Worm algorithms

MW 090525

References

- N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsyn, Phys. Lett. A **238**, 253 (1998)
- N. Prokof'ev and B. Svistunov Phys. Rev. Lett. **87**, 160601 (2001)
- F. Alet and E. S. Sørensen Phys. Rev. E **67**, 015701(R) (2003)
- F. Alet and E. S. Sørensen Phys. Rev. E **68**, 026702 (2003)

Idea

- Map problem to a loop model
- Previous loop algorithms use local moves
+ nonlocal moves having exponentially low acceptance rates
- Sample loops as random walks using local moves only, producing high acceptance rates
- Drastically reduces critical slowing down
- Works for both discrete and continuous systems
- Improved estimators available for correlation functions

Worm algorithm is a main method for quantum many body physics

- The worm algorithm is one of the best methods available to study thermodynamic properties of various interacting quantum many body systems
- It is essentially exact for Bose systems and goes far beyond previously available methods

Remaining problems:

- It does not help for the minus sign problem
- A general method to handle fermions is still missing
- It does not give time dependent properties

Loop representation of 2D Ising model

$$\beta E = -\sum_{\langle ij \rangle} K S_i S_j$$

$$Z = \sum_{\text{all states}} e^{-\beta E} = \sum e^{\sum K S_i S_j} = \sum \prod e^{K S_i S_j}$$

$$S_i S_j = \pm 1 \;\Rightarrow\; \frac{e^K + e^{-K}}{2} + S_i S_j \frac{e^K - e^{-K}}{2} = e^{K S_i S_j}$$

$$\Rightarrow\; e^{K S_i S_j} = \cosh K + S_i S_j \sinh K = \cosh K \left(1 + T S_i S_j\right)$$

$$T = \tanh K \quad \text{(not temperature here!)}$$

$$Z = \sum \prod \cosh K \left(1 + T S_i S_j\right)$$

For N spins there are $2N$ bonds : $Z = \cosh^{2N} K \sum \prod \left(1 + T S_i S_j\right) = 2^N Z' \cosh^{2N} K$

$$Z' = 2^{-N} \sum \prod \left(1 + T S_i S_j\right) = 2^{-N} \sum_{S_1 = \pm 1} \dots \sum_{S_N = \pm 1} \left[1 + T \sum\nolimits_1^* S_i S_j + T^2 \sum\nolimits_2^* (S_i S_j)(S_{i'} S_{j'}) + \dots\right]$$

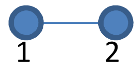
$$\sum\nolimits_l^* = \text{sum over all sets of } l \text{ different NN bonds}$$

Ising loop model (cont)

$$Z' = 2^{-N} \sum_{S_1=\pm 1} \dots \sum_{S_N=\pm 1} \left[1 + T \sum\nolimits_l^* S_i S_j + T^2 \sum\nolimits_l^* (S_i S_j)(S_{i'} S_{j'}) + \dots \right]$$

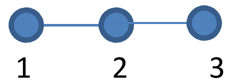
Examples of terms:

$(S_1 S_2)$



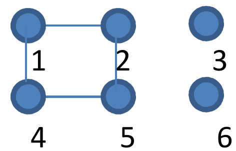
open graph

$(S_1 S_2)(S_2 S_3)$



open graph

$(S_1 S_2)(S_2 S_5)(S_5 S_4)(S_4 S_1)$



closed graph

Since $\sum_{S_i=\pm 1} S_i = 0$, only closed graphs contribute to Z'

Nonzero terms contain S_i to power 0,2 or 4 and equal T^L, $L =$# bonds in term.

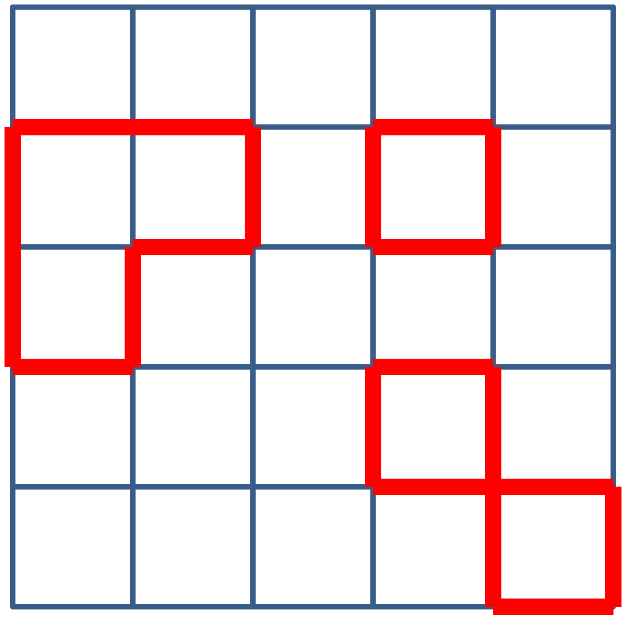
The sum over all S_i gives a factor 2^N (which cancels the 2^{-N} prefactor)

