International Summer School on Numerical Methods for Strongly Correlated Systems in Condensed Matter

Sherbrooke, May 26 -June 7 2008

The Worm Algorithm

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Credit

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Additional reading material at *http://montecarlo.csi.cuny.edu/umass/*

Outline of the lectures

- Motivation and general ideas
- A simple case study: the **Ising** model
- Quantum many-body problems

1. Discrete space and continuous time: lattice bosons
2. Continuous space and discrete time: condensed Helium
3. Long-ranged interactions: Diagrammatic Monte Carlo
4. Applications

Monte Carlo basics

Goal of most Monte Carlo simulation of condensed matter: study of *equilibrium statistical* properties (no time dependence yet)

- Evaluation of **thermal averages**

  Multi-dimensional sums/integrals : typical dimension is $d \times N$

  Not factorizable due to particle interactions

  Straightforward grid integration impossible

- Strategy: turn calculation into "synthetic" **measurement**

  Generate on a computer a *statistically representative sample* of many-particle configurations, drawn from the physical probability distribution (Gibbs)

Compute desired thermal expectation value as statistical average

Monte Carlo basics (cont'd)

(*M. Troyer's notes*)

Statistically representative set of configurations must be generated *sequentially* for any non-trivial system.

Efficiency considerations important

Random walk through configuration space

Metropolis Algorithm (N. Metropolis *et al*., 1953)

Key : Efficient Sampling ☞ Small auto-correlation time

(unbiased statistics: configurations *should* quickly lose memory of progenitors)

Monte Carlo basics (cont'd)

- **Detailed Balance**

  *A random walk is **guaranteed** to sample asymptotically the desired distribution P(c) of configurations **if** the following conditions are satisfied:*

  1) ***Ergodicity***: *rules that govern random walk **must** allow each physical configuration to be visited* ("*paths from anywhere to anywhere*")

  2) ***Detailed balance***: *if* $W(c \longrightarrow d)$ *is the probability of making transition between any two configurations, then it must be*

$$\frac{W(c \to d)}{W(d \to c)} = \frac{P(d)}{P(c)}$$

- **Sampling strategy**

  Elementary move

  *Simple (single-particle), fast but **long** auto-correlation time (ergodicity ?)*

  *Complex (many particles), **shorter** auto-correlation time but **slower***

  or... both simple and with short auto-correlation time ?

Simple case: spin-1/2 Ising model

Classical lattice spin model : $E(c) = -J \sum_{\langle ij \rangle} s_i s_j, \quad s_i = \pm 1$

$c \equiv \{s_1 s_2 ... s_N\}$ generic configuration

$Z = \sum_c \prod_{\langle ij \rangle} \exp(K s_i s_j)$ Partition function $(K = J/T)$

- Equilibrium phase diagram known analytically in 2D (Onsager, 1944)
- Second order ferromagnetic phase transition
- Regarded as *test bench* for MC simulation methods

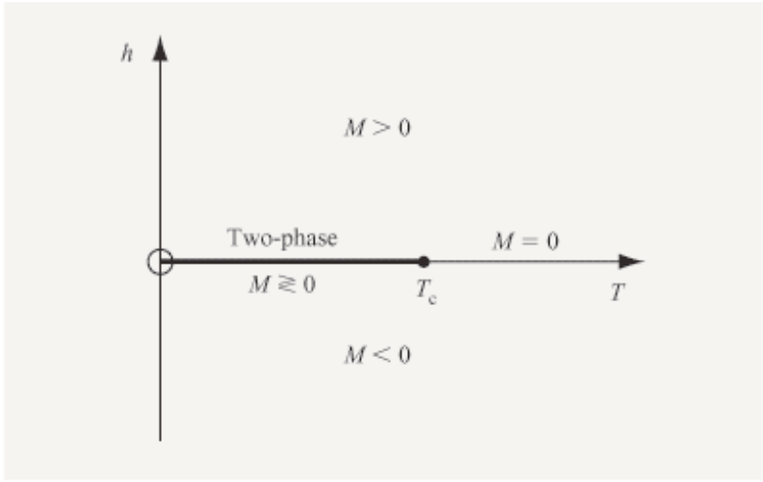
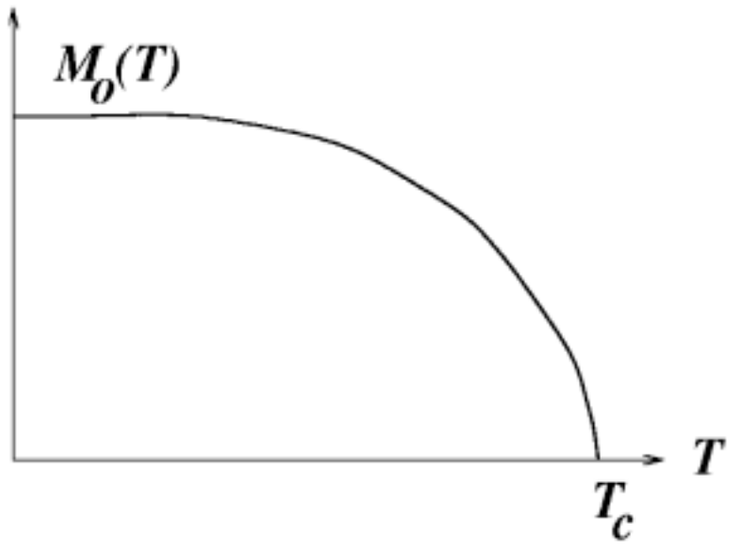


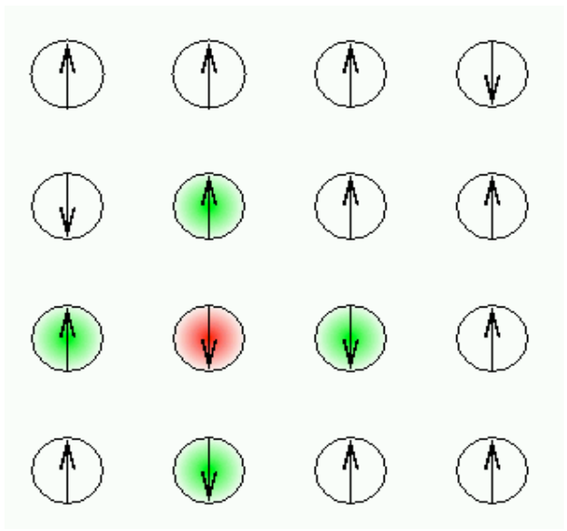
Figure 2

Phase diagram for the Ising model as a function of temperature (T) and magnetic field (h); dark portion of $h = 0$ axis represents two-phase region; T_c denotes critical point.



$$m(T) = (1 - (\sinh(2J/T))^{-4})^{1/8}$$

Monte Carlo simulation

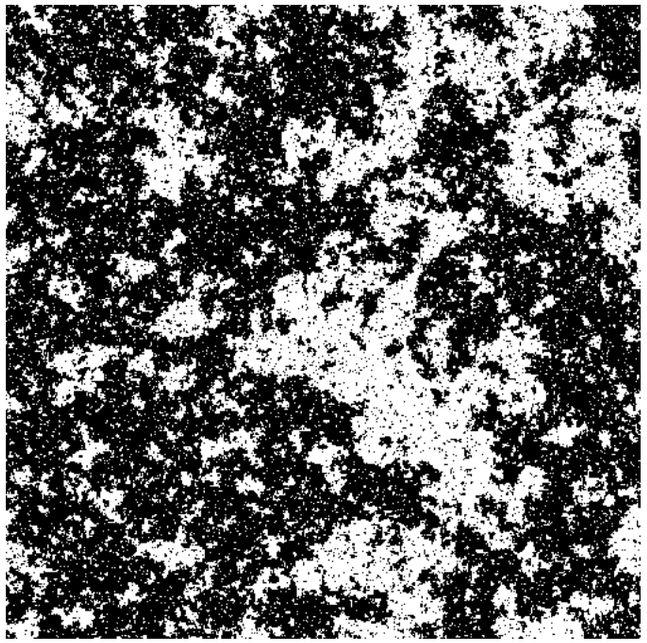


Sampling of configurations

- Local: Flip single spin in c, and accept with probability

$$P = min\{1, \exp[-2Ks \, \Sigma_j s_j]\}$$

Efficient at $T \geq T_c$
Suffers from critical slowing down as $T \rightarrow T_c$
Physical reason: as system approaches critical temperature, correlations on very long distances set in, and large "islands" of ferromagnetically aligned spins appear.



- Cluster update (Swendsen-Wang, 1987, Wolff, 1989)
  Flip clusters of connected equal spins at same time
  Clusters are grown from a seed site, based on a sequential (non-Metropolis) probabilistic procedure, satisfying *detailed balance*
  No critical slowing down at T_c
  Not as efficient as single spin flip at high T
  Physical reason: cluster algorithms owe their efficiency to the proximity to criticality

Worm Algorithm for Ising model

N. Prokof'ev, B. Svistunov and I. Tupitsyn (1991)

$$Z = \sum_{s_1 \ldots s_N} \prod_{\langle ij \rangle} e^{K s_i s_j} = \sum_{s_1 \ldots s_N} \prod_{\langle ij \rangle} \Big[\cosh(K) \Big(1 + \tanh(K) s_i s_j \Big) \Big]$$

i.e.

$$Z = \cosh(K)^{2N} \sum_{s_1 \ldots s_N} \prod_{bonds} \sum_{n_b=0}^{1} \Big[\tanh(K)]^{n_b} s_i^{n_b} s_j^{n_b} \Big] \propto \sum_{\{n_b\}} \tanh(K)^{\sum n_b} \sum_{s_1 \ldots s_N} \prod_{bonds} s_i^{n_b} s_j^{n_b}$$

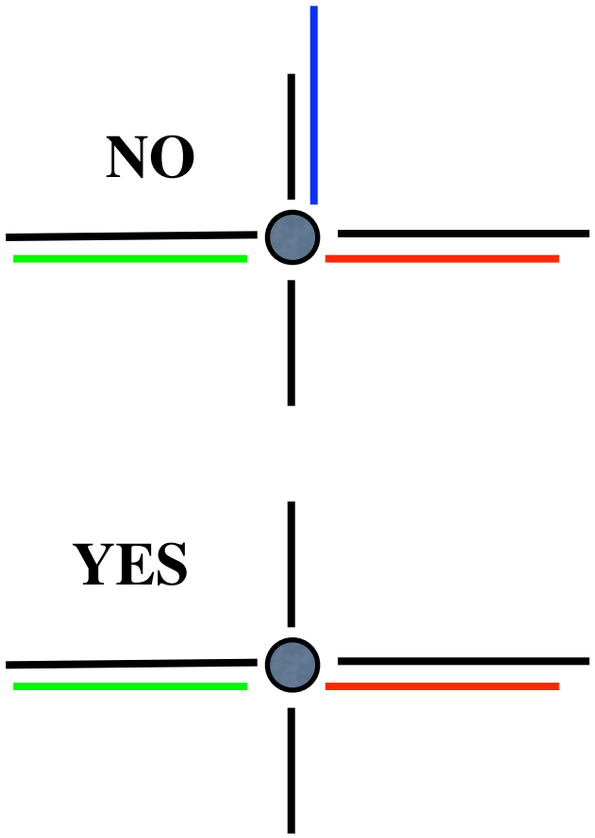
$n_b = 0, 1$: **power** associated to *bond* $\langle ij \rangle$

$$\sum_{s_1 \ldots s_N} \prod_{\langle ij \rangle} s_i^n s_j^n \equiv \prod_i \sum_{s_i} s_i^{p_i}, \quad p_i \quad \text{total power associated to site i}$$

For a spin-1/2 system one has $\sum_s s^p = 2$ if p is even, zero otherwise

$$\text{Hence,} \quad Z = 2^N \sum_{\{n_b\}} \Big[\tanh(K) \Big]^{\sum n_b} \qquad (\textit{closed loops})$$

Closed loops ? *What* loops ?



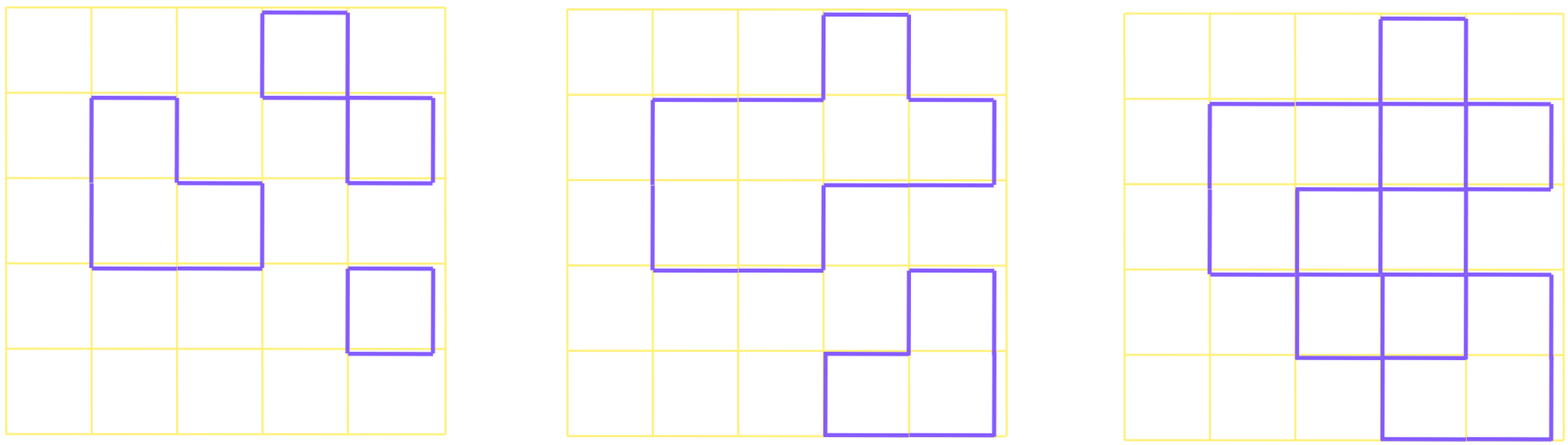
Number of times each site occurs in the product must be **even**

Sum of all occupied bonds involving that site must be **even**

(no bond can be invoked *twice*)

Consequently, bonds connecting sites *necessarily* must form <u>closed loops</u> (not necessarily connected)

Examples



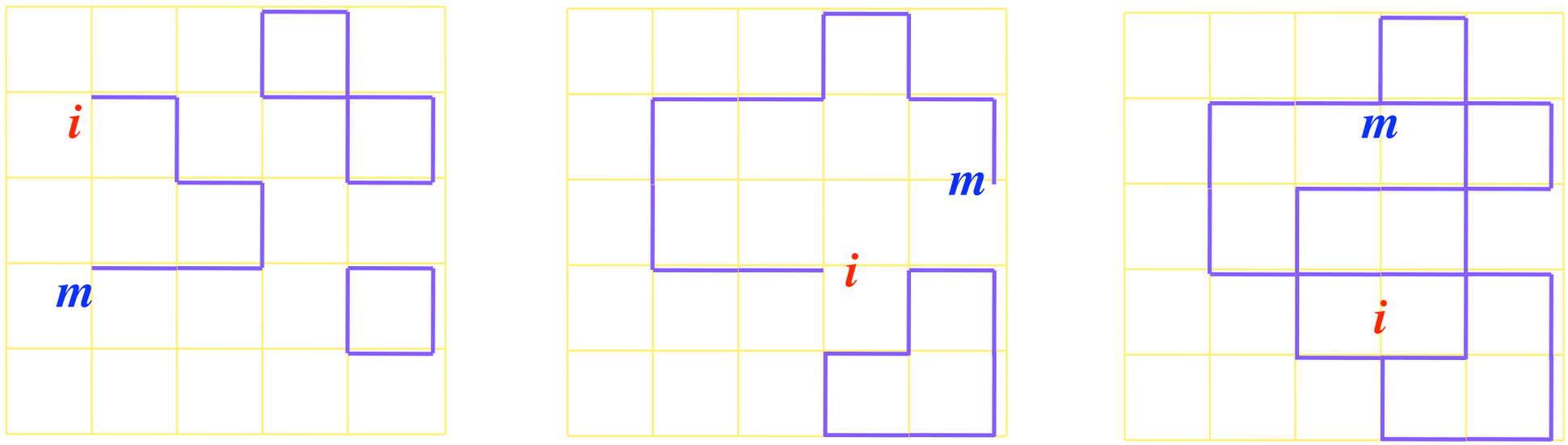
Enter "Ira" and "Masha"

Consider the 2-point *spatial correlation function*

$$g(i-m) = Z^{-1} \sum_{s_1 \ldots s_N} s_i s_m \, e^{K \sum_{\langle jl \rangle} s_j s_l} = Z^{-1} \, G(i-m)$$

