Worm Algorithm PIMC Application to Liquid and Solid ^{4}He

KITP - Santa Barbara, 2/8/06

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Outline of the talk

- Theoretical problem: investigation of superfluid behavior of matter in unusual settings
  - Bulk solid ^4He 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 fnctn
  - 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 $N \gtrsim 100$)
  - 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 $T=1/\beta$

  $\langle \hat{O} \rangle = Tr(\hat{O}\rho) = \int dR\ O(R)\ \rho(R,R,\beta)$

  - $\rho(R,R,\beta)$ many-body density matrix (unknown in general)
  - Feynman's recipe: $\rho(R,R,\beta) \approx \int dR_0 \ldots dR_{P-1}\ \{\Pi_i\ \rho_o(R_i,R_{i+1},\tau)\}$, $\tau = \beta/P$
  - Exact as $P \to \infty$, $\tau \to 0 \Rightarrow \rho_o(R,R',\tau)$ high-T approximation to exact ρ

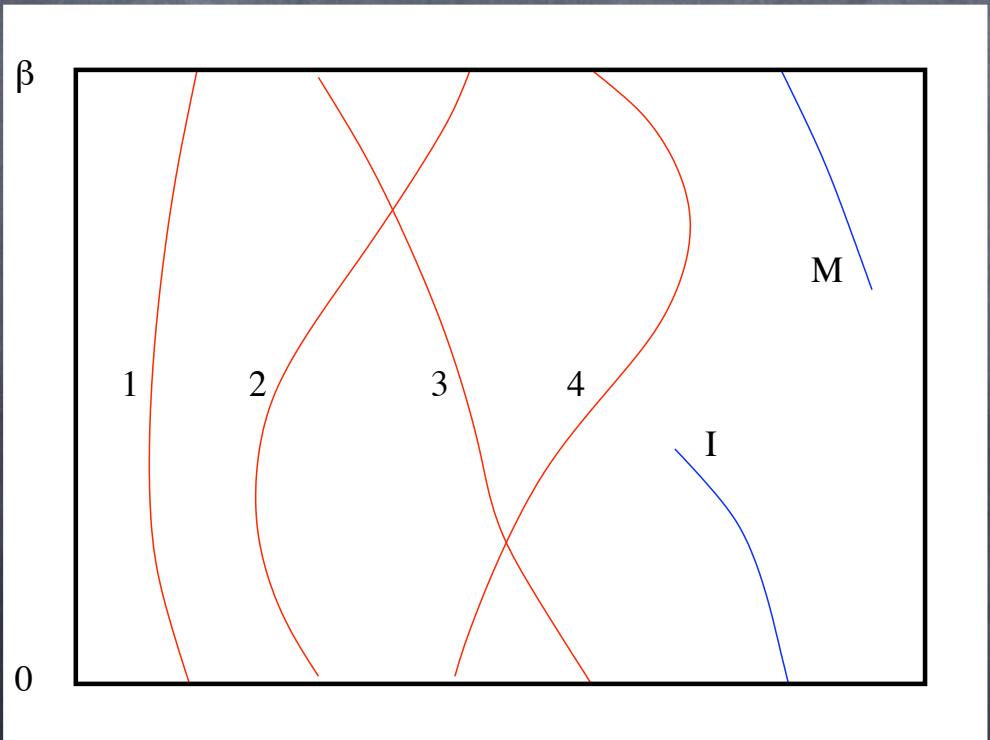
- Monte Carlo scheme to path integration:
  - Generate on a computer set of paths $\{X_i = R_{0i} R_{1i} R \ldots R_{P-1}\}$ sampled with probability $\{\Pi_i\ \rho_o(R_i,R_{i+1},\tau)\} \Rightarrow$ Metropolis algorithm
  - Evaluate $\langle \hat{O} \rangle$ as statistical average of $O(R_i)$
  - **Crucial** to efficiency of method is path sampling strategy