$$Z' = \sum_L g(L) T^L \qquad g(L) = \text{\# closed graphs with length } L$$

$g(L = \text{odd}) = 0 \Rightarrow$ sign of T (and of K) irrelevant as expected

High temperature loop expansion

$$Z = \sum_{b} (\tanh K)^{\sum b_{ij}} \qquad K = J/T \quad b_{ij} = 0,1 \quad \sum_{j} b_{ij} = \text{even, forming closed loops}$$



$$\sum_{j \in nn \text{ of } i} b_{ij} = 0, 2, 4$$

Ising worm algorithm: mark and erase

1. Select a random site i=i_0
2. Select a random link from site i to j
3. Move there and set i=j with probability p=(tanh K)$^{1\text{-}bij}$
   If accepted flip b_{ij} : change 1 to 0 or 0 to 1
4. Update correlation function on the fly:
   add +1 to $G(i\text{-}i_0)$ for the open path from i_0 to i
5. If $i \neq i_0$: repeat from 2
6. If i=i_0: loop closes and move finishes
7. Update averages: add +1 to $G(0)$
   add current loop length to <L>
8. Repeat from 1 until enough data has been collected

- Example of averages:
  - energy: $E = -J \tanh(K)\ [dN + \langle L\rangle/\sinh^2(K)]$
  - susceptibility: $\chi = (1/T)\ \Sigma_i\ g(i),\ g(i)=G(i)/G(0)$

Loop representation of XY model

$$\beta H = -\sum_{\langle ij \rangle} K \cos(\theta_i - \theta_j) \quad , \quad Z = \prod_k \int_0^{2\pi} \frac{d\theta_k}{2\pi} e^{-\beta H} = \prod_k \int_0^{2\pi} \frac{d\theta_k}{2\pi} \prod_{\langle ij \rangle} e^{K\cos(\theta_i - \theta_j)}$$

$$e^{K\cos\theta} \approx \sum_{n=-\infty}^{\infty} e^{-\frac{K}{2}(\theta + 2\pi n)^2} = e^{V(\theta)} = \sum_{J=-\infty}^{\infty} e^{-iJ\theta + V(J)} \quad \text{(Villain model)}$$

$$e^{V(J)} = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{iJ\theta + V(\theta)} = \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} e^{iJ\theta - \frac{K}{2}\theta^2} = Ce^{-\frac{1}{2K}J^2}$$

$$Z = \prod_k \int_0^{2\pi} \frac{d\theta_k}{2\pi} e^{-\beta H} = \prod_k \int_0^{2\pi} \frac{d\theta_k}{2\pi} \prod_{\langle ij \rangle} \sum_{J_{ij}=-\infty}^{\infty} e^{-iJ_{ij}(\theta_i - \theta_j) + V(J_{ij})}$$

$$\text{Integrate out phases:} \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-iJ\theta} = \delta_{J,0}$$

$$Z = \prod_{\langle ij \rangle} \sum_{J_{ij}=-\infty}^{\infty}{}' e^{-\frac{1}{2K}J_{ij}^2}$$

$'$ denotes that configurations are divergence free: $\prod_{\mathrm{k}} \delta_{\sum_{e=\pm x, \pm y, \ldots} J_{k,k+e}, 0}$

This is the partition function of an ensemble of closed directed loops.