Identical procedure adopted for Z expresses G as a sum over *open* loops, with the same weights used for the expansion of Z. The presence of two additional spins (i and m) gives rise to the two "dangling ends"

Examples



Monte Carlo evaluation of *g(i-m)*

- Generate on a computer a set of loops corresponding to *drawing* with a pencil along bonds of a square lattice, *without ever detaching the tip of the pencil from the sheet*. Each bond is penciled only *once* at the most, and there are two *dangling ends* (*Ira* and *Masha*)

- Let the probability with which generic loop occurs be proportional to $[\tanh(K)]^{N_b}$

- When *Ira* and *Masha* are at a distance *i* - *m,* contribute +1 to *G*(*i*-*m*)
  When $i = m$ (closed loop), then contribute +1 to $G(0) \equiv Z$

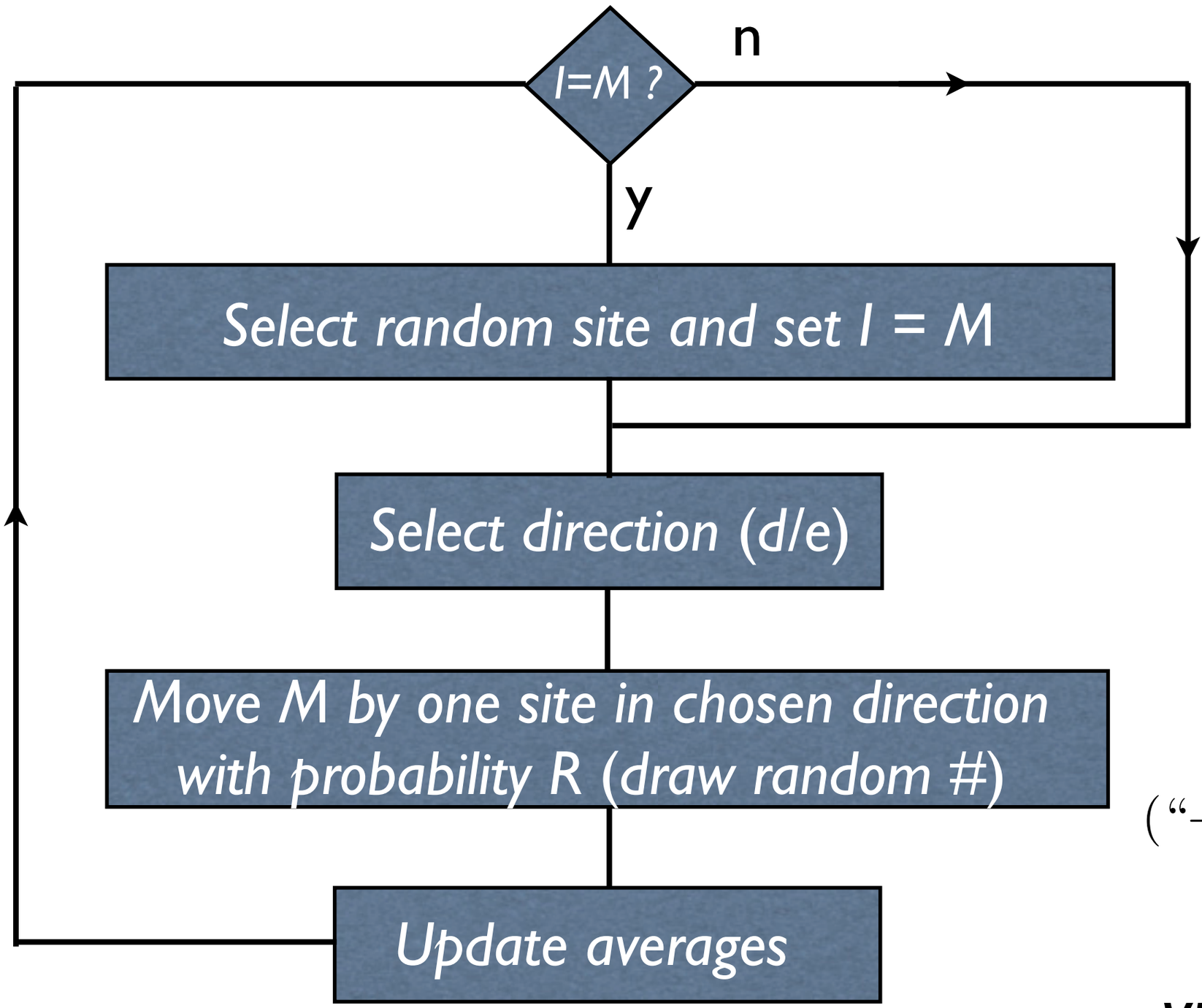
- *Accumulate statistics and evaluate* $g(i\text{-}m)$ as $G(i\text{-}m)/G(0)$

- Other quantities can be computed as well. For example,
  Average *energy*: $-J \tanh(K)\,[dN + \langle N_b \rangle / \sinh^2(K)]$,
  (N_b total number of *penciled bonds*)

  Magnetic susceptibility $\chi = (1/T)\,\Sigma_i\, g(i)$

Structure of Ising Worm code

Simple “draw-and-erase” procedure



$$R = \quad [\tanh(K)]^{\pm 1}$$

(“+” sign if N_b is increased)

yup... that’s it !

How well does it work ?

No critical slowing down *near critical temperature*

Allows to simulate the model efficiently at all temperatures

All *correlation functions available on-the-fly*

Same conclusion established for a rather wide variety of other lattice models (e.g., x-y) and/or universality classes

By now regarded as general algorithm of statistical mechanics

Local moves only

Basic idea easily extended to quantum-mechanical systems

Worm Algorithm and Quantum Many-Body Physics

Worm Algorithm *is currently one of the most powerful methodology to study thermodynamic properties of quantum-mechanical systems comprising many interacting particles*

Essentially exact *for Bose systems (goes* ***far*** *beyond previously existing continuum methodology)*

It does ***not*** *solve/alleviate the infamous "sign" problem*

General Monte Carlo methodology for fermions still lacking

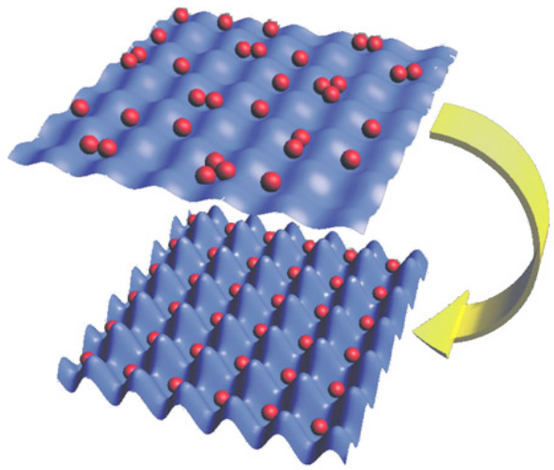
It does ***not*** *represent a step forward toward the computation of time-dependent properties with Monte Carlo*

Worm Algorithm and Lattice Bosons

Bose Hubbard Model (BHM)

$$\hat{H} = \hat{T} + \hat{V}$$
$$\hat{T} = -t \sum_{\langle ij \rangle} (\hat{a}_i^\dagger \hat{a}_j + h.c.); \quad \hat{V} = U \sum_i \hat{n}_i^2 - \sum_i h_i \hat{n}_i \qquad \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$$

h_i site-dependent external potential (e.g., *disorder*)
$U > 0$ (what happens if $U < 0$?)



- BHM subject of much current research
  especially in the context of cold atoms in optical lattices

- Useful *minimal model* and starting point for our discussion
- Methodology described this morning *generally* applicable to lattice bosons

Thermodynamics of BHM

- Calculation of *thermal expectation values*

$$\langle \hat{\mathcal{O}} \rangle = \frac{\mathrm{Tr}\hat{\mathcal{O}}\hat{\rho}}{\mathrm{Tr}\hat{\rho}}, \quad \rho = e^{-\beta \hat{K}}$$

$\hat{K} = \hat{H} - \mu \hat{N}$ *"Grand Canonical" Hamiltonian*

$\beta = 1/T$

$Z = \mathrm{Tr}\hat{\rho} = \sum_c \langle c | e^{-\beta \hat{K}} | c \rangle$, *Grand partition function*

$|c\rangle \equiv |n_1\ n)2\ ...\ n_N\rangle$ generic configuration (occupation number representation)

Matrix elements of $e^{-\beta \hat{K}}$ in $|c\rangle$ basis **not known** analytically

Direct evaluation of Z *unfeasible*

Numerics *required*

Interaction representation

With $\hat{\rho}(\tau) = e^{-\tau \hat{K}}$, it is

$$\frac{\partial \hat{\rho}}{\partial \tau} = -\hat{K}\hat{\rho} \quad (Bloch's\ equation)$$

Set $\hat{\rho}(\tau) = e^{-\tau \hat{V}} \hat{G}(\tau)$, obtain

$$\frac{\partial \hat{G}}{\partial \tau} = -\hat{T}_I(\tau)\hat{G}(\tau), \quad \hat{G}(0) \equiv 1$$

with

$$\hat{T}_I(\tau) \equiv \ e^{\tau \hat{V}} \ \hat{T} \ e^{-\tau \hat{V}}$$

Solution by series expansion

Formal recursive solution of equation for $\hat{G}(\beta)$ yields series for **Partition Function**:

$$Z = \sum_{n=0}^{\infty} (-1)^n \sum_{c,c',\ldots c^{(n-1)}} \int_{\tau=0}^{\beta} d\tau \ldots \int_{\tau^{(n)}=0}^{\tau^{(n-1)}} d\tau^{(n)}$$

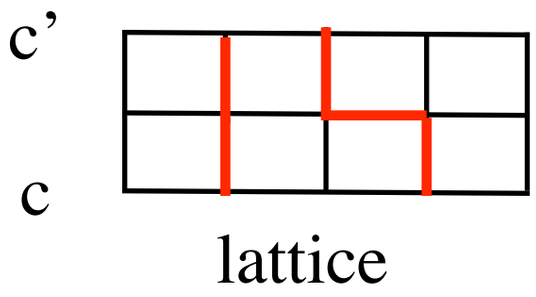
$$\times\ e^{-(\beta-\tau)V(c)}\ \langle c|\hat{T}|c'\rangle\ e^{-(\tau-\tau')V(c')}\ \langle c'|\hat{T}|c''\rangle\ \ldots$$

$$\ldots\ \times\ \ e^{-(\tau^{(n-1)}-\tau^{(n)})V(c^{(n-1)})}\ \langle c^{(n-1)}|\hat{T}|c\rangle\ e^{-\tau^{(n)}V(c)}$$

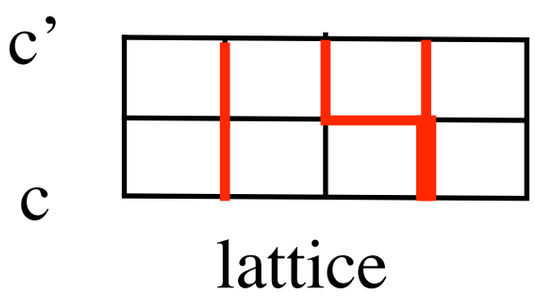
Kinks

Matrix element of kinetic energy operator *only* connects configurations differing *at the most* by the hopping of one particle to NN site

particle

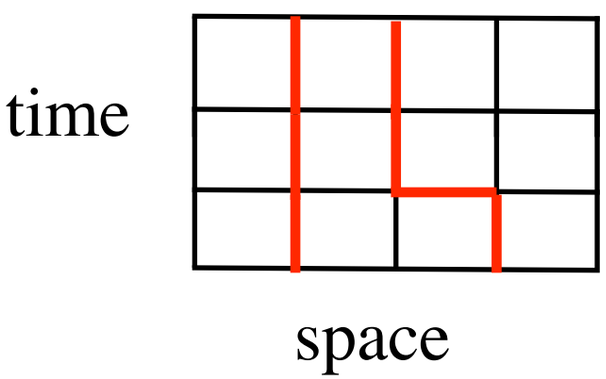


$$\langle c|\hat{T}|c'\rangle = -t$$

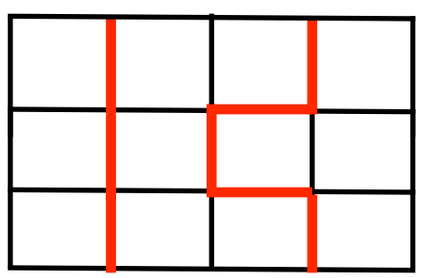


$$\langle c|\hat{T}|c'\rangle = -\sqrt{2}\ t$$

Integrand of *n*th order term in *Z* expansion: *trajectory in imaginary time with n "kinks"*



kink



kink-antikink pair

Monte Carlo integration

Partition function Z *infinite sum* of *multidimensional nested* integrals of increasing order $\Rightarrow$ integral over all *many-particle paths* featuring an arbitrary number of "kinks"

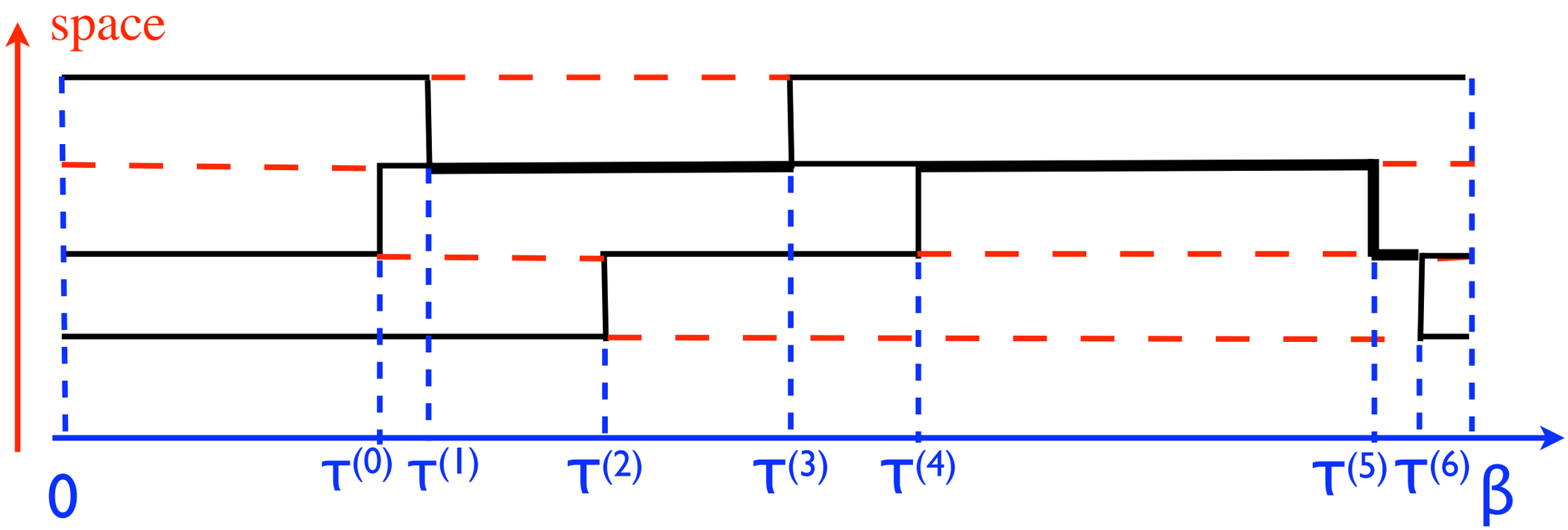
MC evaluation of contributions to Z translates into sampling *paths* with arbitrary numbers of kinks at varying consecutive *ordered* times

Weight of generic configuration proportional to:

$$(\beta t)^n \, \exp\left\{ - \int_{\tau=0}^{\beta} d\tau V[c(\tau)] \right\}$$

Weight is ***positive*** *for* ***bosons***
$c(\tau)$ *piecewise* many-particle path
$V[c(\tau)]$ constant between consecutive kinks

World Line (WL) representation of $\langle c|\, \rho^{(n)} |c\rangle$



Example: **3** particles in **one** dimension (**4**-site lattice)

Particles are all drawn with the same color because of indistinguishability

Dashed lines represent empty lattice sites

Line thickness proportional to number of particles on site

Contribution of order ***7*** (*number of "kinks" occurring at different times*)

Between one kink and the next system propagates "unperturbed" in imaginary time

Initial and final configurations are identical (*in occupation terms*)