Worm Algorithm

N. Prokof'ev, B. Svistunov and I. Tupitsyn, Phys. Lett. A **238**, 235 (1998)

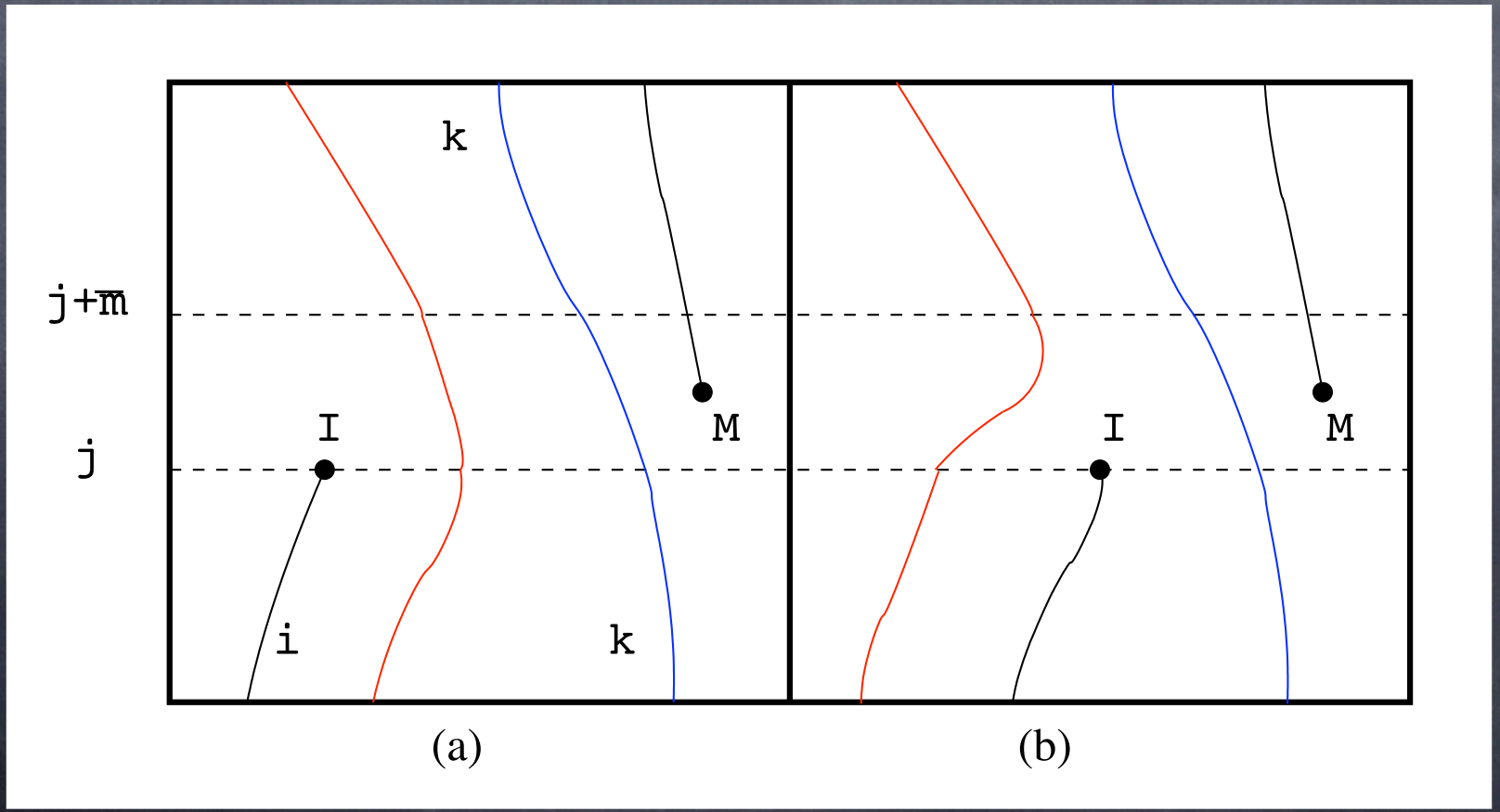
MB, N. Prokof'ev and B. Svistunov, Phys. Rev. Lett. **96**, 10212 (2006)