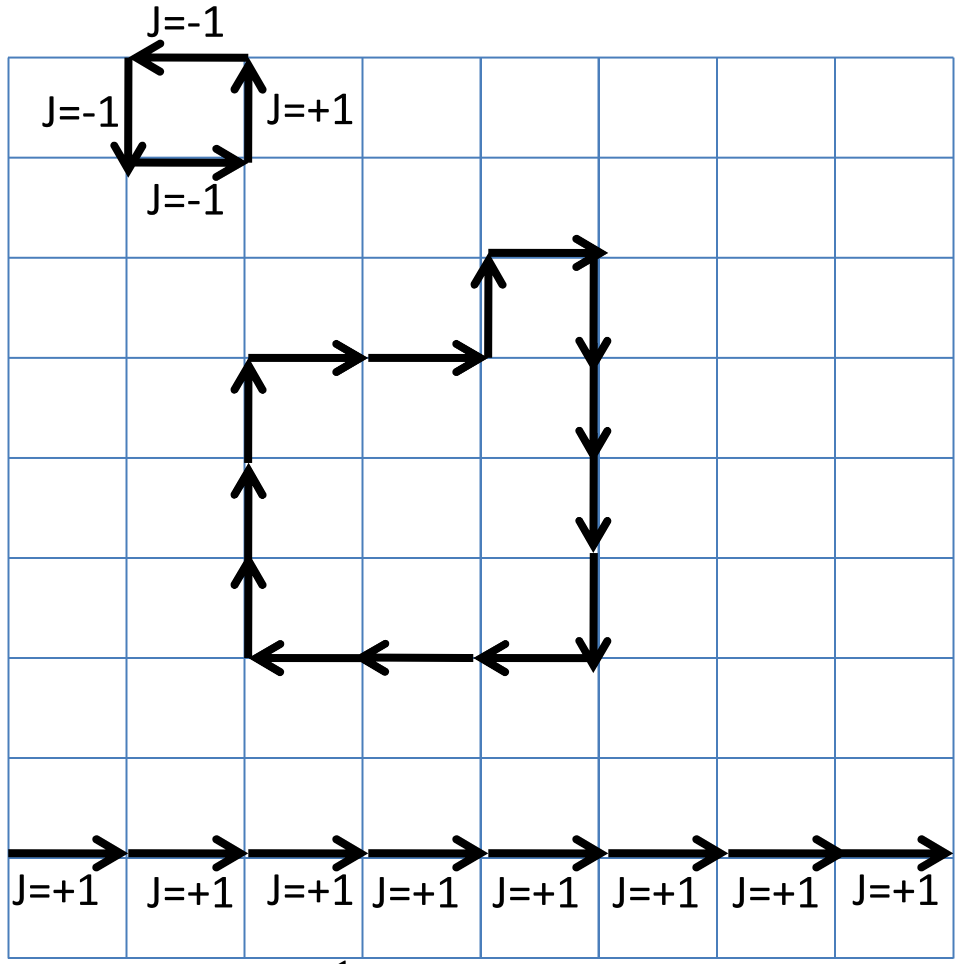
Loop models

- Loops in classical XY model
- XY transition: loops proliferate (”blow out”) and loop size diverges as $\xi \sim t^{-\nu}$
- Worldlines in path integral representation of Bose Hubbard model

$$H = U\sum_i n_i^2 - \sum_i h_i n_i - t\sum_{\langle ij \rangle}(a_i^+ a_j + cc) \quad , \quad n_i = a_i^+ a_j$$

$$Z = \int Dr(\tau)\exp\left[-S[r(\tau)]\right] \quad , \quad S[r(\tau)] = \int_0^{\hbar\beta} d\tau \left[\sum_{i=1}^N \frac{m}{2\hbar^2}\left(\frac{dr}{d\tau}\right)^2 + V(r(\tau))\right]$$

Loop configurations



$$\text{Winding number}: W_\mu = \frac{1}{L_\mu}\sum_k J_k^\mu \quad , \quad \left\langle \Delta W_\mu^2 \right\rangle = \left\langle W_\mu^2 \right\rangle - \left\langle W_\mu \right\rangle^2 = L^{d-2}\beta\rho_s^\mu$$