World Line Monte Carlo

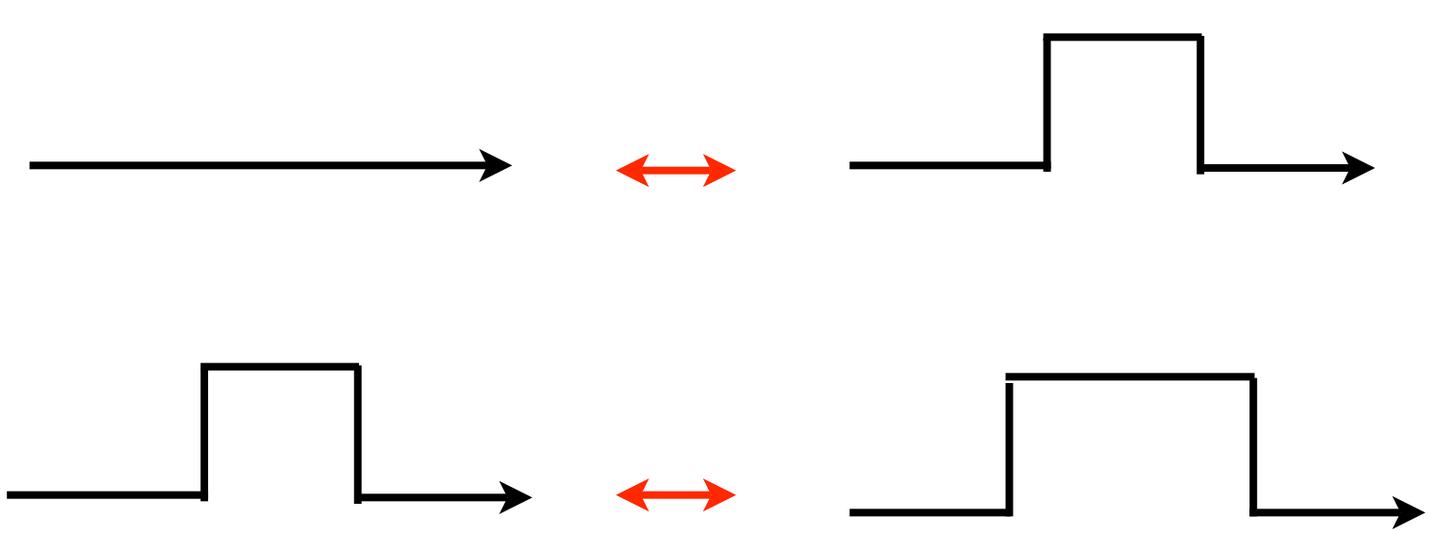
Sampling of many-particle paths ***restricted to*** **the space of closed WLs**

Limited number of updates (*kink-antikink creation and removal, time shifts*)

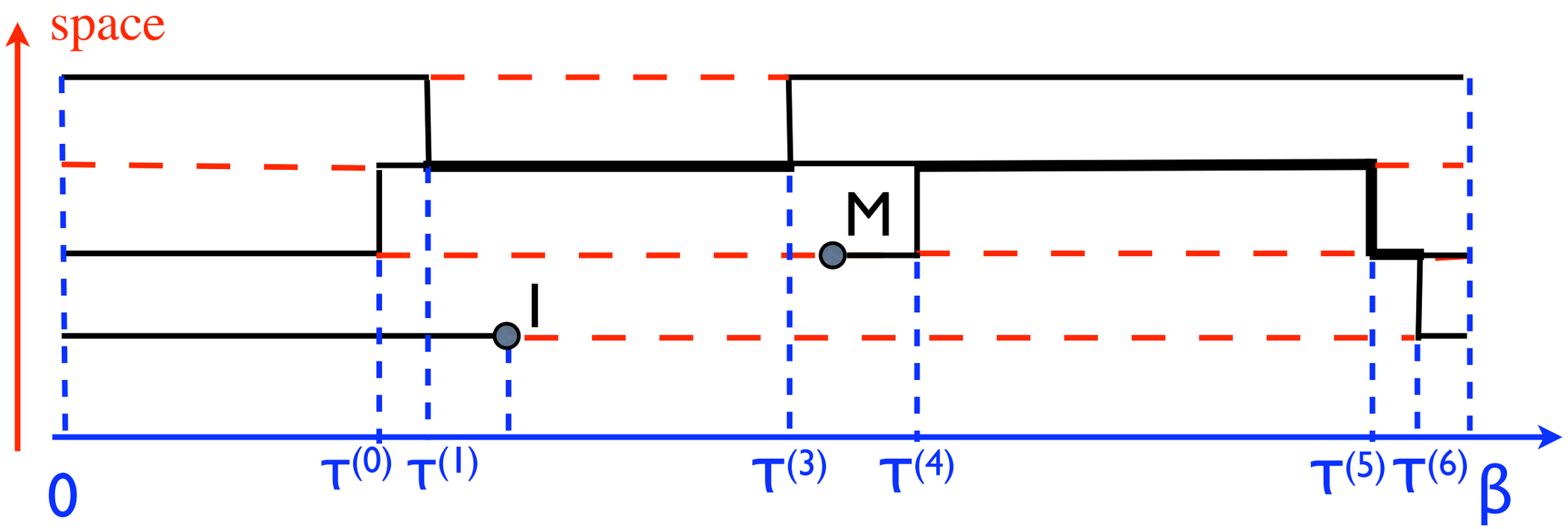
Slow convergence -- size limitation

Ergodicity problematic (*impossible to change* ***winding number*** *on large lattices*)

Also generally impossible to change number of particles (add entire WLs at once)



Ira and *Masha*, again...



- Generalize configuration space to allow for a single WL that ends at $\tau_{\rm I} < \beta$ and resumes at $\tau_{\rm M} < \beta$, with $\tau_{\rm I} < \tau_{\rm M}$

- Formally equivalent to sampling configurations from a probability distribution proportional to the ***single particle Matsubara Green function***

$$g(I-M,\tau_M-\tau_I) = \tfrac{1}{Z}\langle -\hat{\mathcal{T}}[\hat{a}^\dagger(M,\tau_M)\hat{a}(I,\tau_I)]\rangle$$

Worm engine

- Sampling of configuration occurs through **simple set of local updates** *all involving I or M* (other WLs are not touched)

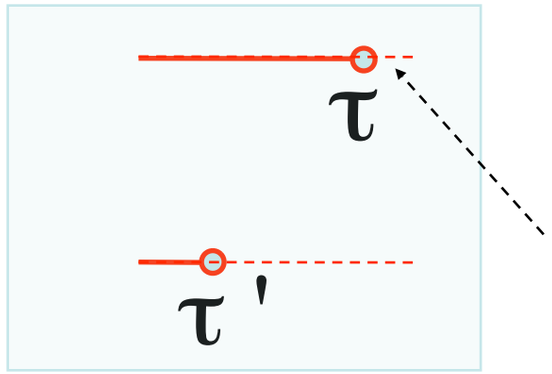
- Identify two *sectors*: *Z-sector* (no open line, or "Worm", i.e., *I* and *M* have reconnected); *G-sector* (one Worm is present)

- Measurements taken in the *G-sector* contribute to g, those taken in *Z-sector* contribute to physical observables

- According to the Metropolis prescription, acceptance ratios for all the moves are proportional to the ratio of the value of the probability distribution to be sampled at the *proposed* over the *current* configurations

Updates (complementary pairs)

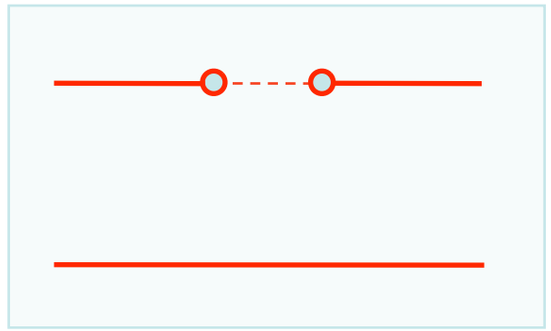
time shift:



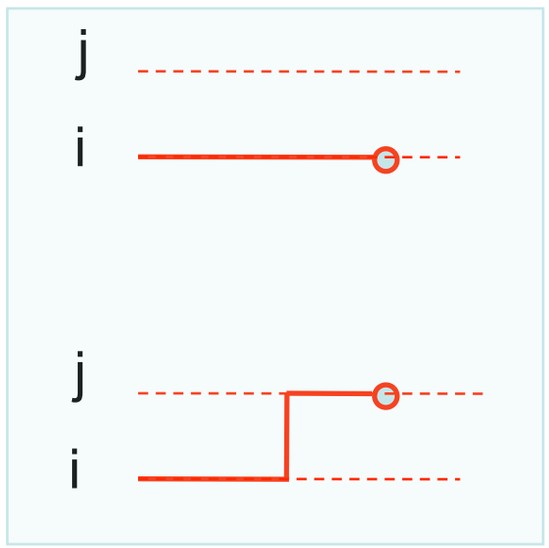
Ira or Masha

Insert/delete Ira and Masha:

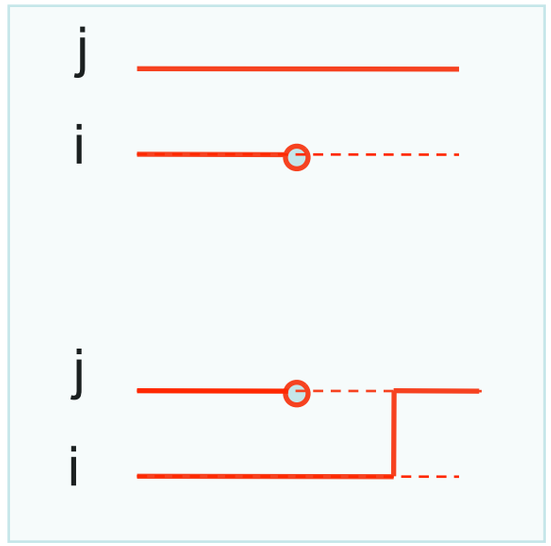
$Z \rightleftarrows G$



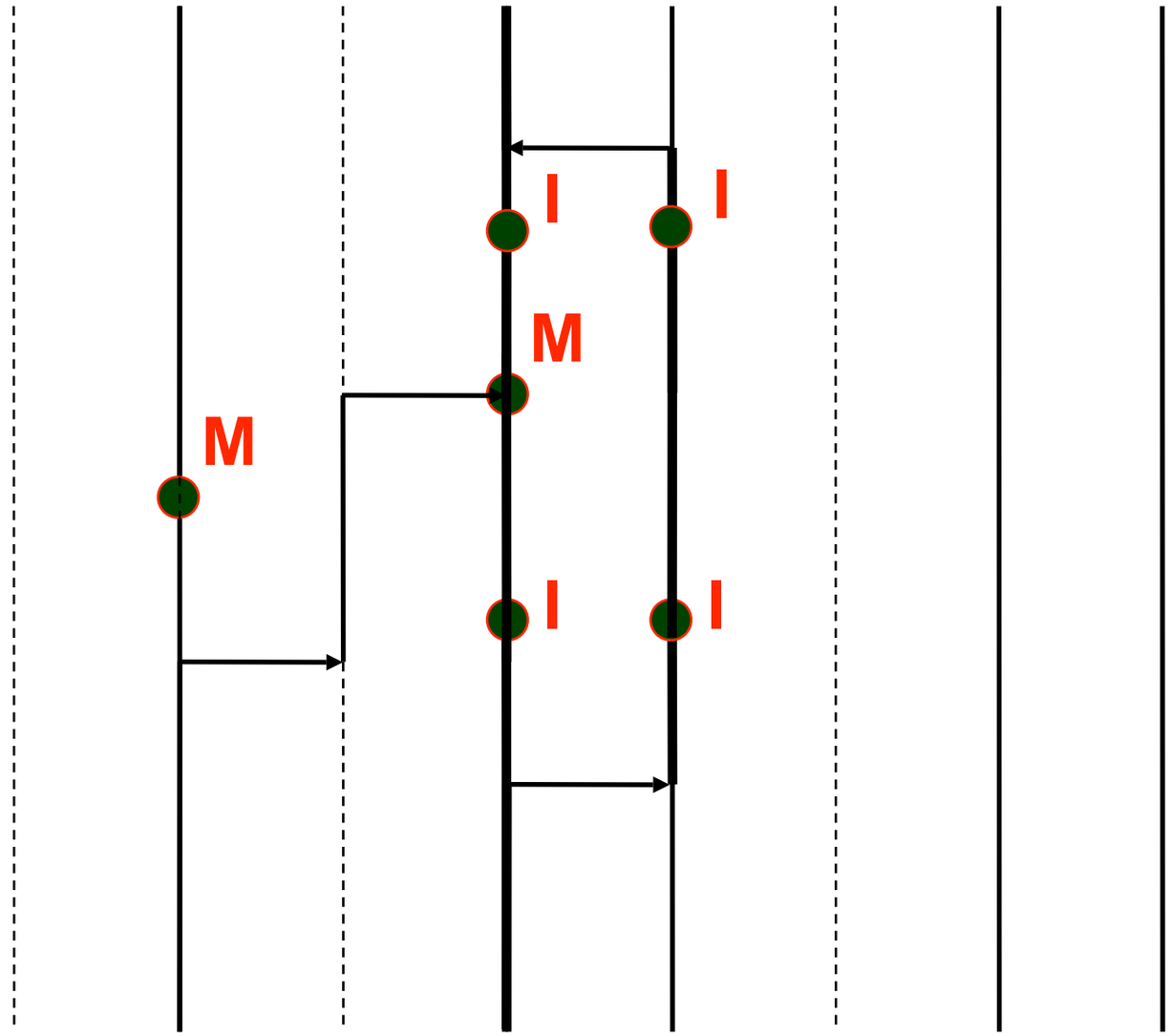
space shift ("particle"):



space shift ("hole" type):



- Two additional moves:
  - *Insert Worm at random lattice site* (*I*=*M*)
  - *Remove Worm when its length is zero*
- Together with the fact that *I* can advance past *M*, these two moves cause number of particles to fluctuate (**grand canonical ensemble**)
  - *Canonical implementations possible*


I
I
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I

Superfluid density and winding number

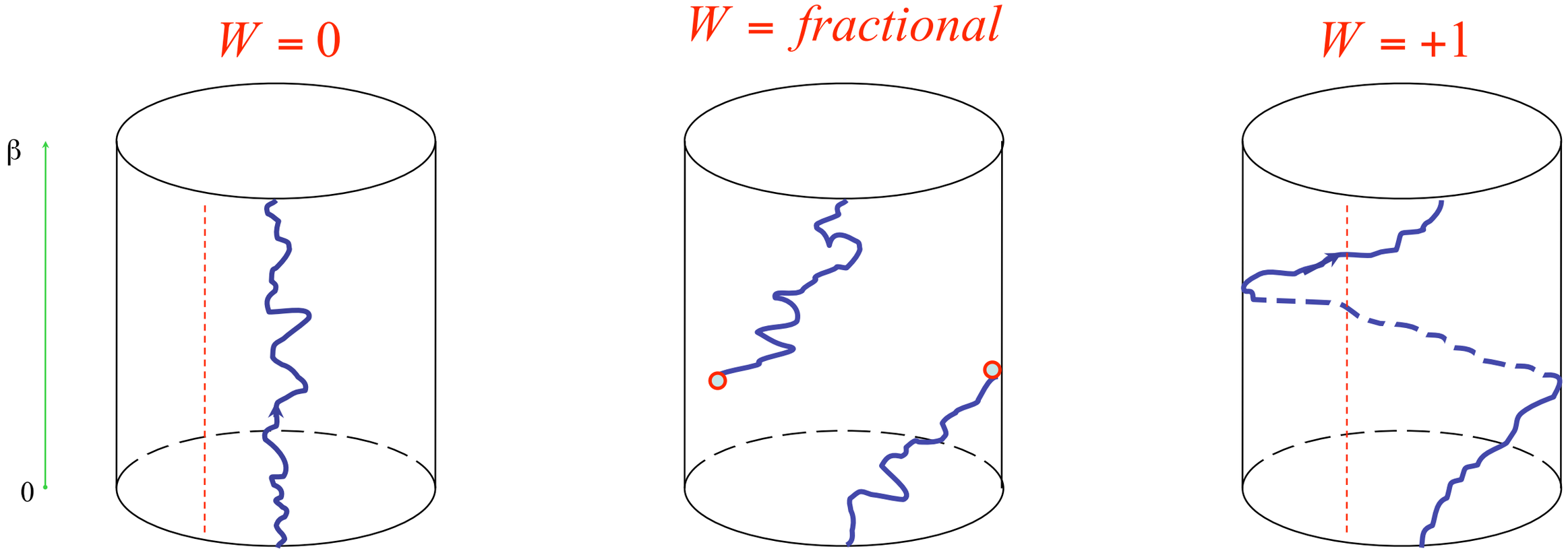
- Study of superfluid response of many-body system can be performed by numerical simulation with <u>periodic boundary conditions</u> via the computation of the **superfluid density** as a function of *T*

- Superfluid density related to *winding number W* (Pollock and Ceperley, 1987)

  counts number of times single-particle paths "wrap" around PBC

  *essentially **impossible** to create paths with non-zero winding without using Worms*

$$\rho_S \propto \langle W^2 \rangle$$



Remarks

- *No time discretization or "time step errors"*

- Lattice simulations with a number of particles of order 10^6 *standard* (no unusual computational resources required)