- 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



Worm Algorithm (cont'd)

- 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)

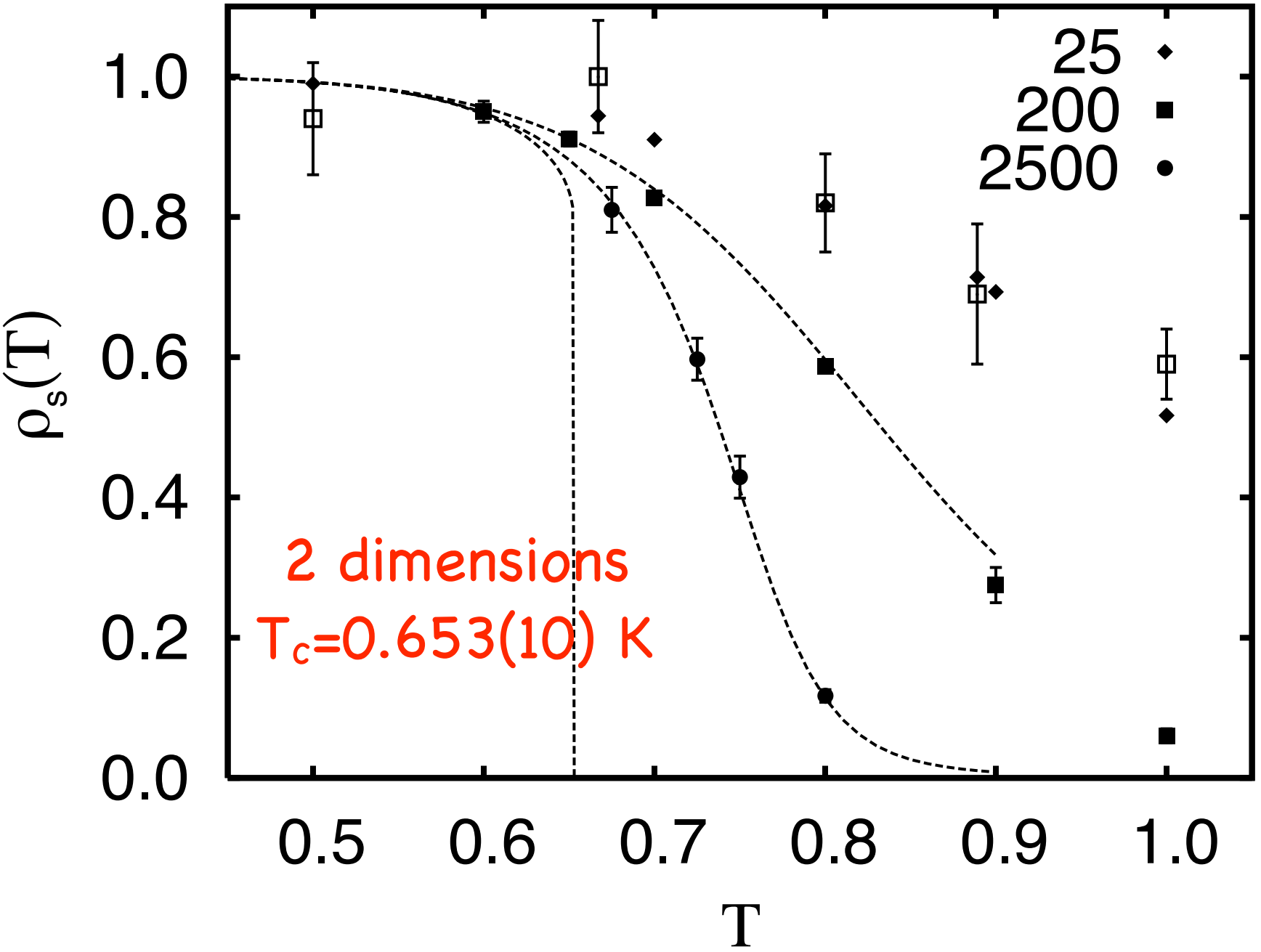