ρ_s^μ superfluid density in direction $\mu = x, y, \ldots$

Correlation function

Matsubara Green function given by open worm as

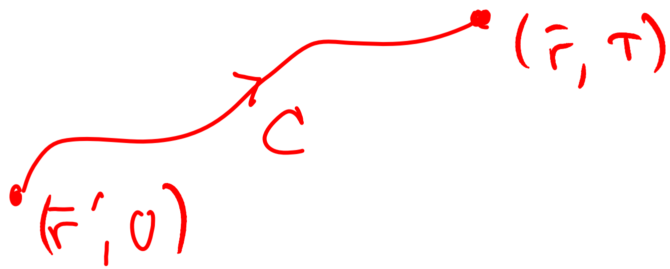
$$G(r,r',\tau) = -\left\langle T\psi^{+}(r,\tau)\psi(r',0)\right\rangle = \left\langle e^{i(\theta(r,\tau)-\theta(r',0))}\right\rangle$$

$$= \frac{1}{Z}\int D\theta \sum_{\{J\}} \exp\left[\sum_{\langle ij\rangle} -iJ_{ij}(\theta_i-\theta_j) - \frac{J_{ij}}{2K} - i(\theta_{r,\tau}-\theta_{r',0})\right]$$

$$= \frac{1}{Z}\int D\theta \sum_{\{J\}} \exp\left[\sum_{\langle ij\rangle\notin C}\left(-iJ_{ij}(\theta_i-\theta_j) - \frac{J_{ij}^2}{2K}\right) + \sum_{\langle ij\rangle\in C}\left(-i(J_{ij}-1)(\theta_i-\theta_j) - \frac{J_{ij}^2}{2K}\right)\right]$$

$$= \frac{1}{Z}\int D\theta \sum_{\{J\}} \exp\left[\sum_{\langle ij\rangle\notin C}\left(-iJ_{ij}(\theta_i-\theta_j) - \frac{J_{ij}^2}{2K}\right) + \sum_{\langle ij\rangle\in C}\left(-iJ_{ij}(\theta_i-\theta_j) - \frac{(J_{ij}+1)^2}{2K}\right)\right]$$

$$= \left\langle \exp\left[-\sum_{\langle ij\rangle\in C} \frac{J_{ij}+\frac{1}{2}}{K}\right]\right\rangle$$



Worm algorithm for XY model

1. Select a random site $i=i_0$
2. Select a random direction $\mu= \pm x, \pm y,\ldots$ and a trial increment $J_i^\mu \rightarrow J_i^\mu \pm 1$
3. Accept the trial move with probability $p=\min\{1,\exp(-\beta\Delta H)\}$ and set $i \rightarrow i+\mu$
4. Collect data to correlation function $G(i-i_0)$ on the fly
5. If $i \neq i_0$ repeat from 2
6. If $i=i_0$ the worm closed. Gather data to averages
7. Repeat from 1 until enough data has been generated

Reduced critical slowing down

Cluster Monte Carlo algorithm for the quantum rotor model
Fabien Alet and Erik S. Sorensen
PHYSICAL REVIEW E **67**, 015701(R), 2003