  Accurate finite-size scaling and determination of critical points possible

  Realistic *simulations of experimental systems realizable in Optical Lattices*

- Extension to long-range interactions possible through *Diagrammatic Monte Carlo* (continuum part)

- Also possible to work with more than one worm (pairing)

- *Grand Canonical*

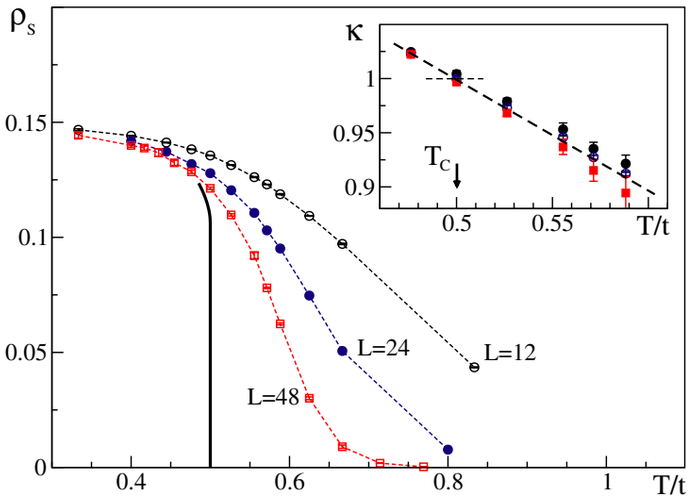
- Other extensions (*multicomponent systems, flavor-changing interactions etc*.) have been worked out

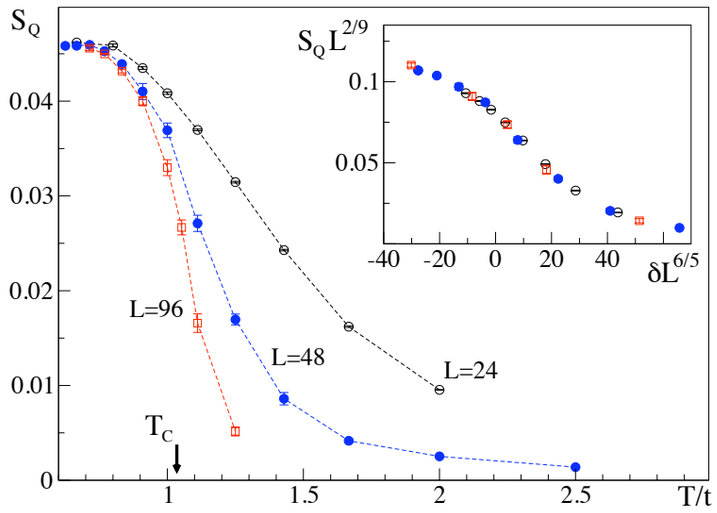
- Similar in spirit to Stochastic Series Expansion (SSE)

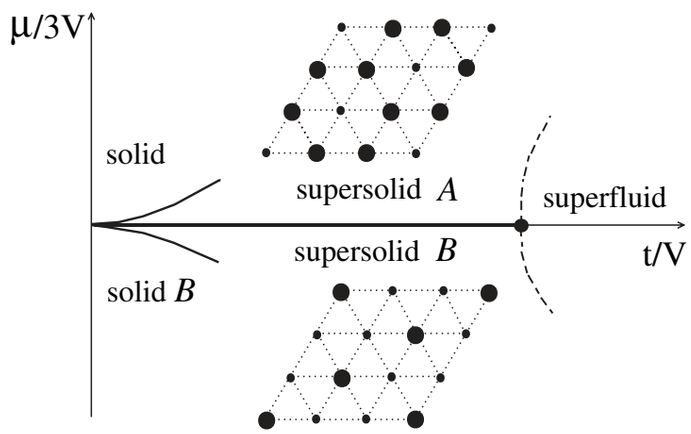
Application: Supersolid phase of hard core Hard core bosons on triangular lattice

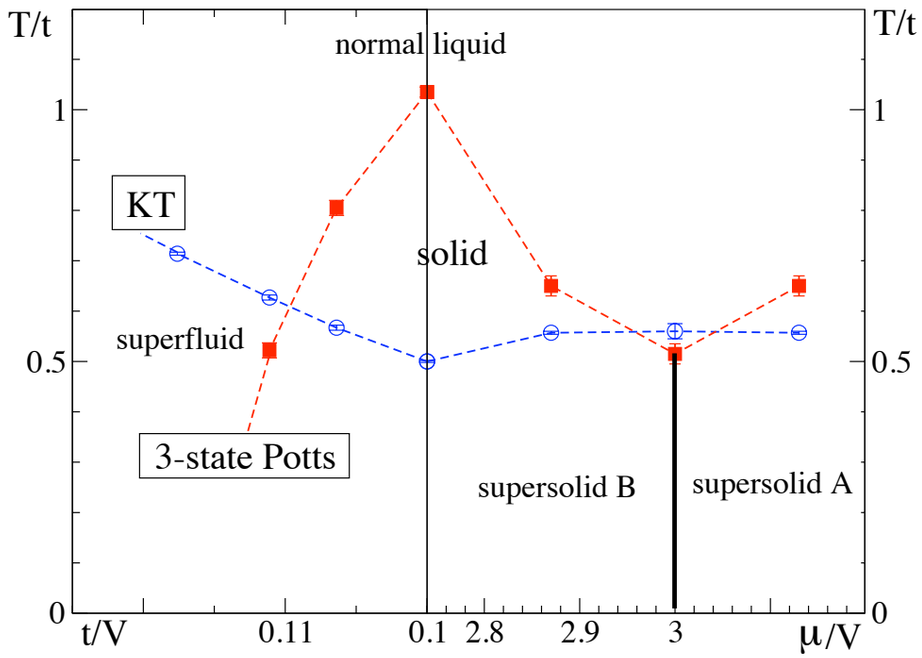
*MB and N.V. Prokof'ev, PRL **95**, 237204 (2005)*

Goal: search and characterization of *Supersolid phase*









Application: two-component lattice model with flavor-changing interaction

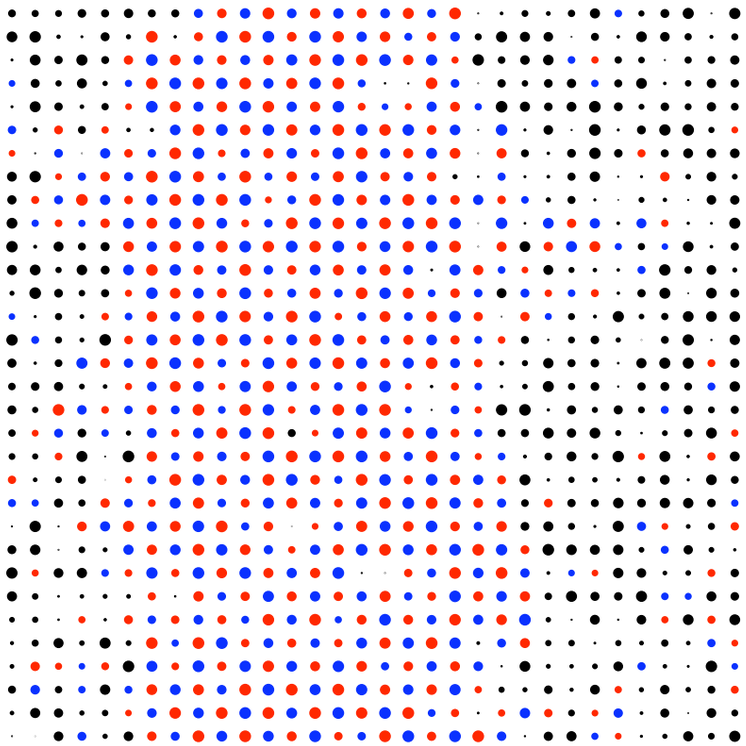
MB and N.V. Prokof'ev, PRB ***77****, 092502 (2008)*

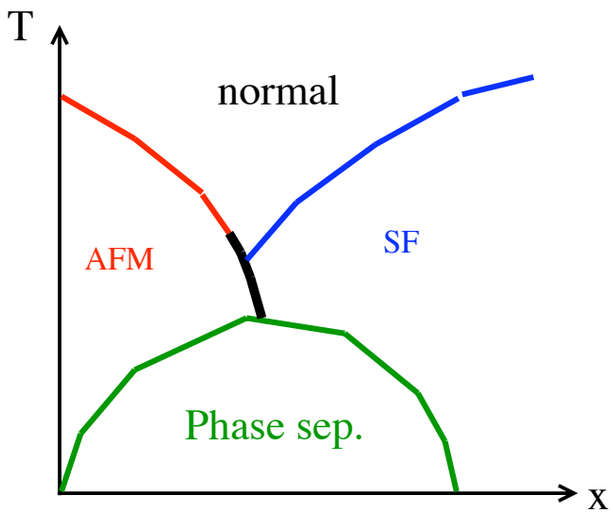
Boson *t-J* model

Hamiltonian of system of isotopic mixture of hard core bosons

Interaction allows mixing of species

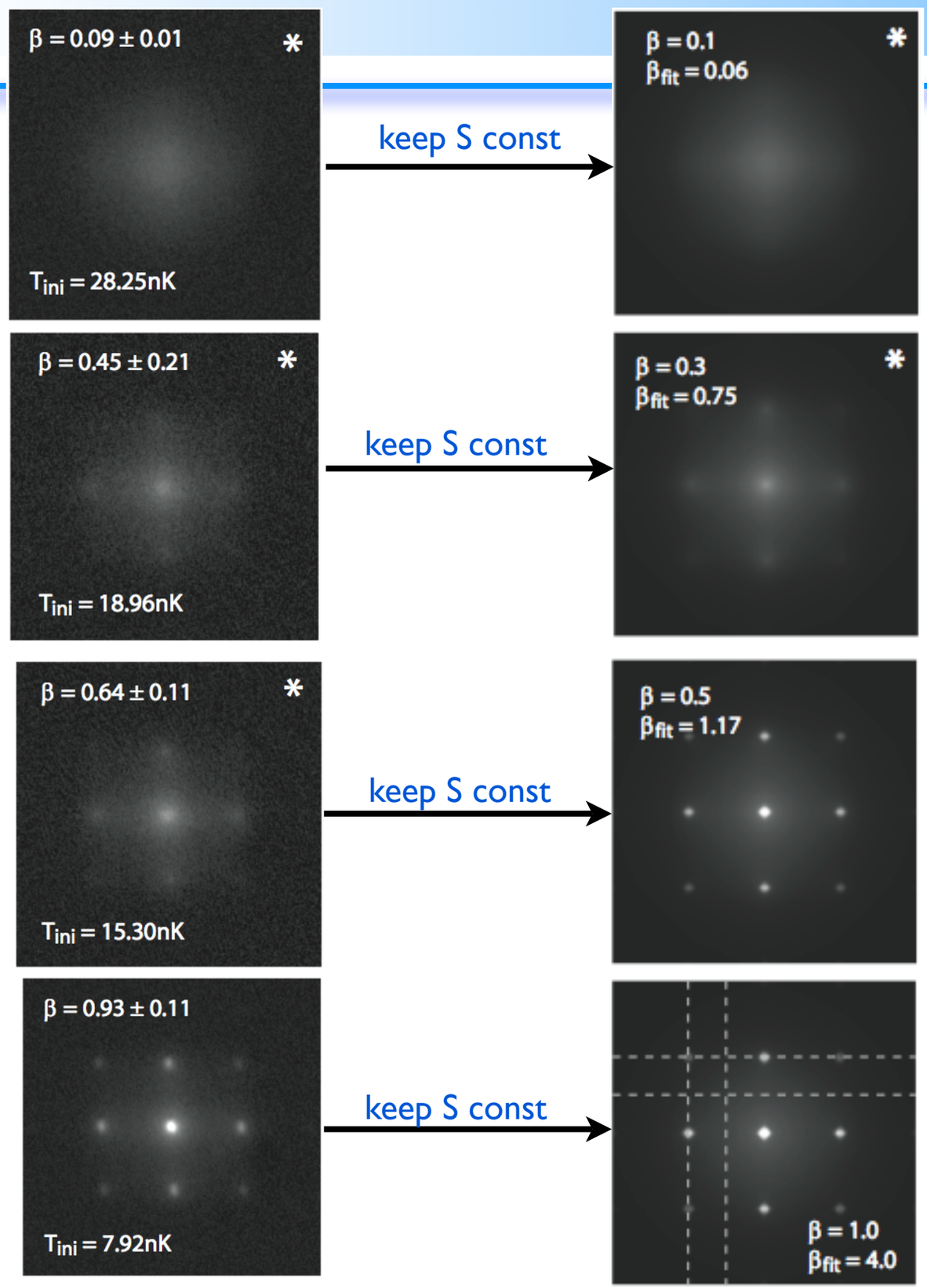
Rich phase diagram





small mismatch in temperature

L. Pollet, C. Kollath, K.Van Houcke and M.Troyer
ArXiv:0801.1887 (2008)



Tc

left column : experiment in Mainz; right column : simulations (or was it the other way around?) Temperature determined by keeping the entropy constant

QMC is too accurate, no noise from CCD, QMC can be made more noisy by running for a shorter period of time

End of first part

Next: continuum

but first: coffee (lot of it)

Continuous-space Worm Algorithm

- **Goal**: obtaining accurate thermodynamics for many-particle systems

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i\langle j} v(|\mathbf{r}_i - \mathbf{r}_j|)$$

- Feynman's **Space-time** formulation of quantum statistical mechanics
  Statistical Mechanics: A set of Lectures, Addison-Wesley (1972)

- **Thermal averages** of physical operators at finite temperature $T = 1/\beta$

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

$\rho(R,R,\beta) = \langle R|e^{-\beta\hat{K}}|R\rangle$ *many-body density matrix*
$|R\rangle \equiv |\mathbf{r}_1 ... \mathbf{r}_N\rangle$ system configuration
$\hat{K} = \hat{H} - \mu\hat{N}$ *grand canonical Hamiltonian*
$Z = \int dR\ \rho(R,R,\beta)$ grand partition function

Path Integrals

- **Same basic strategy** as on lattice:

  Many-body density matrix not known for any non-trivial many-body system

  Obtained through path integration (*A.-M. Tremblay's notes*)

$$Z = \int \mathcal{D}R(u)\, \exp\left[-S[R(u)]\right]$$

$(u\hbar \; imaginary \; time)$

Integration over all possible *continuous*, β-periodic many-particle paths with

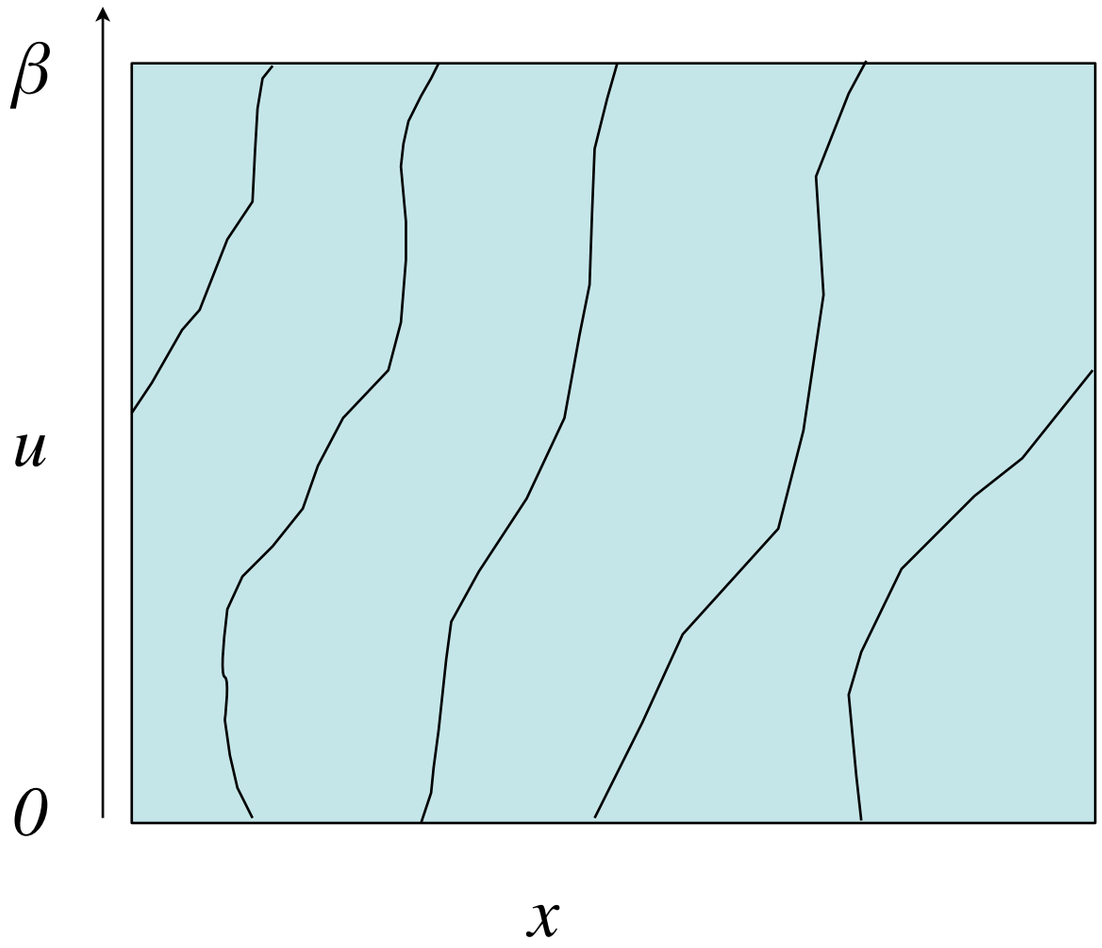
$$S[R(u)] = \int_0^\beta du \left\{ \sum_{i=1}^{N} \frac{m}{2\hbar^2} \left(\frac{d\mathbf{r}_i}{du} \right)^2 + V(R(u)) \right\} \quad \text{“}Euclidean\ Action\text{”}$$