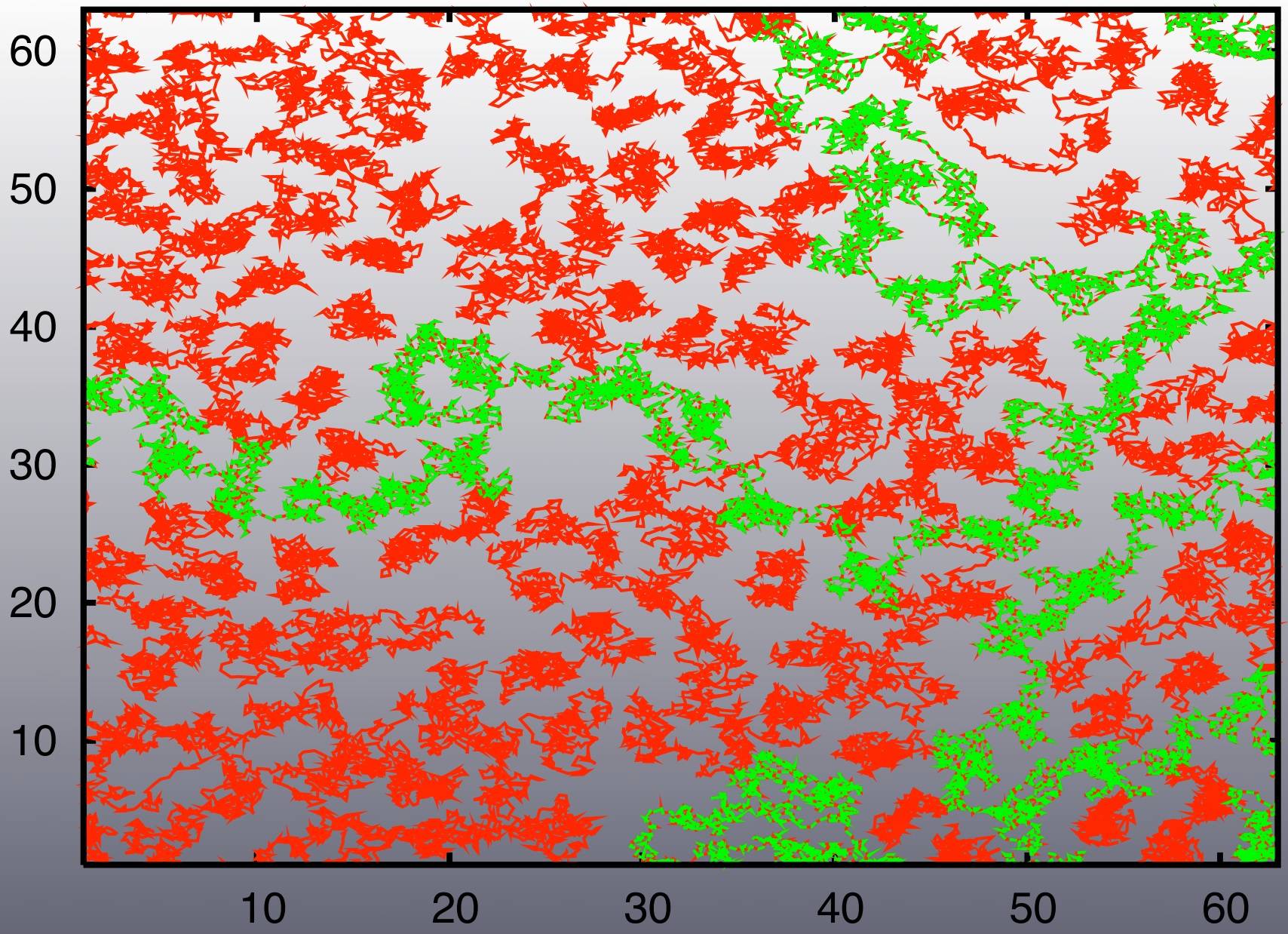
Worm Algorithm (cont'd)

- Configurations with an open WL contribute to the **Matsubara Green function** (G-sector) ⇒ **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

