R,\beta) \approx \int dR_0...dR_{P-1} \{ \prod_i \rho_o(R_i,R_{i+1},\tau) \}, \; \tau = \beta/P \]

Exact as $P \to \infty$, $\tau \to 0 \Rightarrow \rho_o(R,R',\tau)$ high-T approximation to exact \( \rho \)

Monte Carlo scheme to path integration:

- Generate on a computer set of paths \( \{X_i=R_{0i}R_{1i}R...R_{P-1}\} \) sampled with probability \( \{ \prod_i \rho_o(R_i,R_{i+1},\tau) \} \Rightarrow \text{Metropolis algorithm} \)
- Evaluate \( \langle \hat{O} \rangle \) as statistical average of \( O(R_i) \)

Crucial to efficiency of method is path sampling strategy
Worm Algorithm


Basic idea: work in extended configuration space

Include 1 open Word Line (worm) whose head and tail can advance and recede in imaginary time ⇒ Grand Canonical ensemble
Local moves only-- all involving worm

- Head and tail of worm can “swap” with other World Lines
  ⇒ efficient sampling of long permutation cycles

- Complementary pairs of moves Open/Close, Advance/Recede
  ⇒ detailed balance (swap move self-complementary)
Worm Algorithm (cont’d)

- Configurations with an open WL contribute to the Matsubara Green function (G-sector) \(\Rightarrow\) nontrivial modifications of WL
- Swap moves enjoy relatively high acceptance, even with hard core potentials
- Head and tail can reconnect, resulting in a diagonal configuration, which contributes to the partition function (Z-sector)
- Reconnection is attempted periodically (no need to “wait” for it !)
- Number of particles fluctuates (WLs can disappear and be recreated) -- Note, however, that canonical versions are possible

General algorithm of statistical mechanics

- Applied to several quantum and classical lattice models
- No critical slowing down for Ising model
Application: SF transition in $^4$He

2 dimensions

$T_c = 0.653(10)$ K
$^4\text{He}$ in 2 dimensions, $T=0.6$ K, 200 particles
Superfluid Transition in 3D $^4$He

\[ N = 64 \text{ to } 2048 \]
SF transition in $^4$He (cont’d)

$\langle W^2 \rangle / 3$

3 dimensions
$T_c = 2.193(6) \, \text{K}$
OK, but ... Why do we need large systems?

- Some physical quantities **require** large size extrapolation
- Examples: $T_c$, $n_0$
Why is it important to do large systems?

Some **physical phenomena** can **only** be properly formulated or studied on sufficiently large system sizes.
- Possible superfluid layer at solid $^4$He grain boundaries
- Superfluidity in porous media
- Dislocations and extended defects in quantum crystals
- Polycrystalline samples (talk by B. Svistunov next week)
**BEC/SF in solid $^4$He?**

### Graphical Representation

- **Superglass**
  - $\rho=0.0292$ Å$^{-3}$

- **Hcp crystal**
  - $\rho=0.0359$ Å$^{-3}$

**Parameters**
- $T=0.2$ K, $N=800$
- $\rho_s=0$

The graph plots the logarithm of the density $n(r)$ against distance $r$ (Å). The data points and curves illustrate the density distribution for different systems under specified conditions.
Results

- No evidence of BEC/SF found in a perfect hcp crystal at low T
- Ring exchanges do occur, but long permutation cycles yielding nonzero winding (i.e., SF) are not observed
- Through “swap” type moves, worm ends can travel far apart (providing statistics for n(r) at large r). However, they almost invariably reconnect without leaving any permutation behind, unlike in the superfluid.
- Physical result, not artifact of computational/sampling methodology (e.g., possible lack of ergodicity)

Consistent with general theoretical result for commensurate crystals

Current and future research

- Accurate determination of vacancy activation energy in solid $^4$He
  - Application of Green function formalism - no subtraction needed of large energies

- Exploration of novel phases of solid Helium
  - Possible "superglass" phase
  - Superfluidity at grain boundaries (talk by B. Svistunov)

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