- Action associated to path balance between *kinetic* (path curvature) and *potential* energy (depends on interactions) along path

  Smooth, straight paths have generally higher probability

  Paths of high potential energy have low probability

Quantum Statistics



Example
4 particles in 1d

Exchanges occur *only* through PBC

- Paths are *β-periodic*, i.e., $R(\beta)=R(0)$
  - *However, individual particle positions can undergo exchanges*
  - ***Crucial** ingredient of the physics of ensembles of indistinguishable particles*
  - *Underlie phenomena such as BEC and Superfluidity*

- Ascribing *physical content* to paths is tempting but *dangerous*
  - *Least action path: solution of Newton's EOM with **reversed** potential*
  - ***However**: imaginary-time formalism useful for studying tunneling* (***instanton***)

Monte Carlo strategy

- Sample many-particle paths $R(u)$ through configuration space, based on the probability distribution proportional to $\exp[-S(R(u))]$ -- *Metropolis algorithm*

- Evaluate thermal expectation values as *statistical* averages of quantities of interest computed along paths

- **First important difference** with lattice calculation:

  No continuous time (*yet*)

  Action integral must be *discretized* → *time step error inevitable*

  Reason: no expansion for kinetic energy exists in the continuum (no *kinks*)

Discretization: $R(u) \equiv \{R_0, R_1, ..., R_{M-1}\}$, $R_M \equiv PR_0$
(P *permutation of particle labels*)
$M\tau = \beta$, τ is the *time step*
Simplest approximate action (we can do better but it is not needed now):

$$S[R(u)] \approx \sum_{i=1}^{N} \sum_{l=0}^{P-1} \frac{m(\mathbf{r}_{il} - \mathbf{r}_{il+1})^2}{2\tau\hbar^2} + \tau \sum_{l} V(R_l)$$

(*Note*: in the absence of interaction any discretized form is *exact*)

Discrete Action

- Probability with which a *discrete* path $R(u)$ is sampled

$$P \propto \exp\Big[-S[R(u)]\Big] = \prod_{i=1}^{N} \prod_{l=0}^{M-1} \rho_\circ(\mathbf{r}_{il}, \mathbf{r}_{il+1}, \tau) \times \prod_{l=0}^{M-1} e^{-\tau V(R_l)}$$

where

$$\rho_\circ(\mathbf{r}, \mathbf{r}', \tau) = \Big(2\pi\hbar^2\tau/m\Big)^{-1/d} \exp\Big[-\frac{m(\mathbf{r}-\mathbf{r}')^2}{2\hbar^2\tau}\Big]$$

is the density matrix of a *free particle*, and

$$V(R) = U(R, \tau) - \mu N$$

In the simplest version, U is the *total potential energy*, does not depend on τ
(In some approximations, it does)

Path Integral Monte Carlo (PIMC)

- *In principle exact* numerical tool to compute thermodynamics of Bose systems
  D. Ceperley, Rev. Mod. Phys. ***67****, 295 (1995)*

  No adjustable parameter, approximation, a priori input

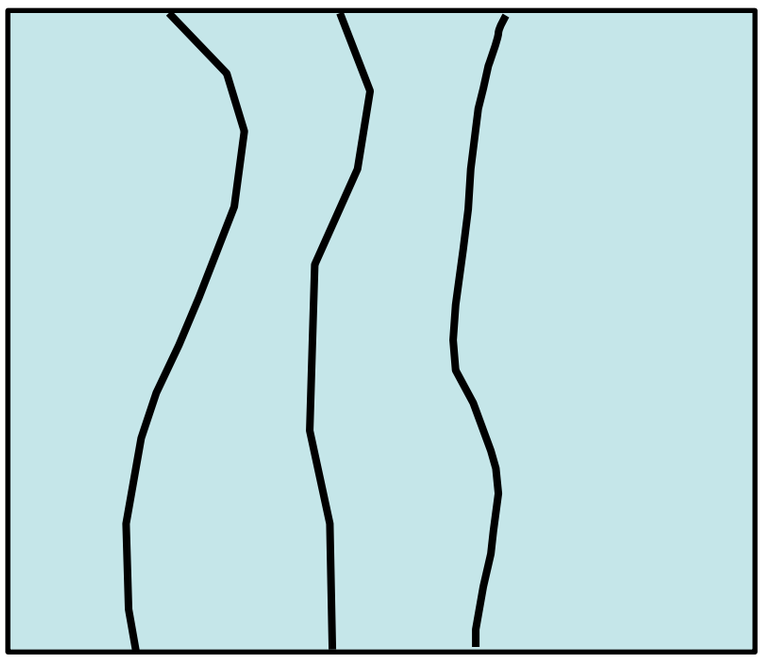
  Works directly on microscopic Hamiltonian

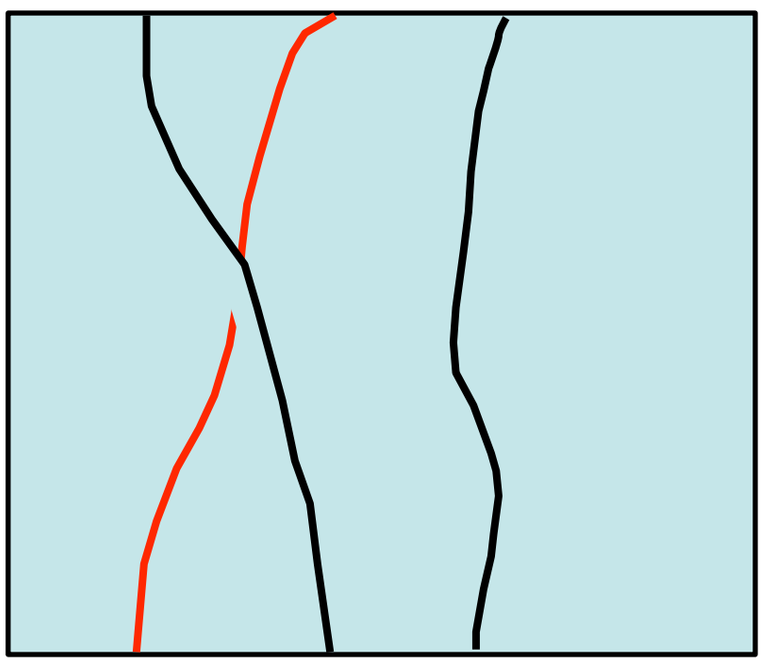
  Direct computation of $\varrho_s(T)$ (superfluid density)

- **Sampling**

  Occurs through elementary move that modifies portions of single-particle paths

  Permutations are sampled by *explicit construction of permutation cycles*





PIMC (*cont'd*)

- **Sampling issues**

  In the presence of *repulsive*, *hard core potentials*, any such sampling of permutations is bound to become inefficient (*high likelihood of rejection*)

  Avoid hard cores through periodic boundary conditions -- yields a *vanishing* contribution

- **Problems**:

  Occurrence of *nonzero* winding requires *macroscopic* permutation cycles (length ~ $N^{1/d}$)

  Effort required to sample macroscopic permutation cycles scales **exponentially** with N

  No simulation of superfluid transition in bulk systems with more than ~100 particles

  Extrapolation to *thermodynamic limit* ($N \to \infty$) often **problematic**

  Ambiguous interpretation of results (*no* superfluidity *or* ergodicity problem ?)

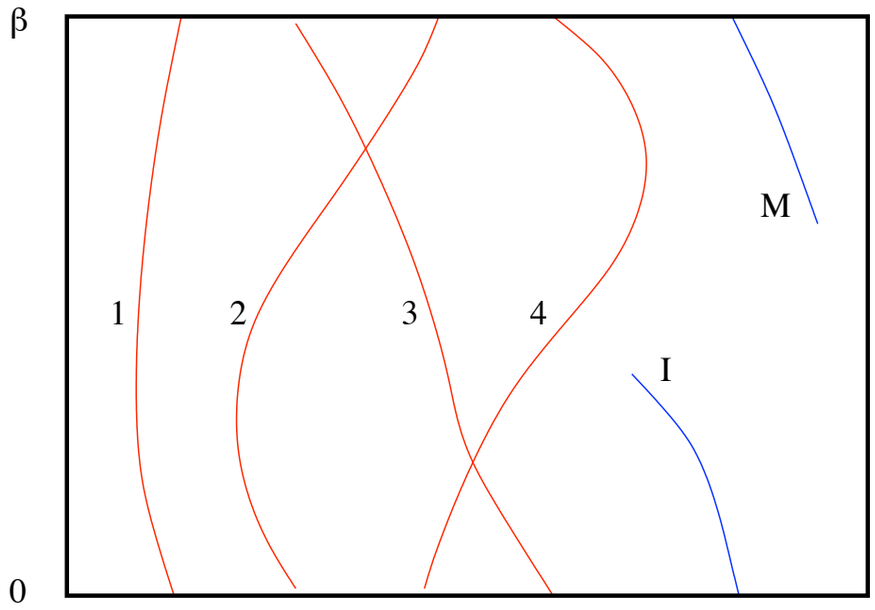
- **Size matters**:

  Some problems cannot even be properly *formulated* if only a few particles can be simulated (example: superfluid layer in solid helium at *grain boundary*)

  Even for *finite-size systems*, however (e.g., quantum droplets), efficient sampling of permutations can be *crucial* to capture the physics

Ira and Masha go to the continuum

MB, N.V. Prokof'ev and B.V. Svistunov, PRL ***96****, 070601 (2006)*
MB, N.V. Prokof'ev and B.V. Svistunov, PRE ***74****, 036701 (2006)*



- *Generalize configuration space, from that of the partition function to that of the* **Matsubara Green function**

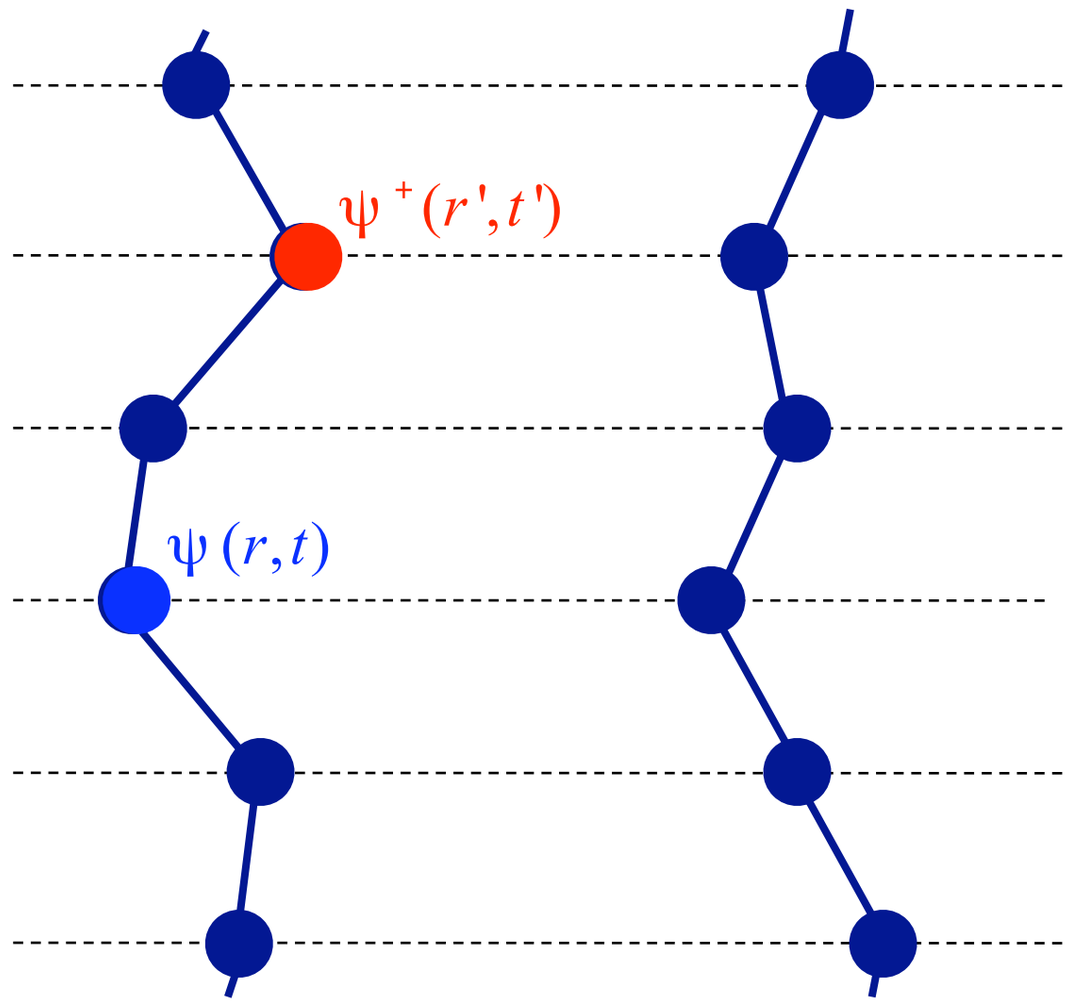
$$G(\mathbf{r}_1, \mathbf{r}_2, t) = \frac{g(\mathbf{r}_1, \mathbf{r}_2, t)}{Z} = -\langle \hat{\mathcal{T}}[\hat{\psi}(\mathbf{r}_1, t)\ \hat{\psi}^\dagger(\mathbf{r}_2, 0)]\rangle$$

- One open path with two dangling ends (*worm*)

  Analogously to lattice methodology, Z- and G-sectors are identified

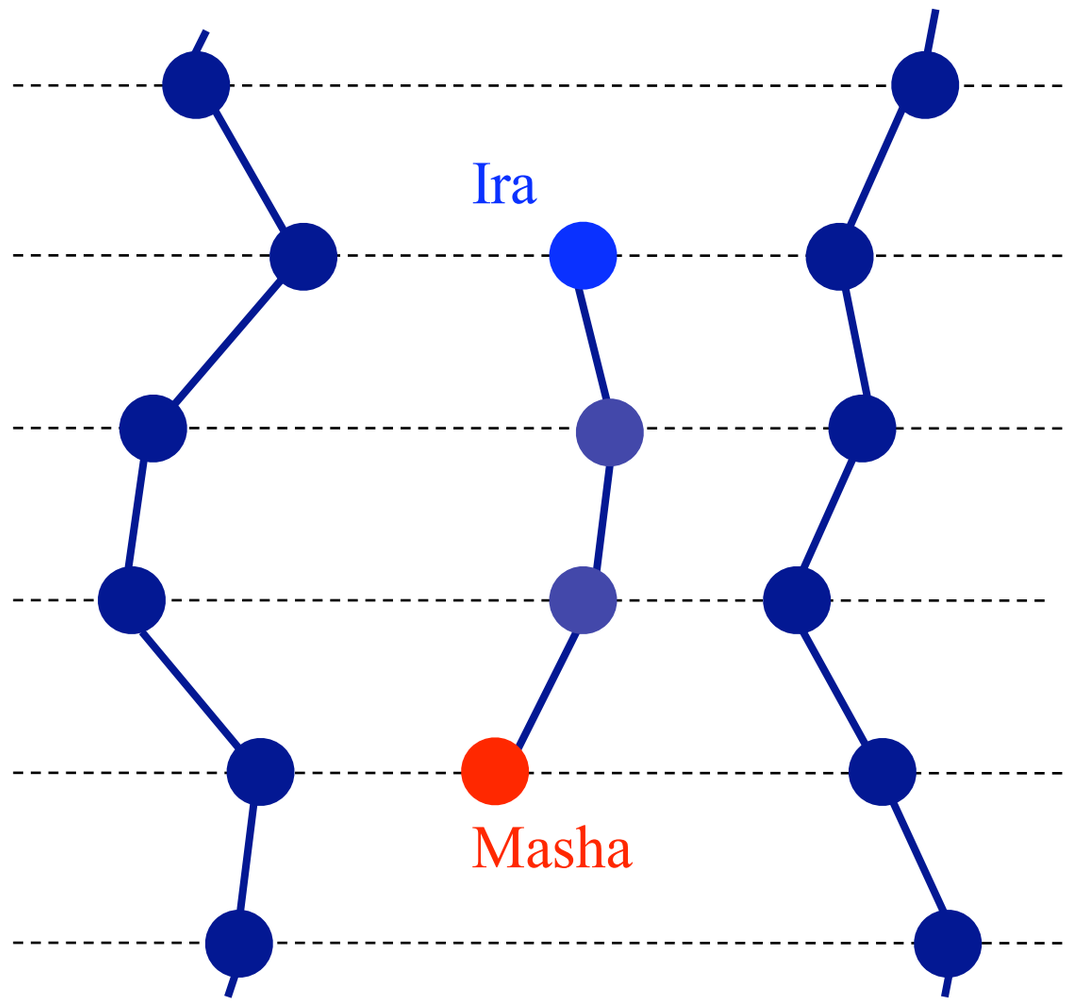
  Sampling of many-particle paths occurs through simple set of complementary moves, only involving the worm