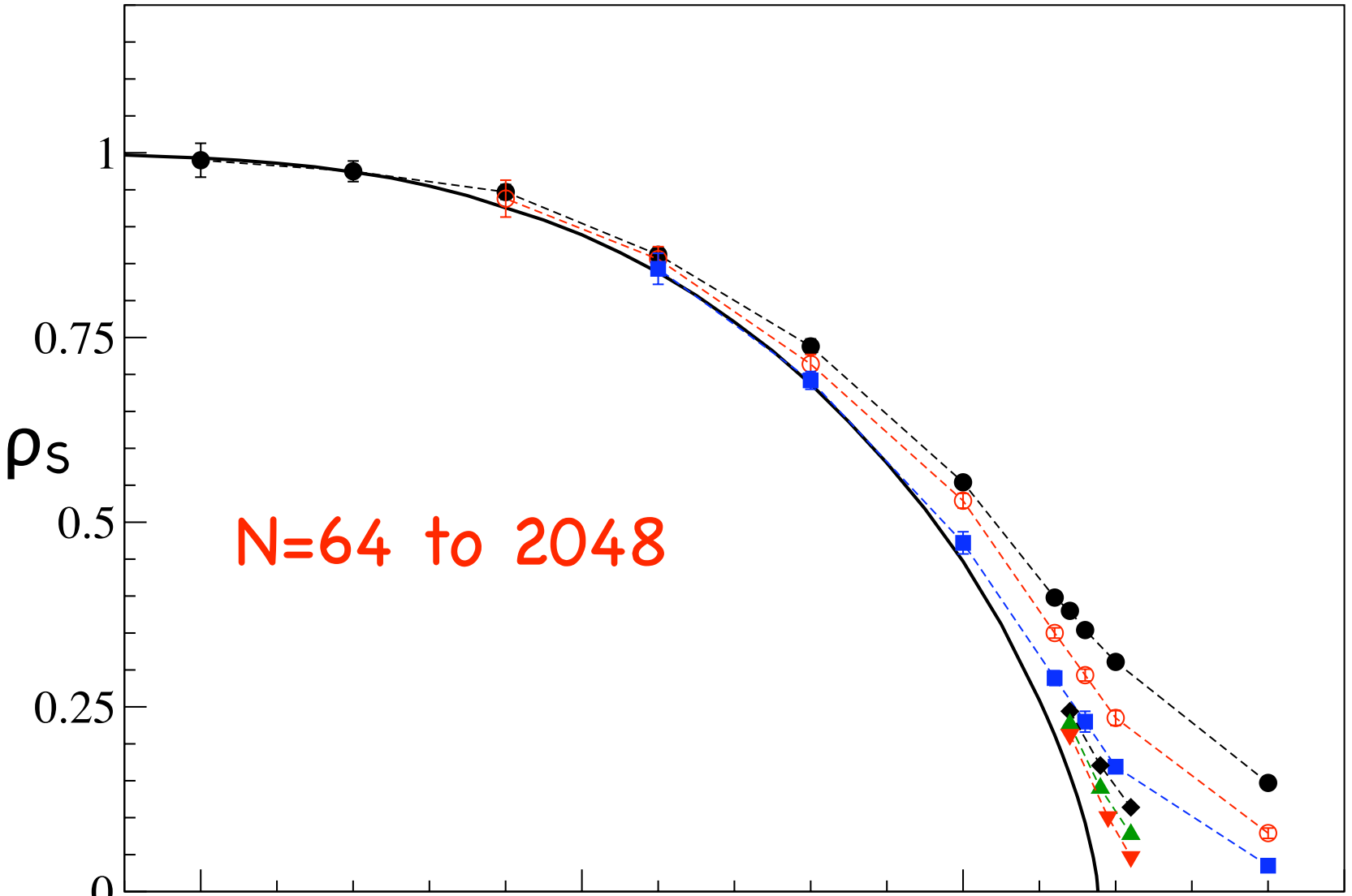
Application: SF transition in ^{4}He



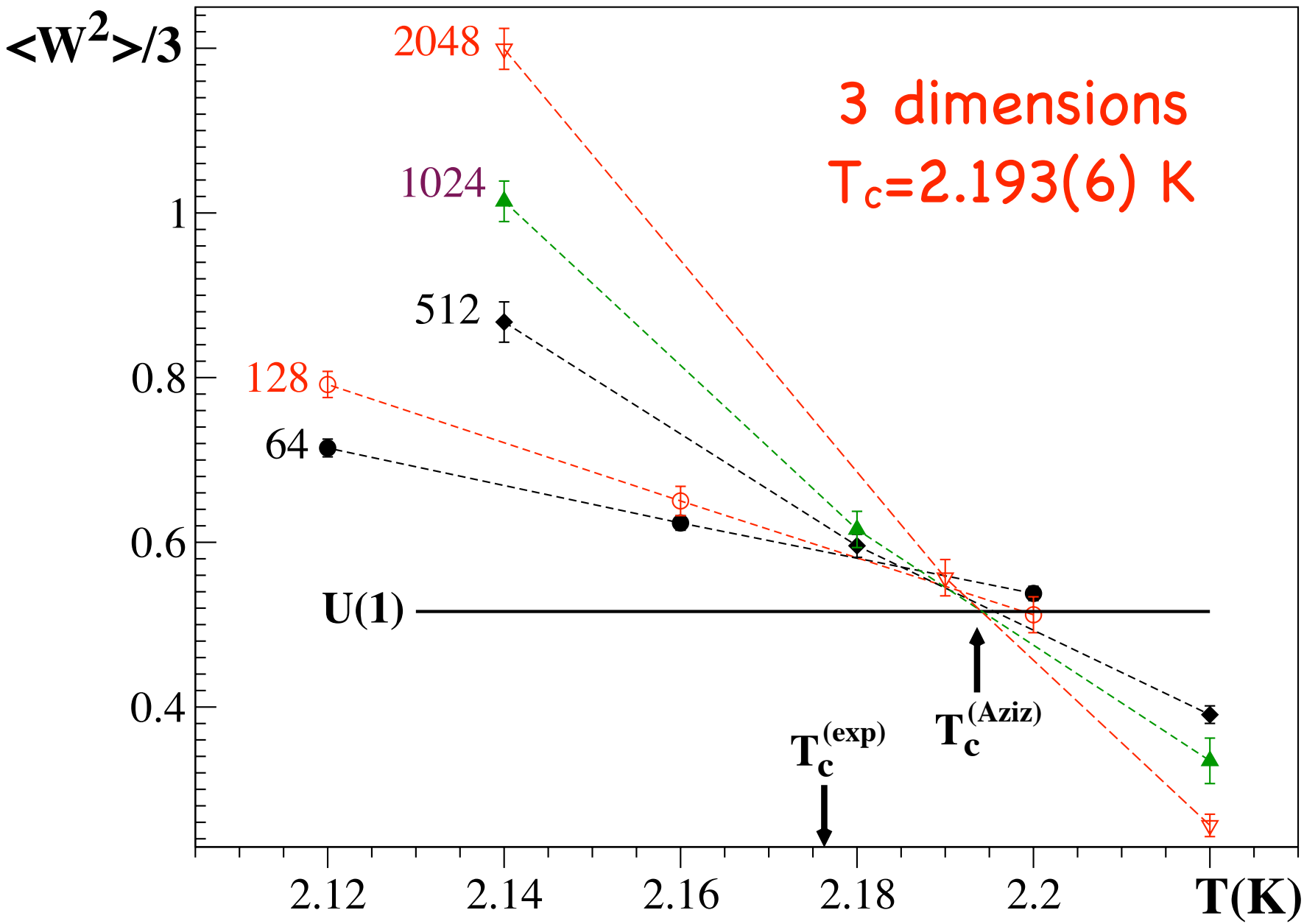