G

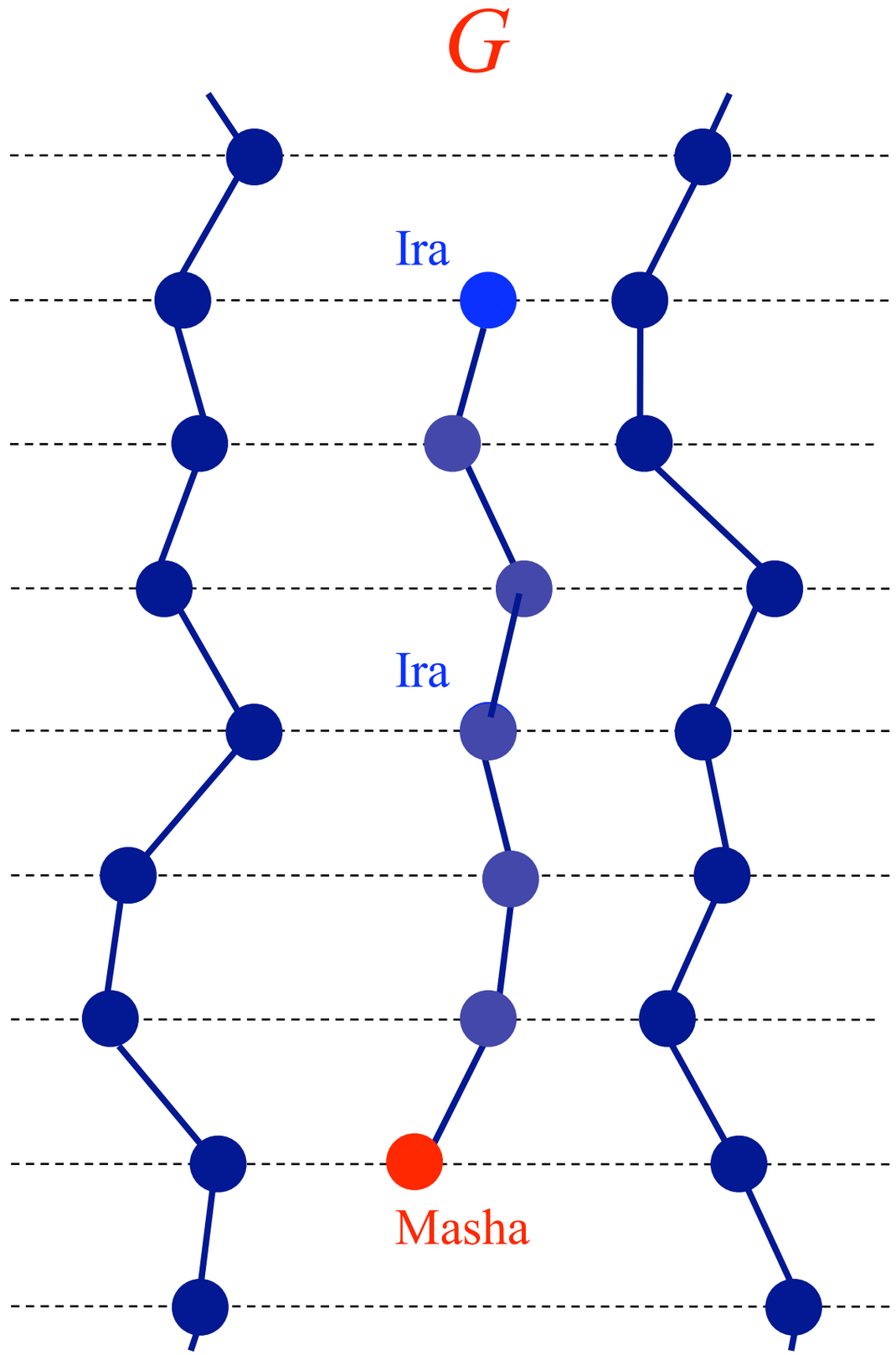


(open/close update)

G

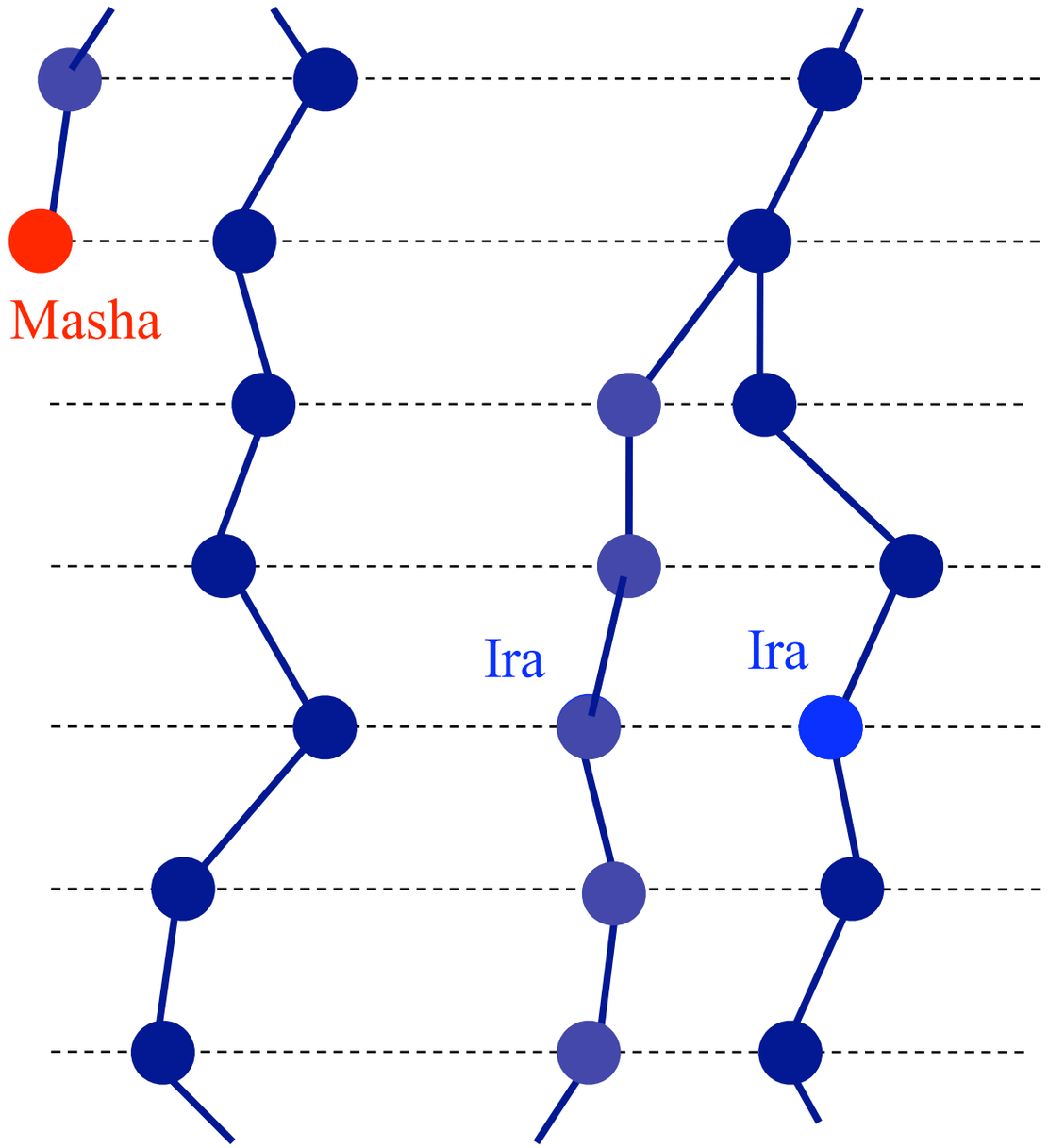


(insert/remove update)



(advance/recede update)

G



swap update (self-complementary)

Remarks

- Configurations with open WL contribute to the Matsubara Green function
  All non-trivial topological path modifications occur in G-sector

- *Swap* moves enjoy relatively high acceptance, even with hard core potentials

- When *Ira* and *Masha* reconnect, a *Z*-sector configuration is obtained, and most observables computed -- large permutation cycles *automatically occur*

- Reconnection is *one of the attempted moves* (no need to wait for it !)

- Number of particles fluctuate (*again, canonical implementations possible*)

Can *I* and *M* get "stuck" far away from each other ?

- Statistics of spatial distances between *I* and *M* given by *one-body density matrix*
  Decaying exponentially in a non-BEC
  Going to a constant in a BEC (but high acceptance probability of reconnection)

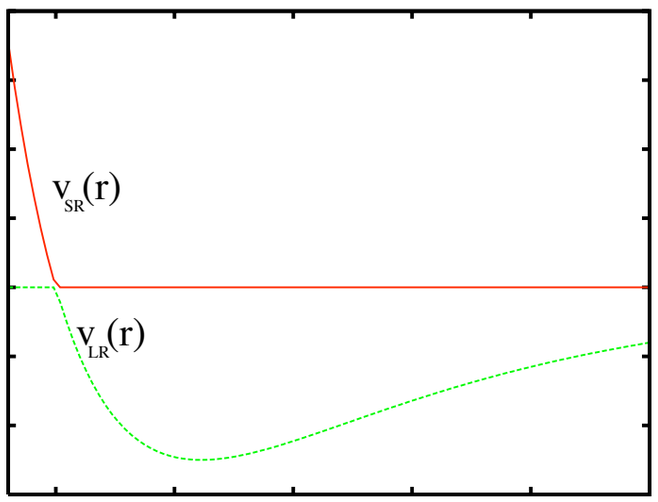
Diagrammatic Monte Carlo: a trick to deal with long-range interactions

- In MC, updates require the calculation of $\exp\left[-\sum_{j\neq i} v(r_{ij})\right]$
  (*omit β for simplicity for a few slides*)
  Scales as the number of particles
  For rapidly decaying potentials, much time spent computing small quantities

- Pair potential with *repulsive core* and *long-range attractive tail*
  e.g., Lennard-Jones

$$v(r) = v_{HC}(r) - v_{LR}(r)$$

both functions are non-negative



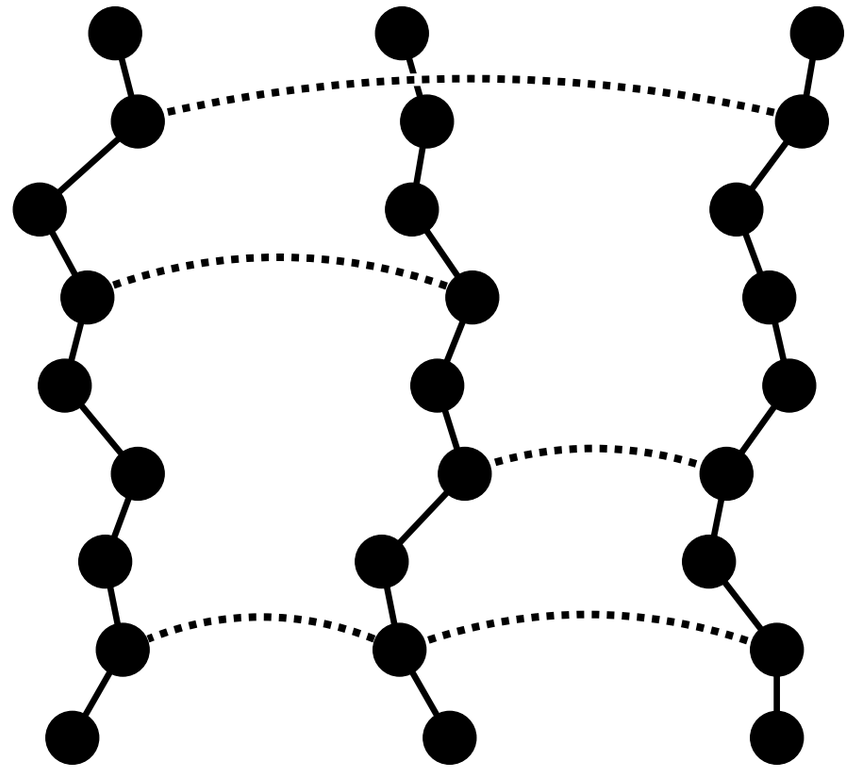
Diagrammatic Monte Carlo (cont'd)

- Trick: treat *short-range* part explicitly, *long-range* one is sampled

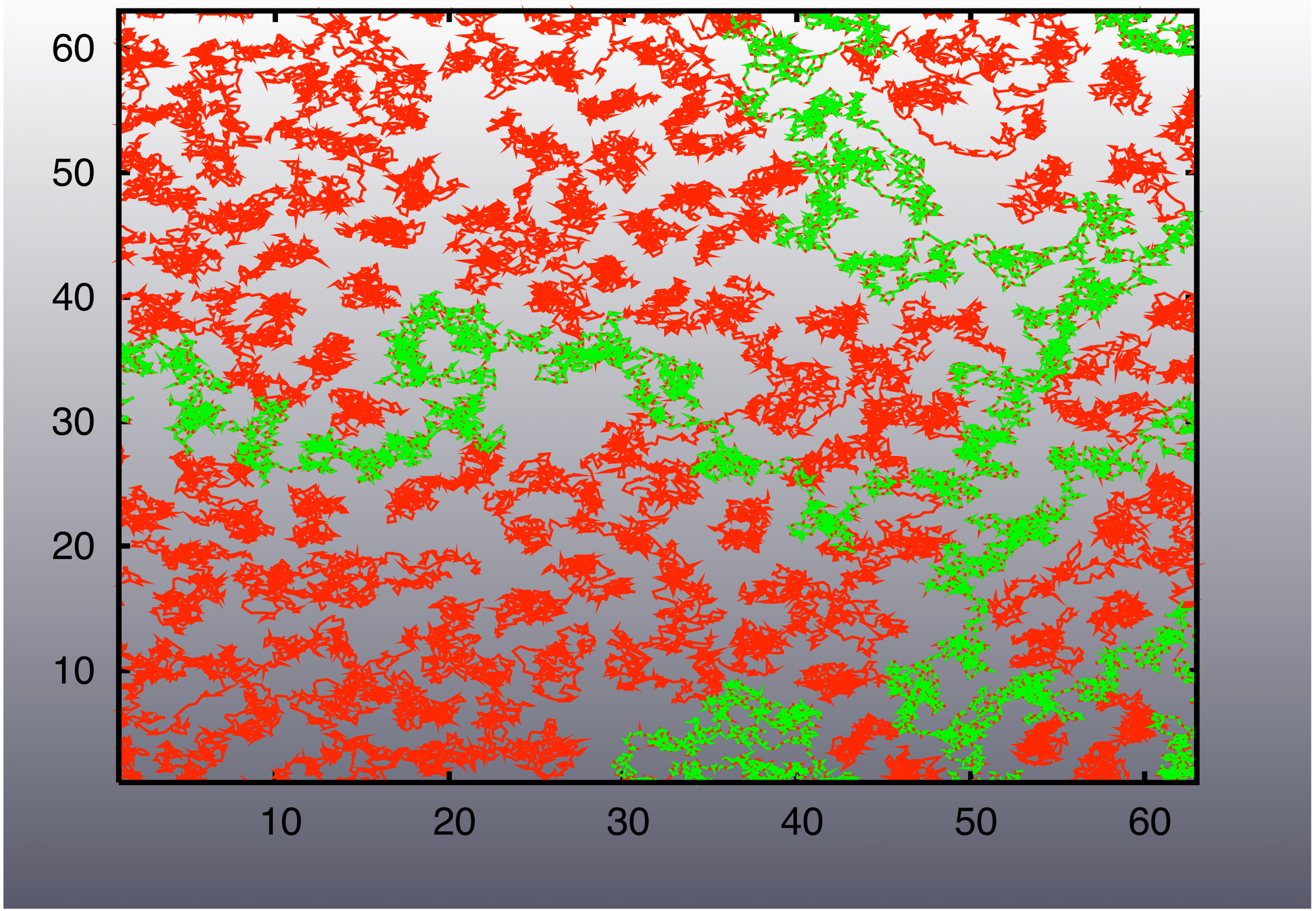
- Simply re-write $\exp\left[v_{LR}(r)\right] = \left[1 + \left(\exp[v_{LR}(r)] - 1\right)\right]$

*Sum of **positive** contributions*
*Can be treated **probabilistically***

*Each particle interacts on average with **few** nearest neighbors and **few** linked distant particles. Links are created and removed dynamically*
Overall scaling is <u>linear</u> with N

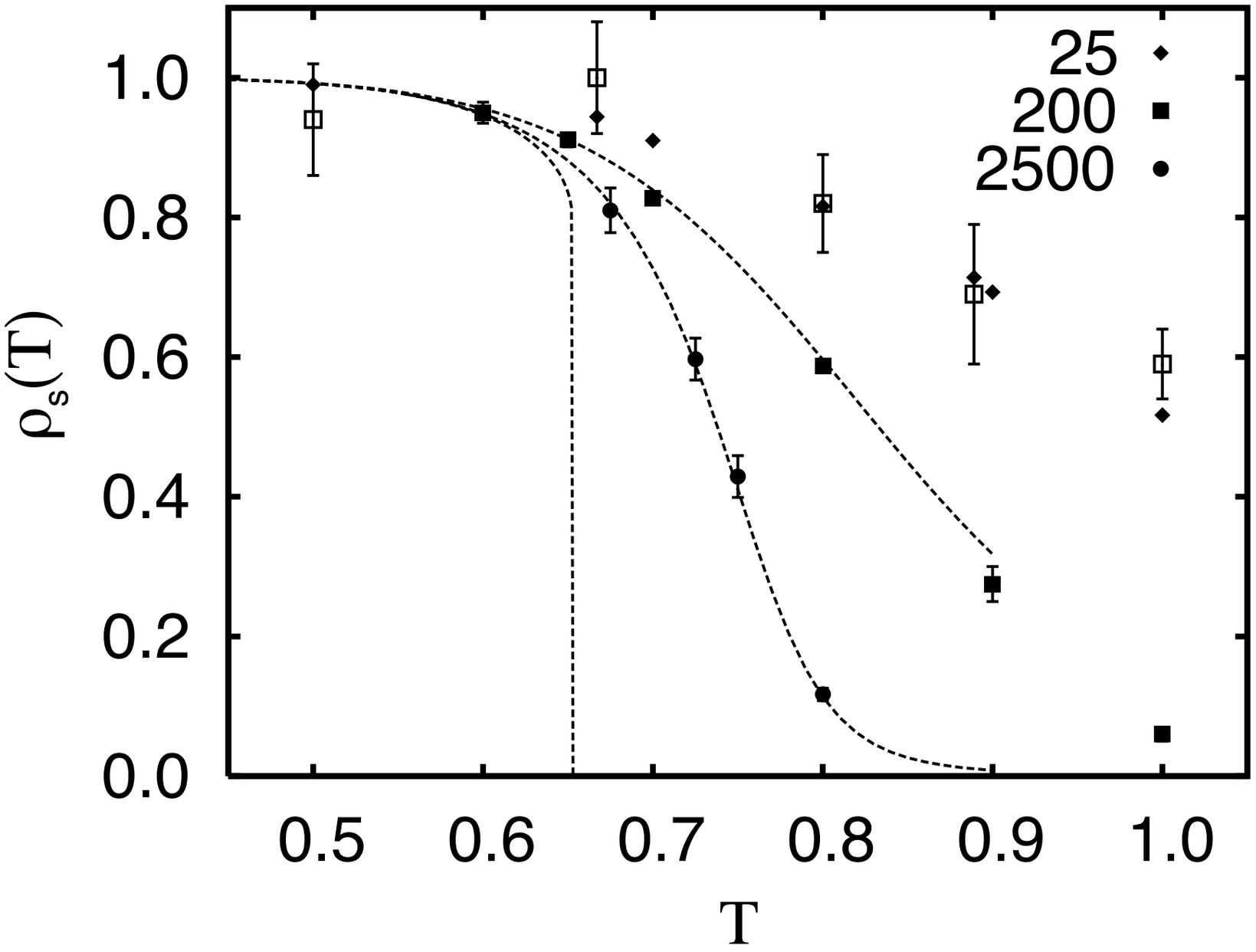


- Switch "on" and "off" interaction between pairs of particles
  interaction switched on with probability proportional to $(\exp[v_{LR}(r)] - 1)$
  with probability proportional to 1, *particles do **not** interact*



^{4}He in two dimensions, T=0.6 K

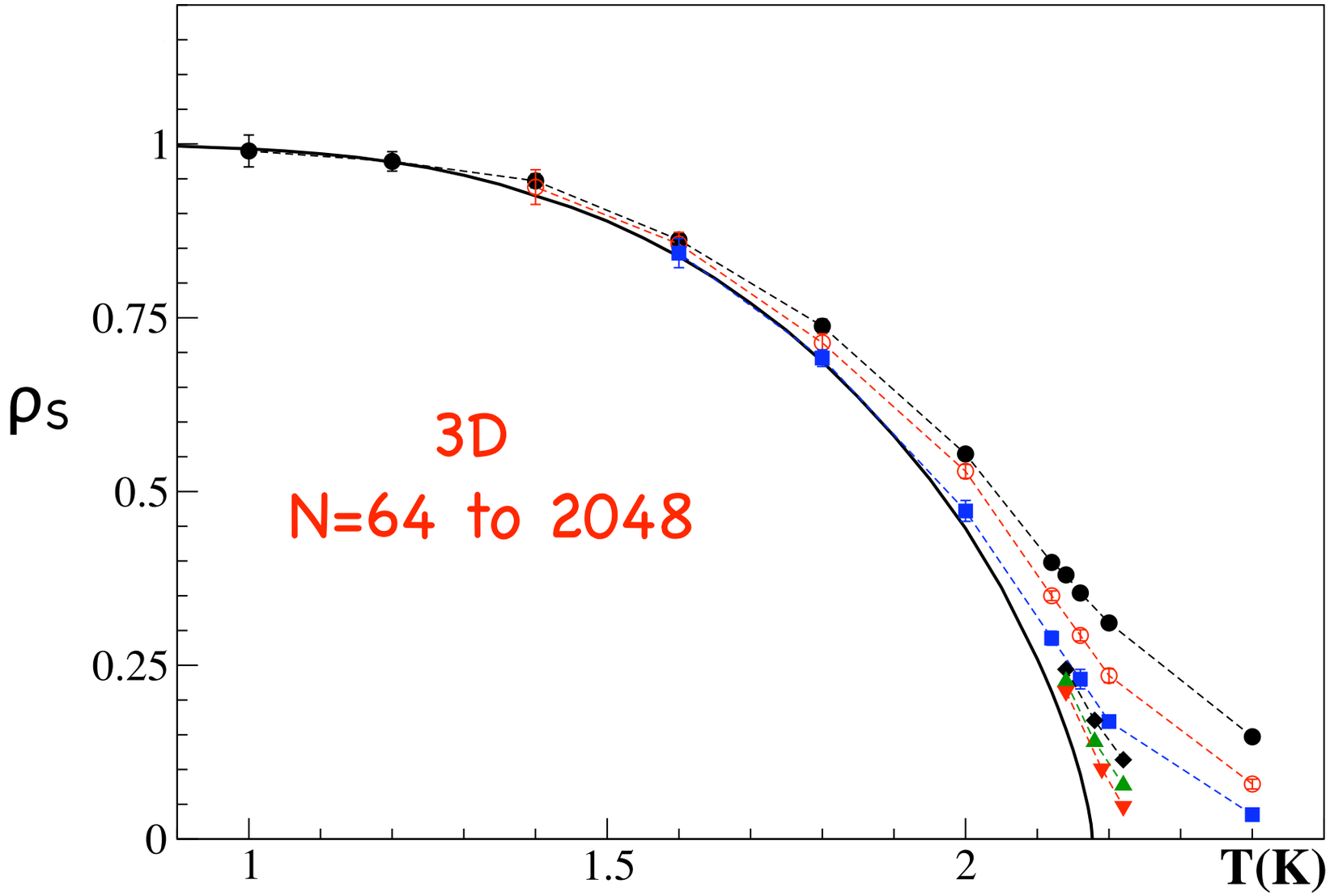
Application: Superfluid transition in ^{4}He



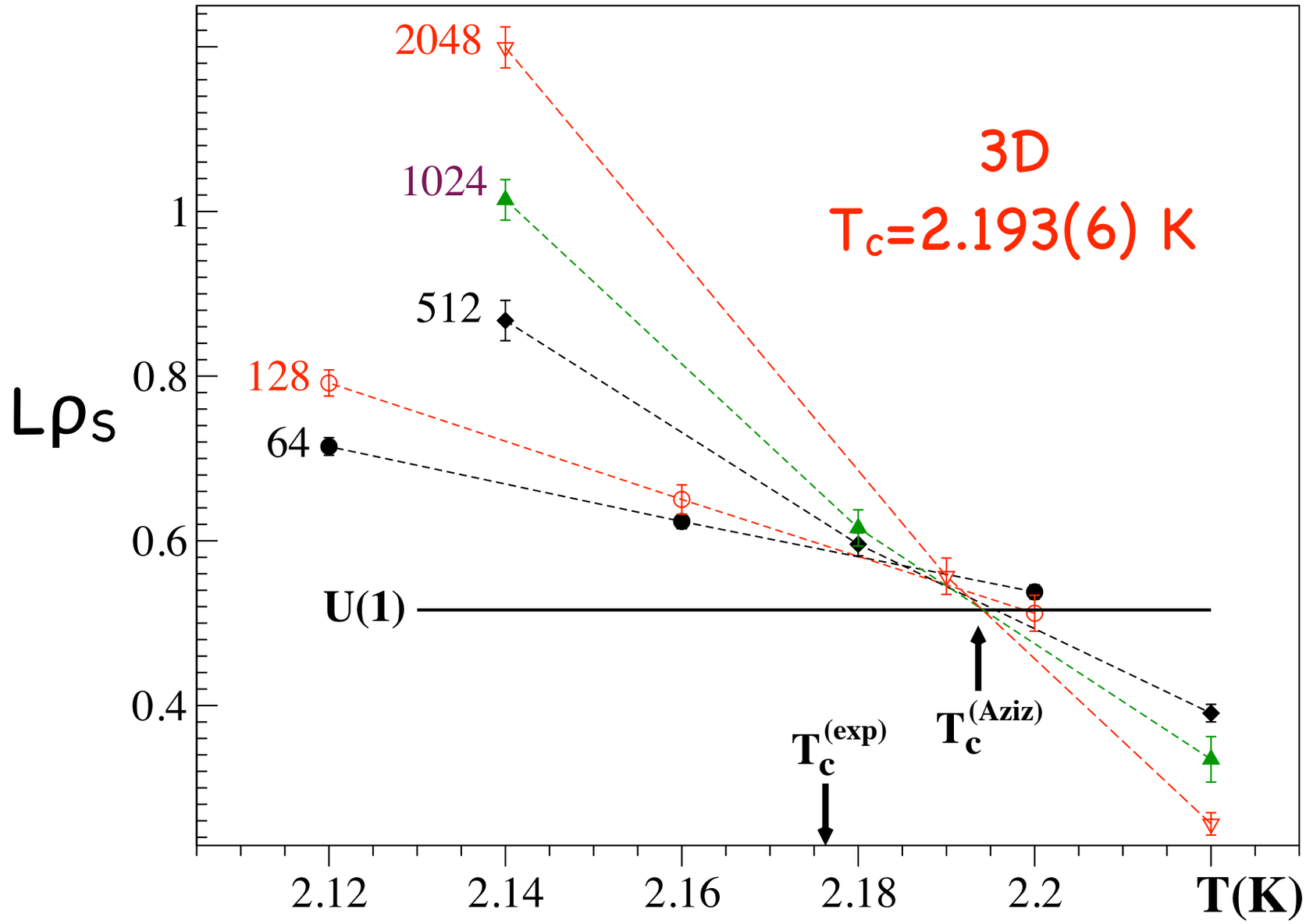
2D

T_c = 0.653 (10) K

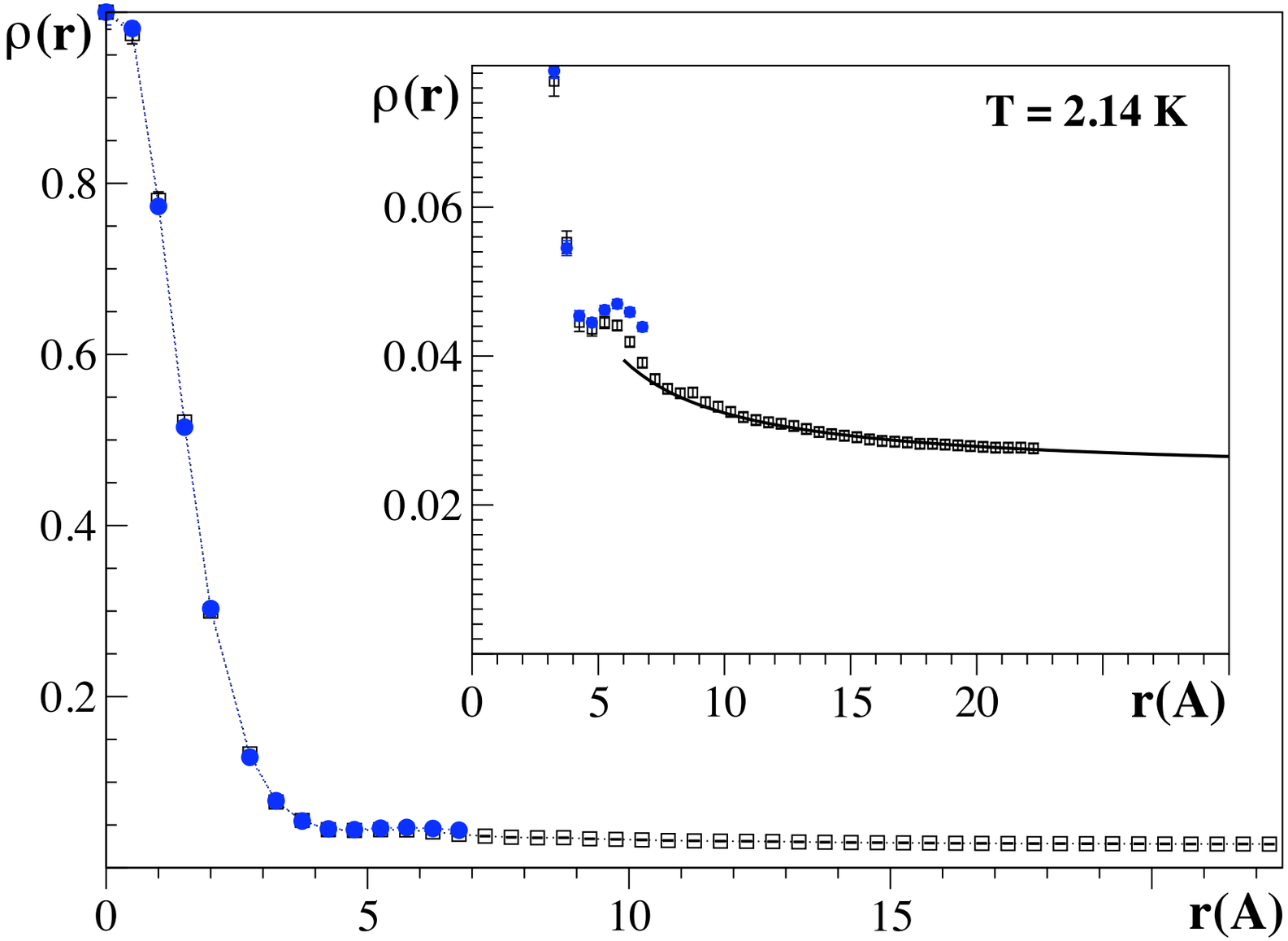
Superfluid transition in ^{4}He (cont'd)