^{4}He in 2 dimensions, T=0.6 K, 200 particles

Superfluid Transition in 3D ^{4}He

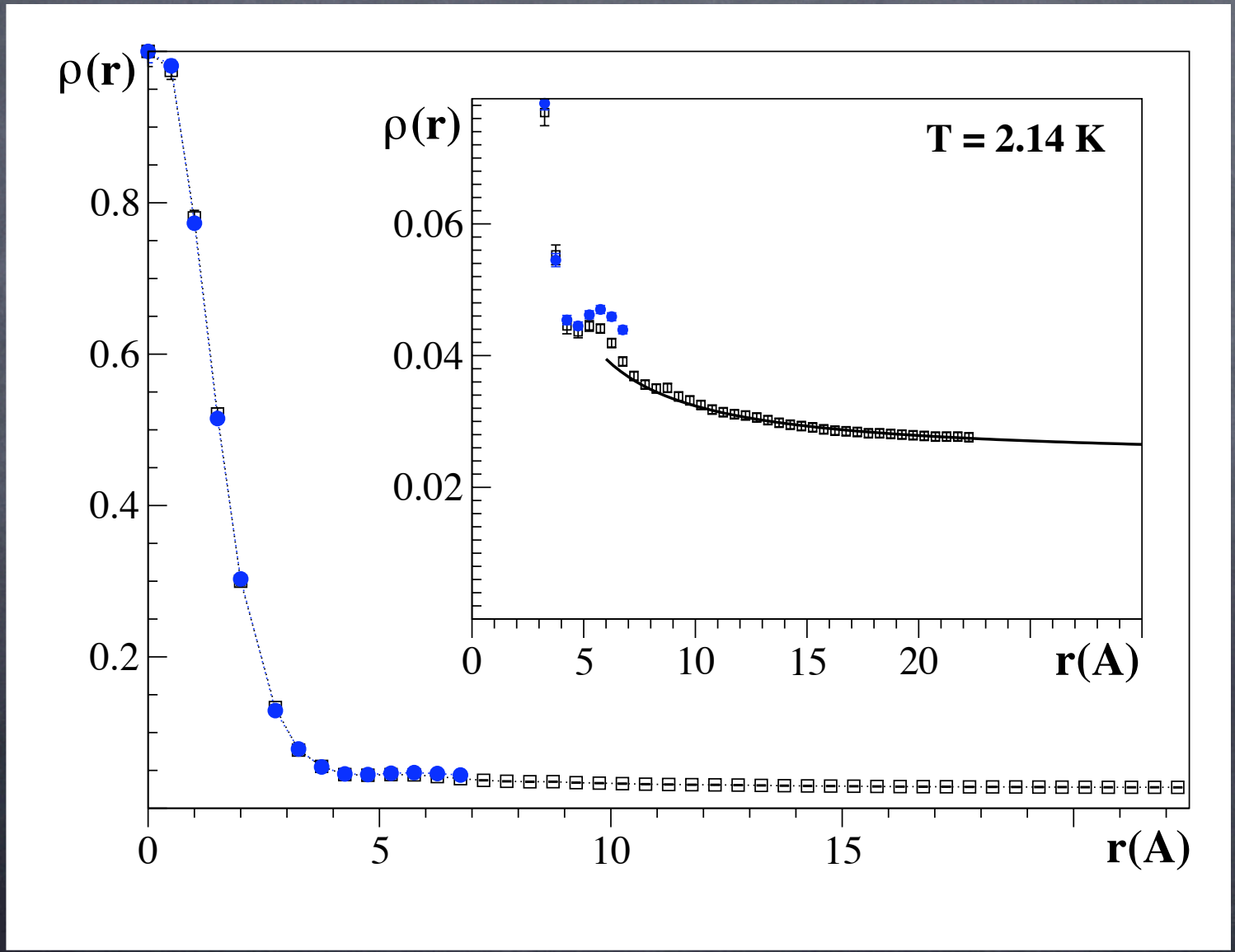


SF transition in ^{4}He (cont'd)



OK, but ...Why do we need large systems ?