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

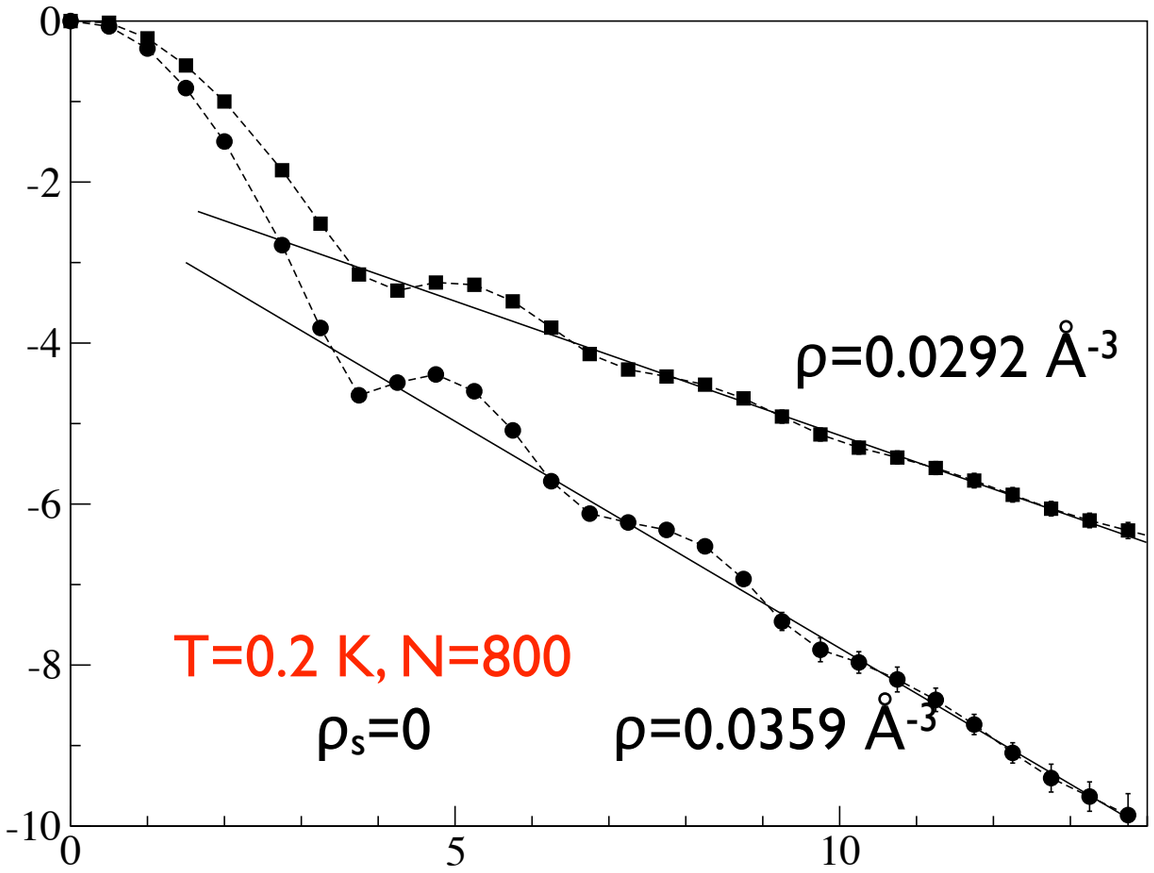


Superfluid transition in ^{4}He (cont'd)



Application: Search for BEC in solid ^{4}He

MB, N. Prokof'ev and B. Svistunov, Phys. Rev. Lett. **96**, 105301 (2006)



Exponential decay of one-body density matrix seen at low T, large r for perfect hcp ^{4}He crystal

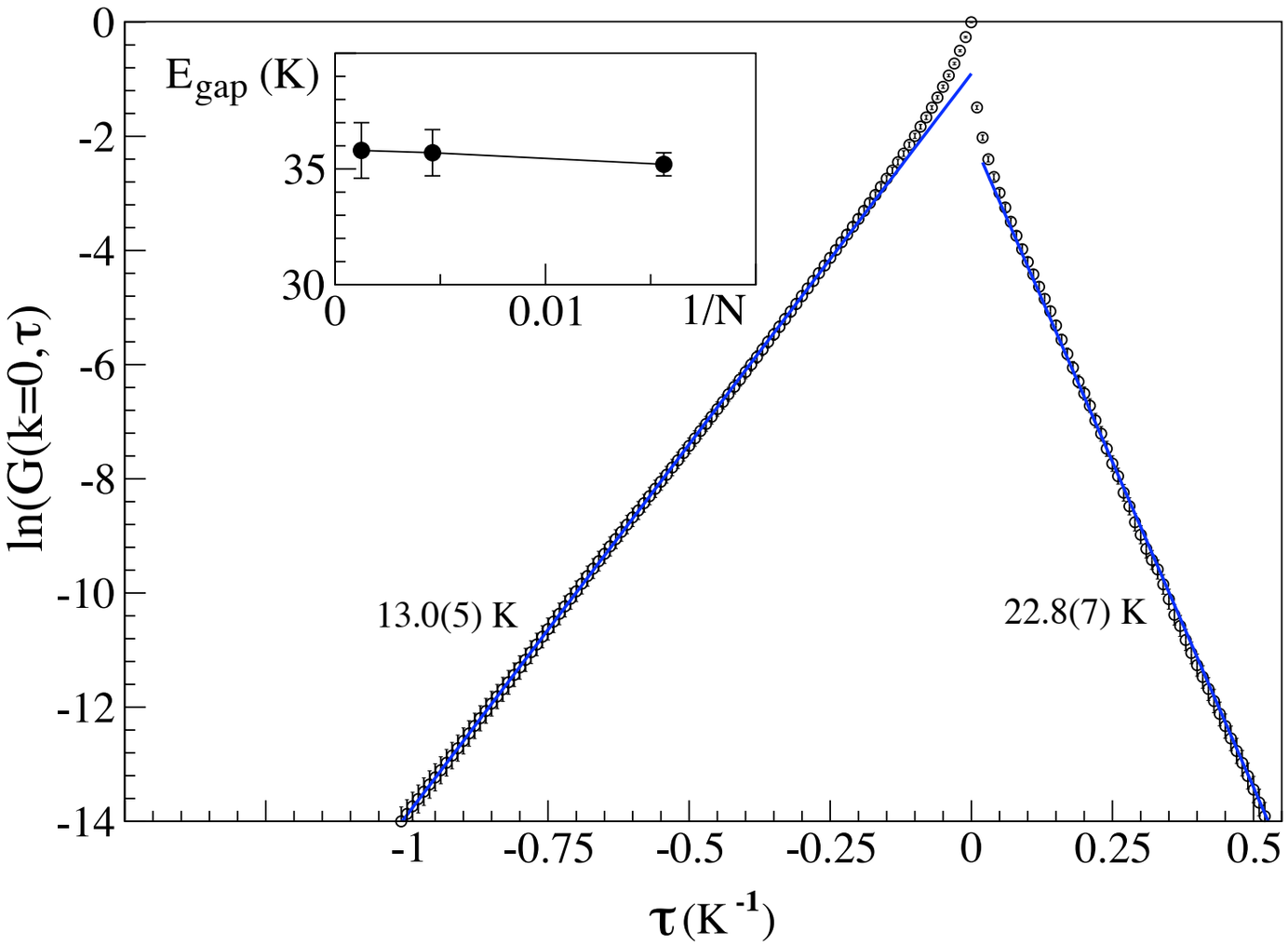
Absence of BEC
Independent of pressure

Absence of SF
No long permutation cycles

Application: vacancies in solid ^{4}He

MB, A. Kuklov, L. Pollet, N. Prokof'ev, B. Svistunov and M. Troyer, PRL **97**, 080401 (2006)

Activation energy for vacancies and interstitials can be obtained straightforwardly from **exponential decay** of Matsubara Green function



$G(\mathbf{k}=0,\tau) \sim e^{-|\tau|\Delta}$, long τ

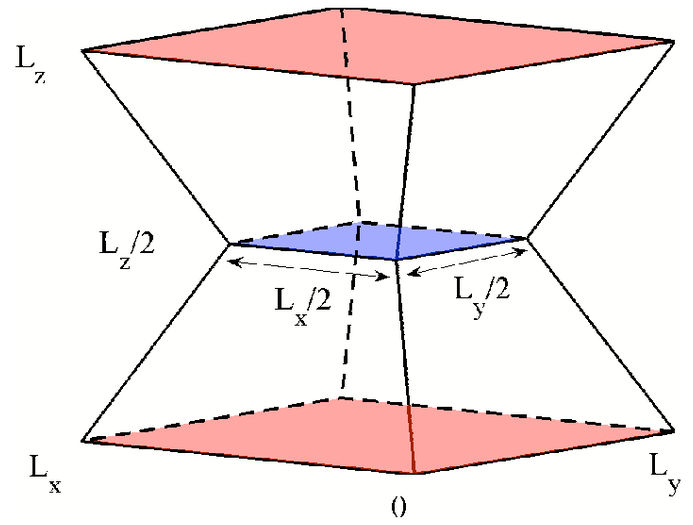
too large for thermal activation at $T < 1$ K

Consistent with **no** vacancies (nor interstitials) in solid He

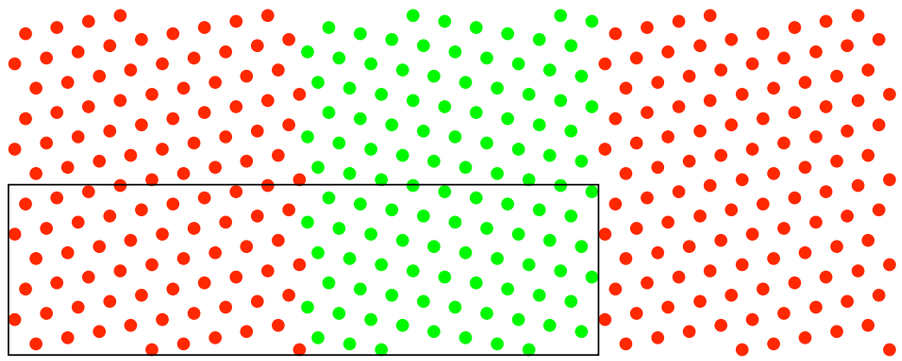
Application: superfluidity at grain boundaries in solid ^{4}He

L. Pollet, MB, A. Kuklov, N. Prokof'ev, B. Svistunov and M. Troyer, Phys. Rev. Lett. ***98****, 135301 (2007).*

By direct simulation, evidence is obtained that a grain boundary in direct contact with a superfluid at the melting pressure is **thermodynamically stable**.



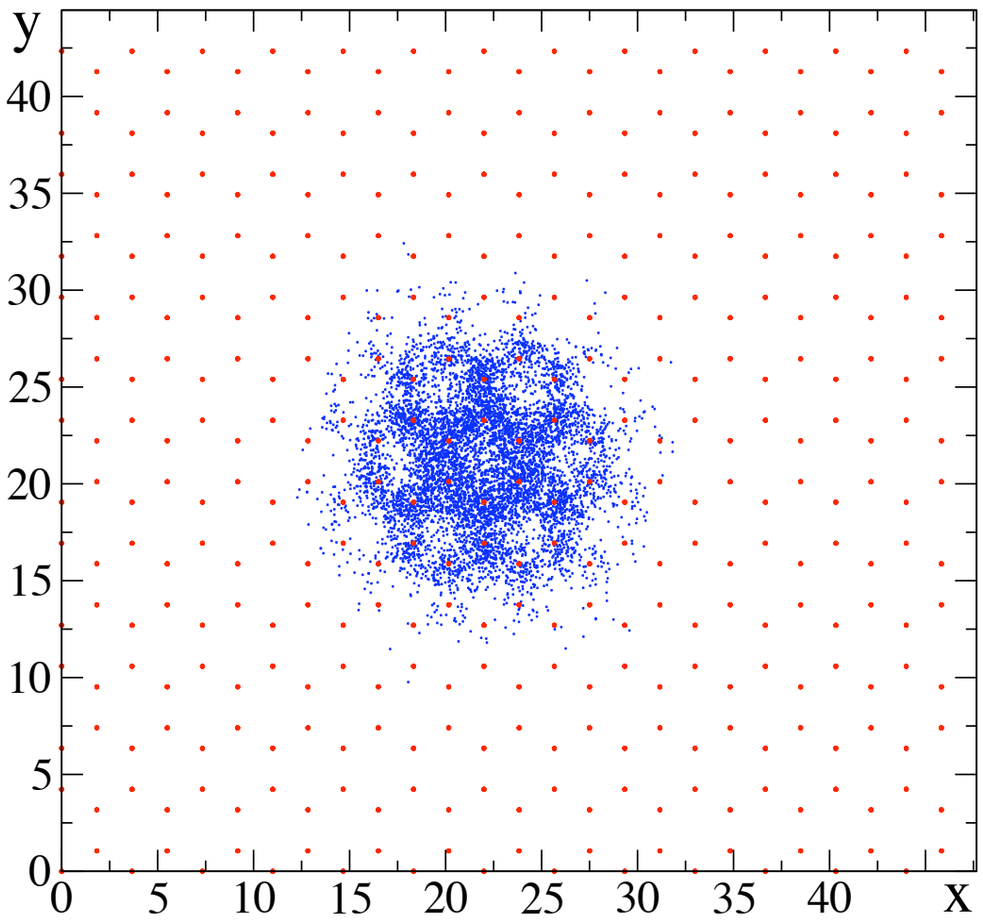
Superfluid behavior of a generic GB at temperatures of the order of 0.5 K is observed. Indeed, a **generic GB is found to be superfluid**, although insulating GBs exist as well, for particular relative orientations of the crystallites

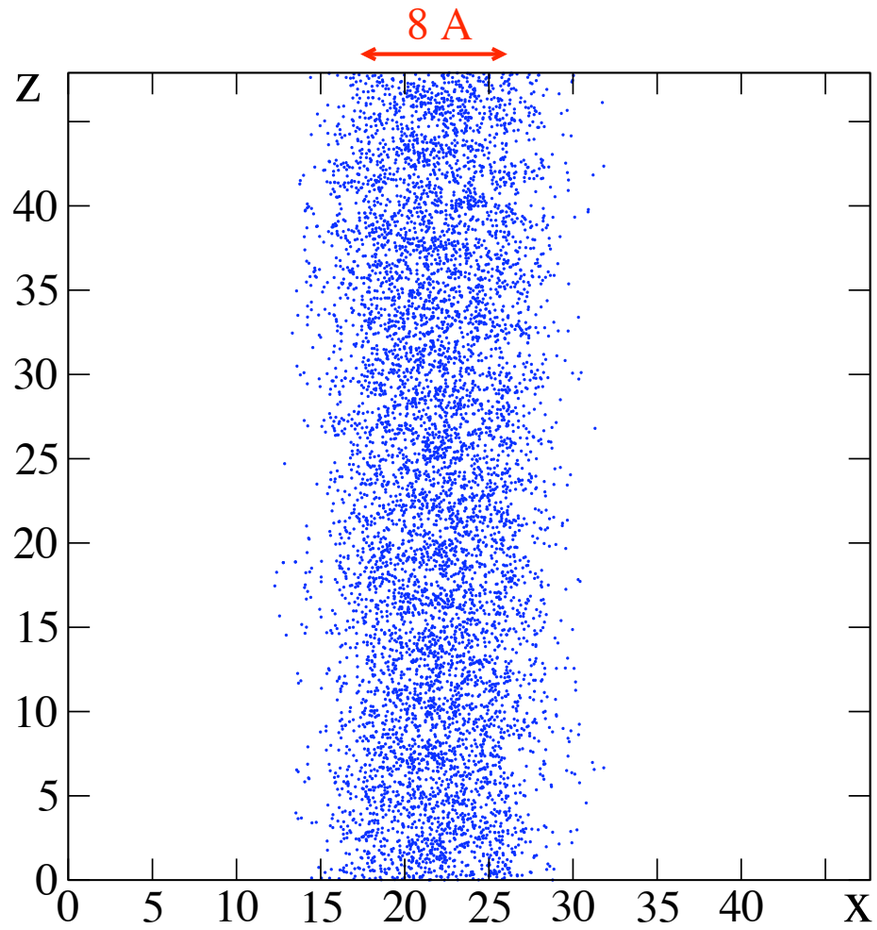


Simulations performed on systems including as many as **13000** particles (*that many are needed*)

Application: superfluidity in the core of a screw dislocation in solid ^{4}He

MB, A. Kuklov, L. Pollet, N. Prokof'ev, B. Svistunov and M. Troyer, Phys. Rev. Lett. ***99****, 035301 (2007).*





Simulations of single screw dislocation inside hcp ^{4}He crystal show evidence of spatially modulated *Luttinger liquid* (1d supersolid ?)

Other applications

- Phase diagram of dipolar systems

  (H.-P. Buchler *et al*., PRL **98**, 060404 (2007))

- *Superfluid properties of para-hydrogen clusters*

  (F. Mezzacapo and MB, PRL **97**, 045301 (2006); PRL **100**, 145301 (2008))

- Momentum distribution of liquid *para*-hydrogen

  (MB, (2008))

Open issues

- *Sign problem* (*neither improved not worsened* by WA)
- *Continuous time (is there any way of avoiding the time step error in continuos space ?)*
- *Can run into problems whenever multi-particle updates are needed (e.g., at first order phase transitions)*
- *Dynamical information* (*linear response theory and analytic continuation)*

lunch... ?