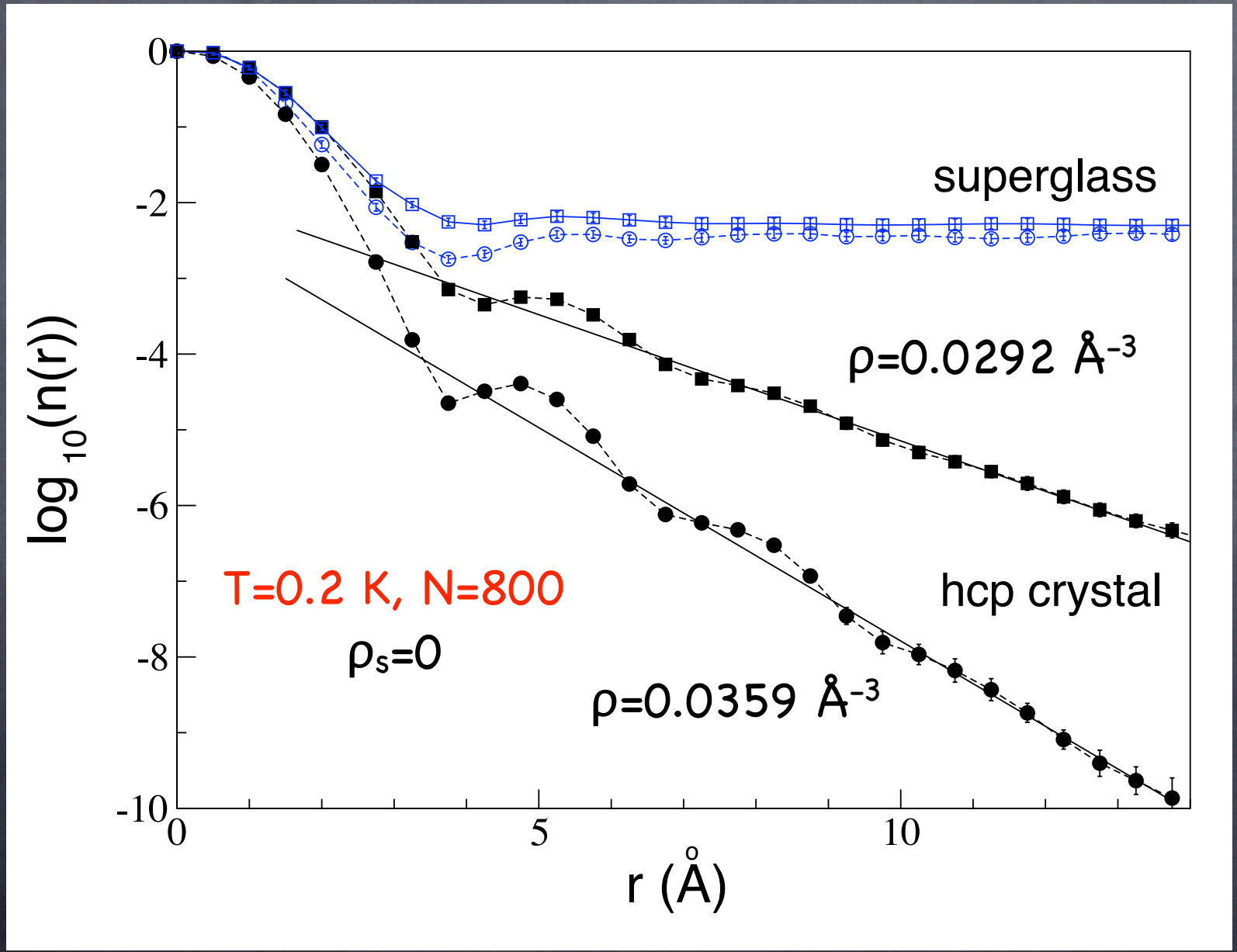
- Some physical quantities require large size extrapolation
  - Examples: T_c, n_0



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 ?



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
  - N. Prokof'ev and B. Svistunov, Phys. Rev. Lett. **94**, 155302 (2005)

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)

- Acknowledgments
  - NSERC (Canada)
  - NSF
  - NASA
  - Sloan Foundation