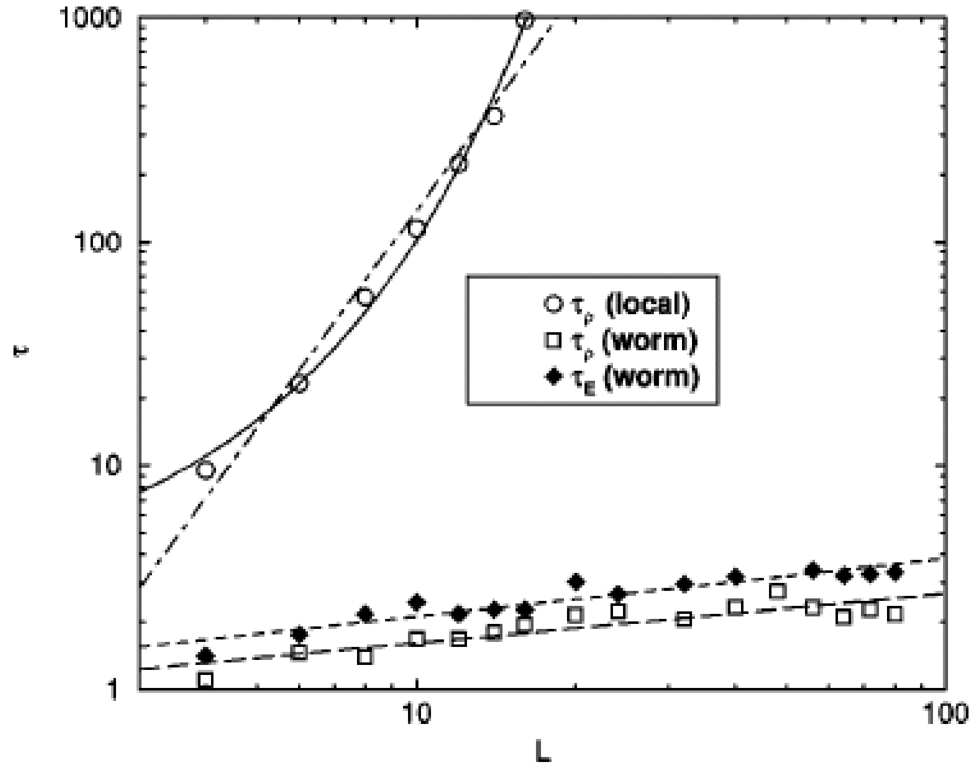


FIG. 1. Autocorrelation times versus lattice size for the conventional and worm algorithm for $\mu = 0$ at $K = 0.333$. The dashed lines indicate power-law fits and the solid line an exponential fit in L.

Undirected worm algorithm

Fabien Alet and Erik S. Sorensen, PHYSICAL REVIEW E **68**, 026702 (2003)

All in all, the geometrical undirected worm algorithm can be summarized by using the following pseudoalgorithm.

(1) Choose a random initial site $s_1=(\mathbf{r}_1,\tau_1)$ in the space-time lattice.

(2) For each of the directions $\sigma=\pm x,\pm y,\pm \tau$, calculate the weights $A_{s_i}^{\sigma}$ with $A_{s_i}^{\sigma}=\min[1,\exp(-\Delta E_{s_i}^{\sigma}/K)]$, $\Delta E_{s_i}^{\sigma}=E_{s_i}^{\prime\sigma}-E_{s_i}^{\sigma}$.

(3) Calculate the normalization $N_{s_i}=\Sigma_{\sigma}A_{s_i}^{\sigma}$ and the associated probabilities $p_{s_i}^{\sigma}=A_{s_i}^{\sigma}/N_{s_i}$.

(4) According to the probabilities $p_{s_i}^{\sigma}$, choose a direction σ.

(5) Update $J_{s_i}^{\sigma}$ for the direction chosen and move the worm to the new lattice site s_{i+1}.

(6) If $s_i\neq s_1$, go to (2).

(7) Calculate the normalizations $\overline{N}_{s_1}$ and N_{s_1} of the initial site s_1, with and without the worm present. Erase the worm with probability $P^{e}=1-\min(1,N_{s_1}/\overline{N}_{s_1})$.

Directed worm algorithm

Fabien Alet and Erik S. Sorensen, PHYSICAL REVIEW E **68**, 026702 (2003)

We can now define a *directed* geometrical worm algorithm with minimal backtracking probability. Using a pseudocode notation, we have the following.

(1) Choose a random initial site $s_1=(\mathbf{r}_1,\tau_1)$ in the space-time lattice.

(2) If $i=1$, then for each of the directions $\sigma=\pm x,\pm y,\pm\tau$, calculate the weights $A_{s_i}^{\sigma}$ with $A_{s_i}^{\sigma}=\min[1,\exp(-\Delta E_{s_i}^{\sigma}/K)]$, $\Delta E_{s_i}^{\sigma}=E_{s_i}^{\prime\sigma}-E_{s_i}^{\sigma}$. Calculate the normalization $N_{s_i}=\Sigma_{\sigma}A_{s_i}^{\sigma}$ and the associated probabilities $p_{s_i}^{\sigma}=A_{s_i}^{\sigma}/N_{s_i}$. Else: According to the incoming direction σ_l, set $p_{s_i}^{\sigma}$ equal to the lth column of P_{s_i}.

(3) According to the probabilities $p_{s_i}^{\sigma}$, choose a direction σ.

(4) Update $J_{s_i}^{\sigma}$ for the direction chosen and move the worm to the new lattice site s_{i+1}.

(5) If $s_i\neq s_1$, go to (2).

(6) Calculate the normalizations $\overline{N}_{s_1}$, of site s_1 with the worm present, and N_{s_1}, without the worm. Erase the worm with probability $P^e=1-\min(1,N_{s_1}/\overline{N}_{s_1})$.

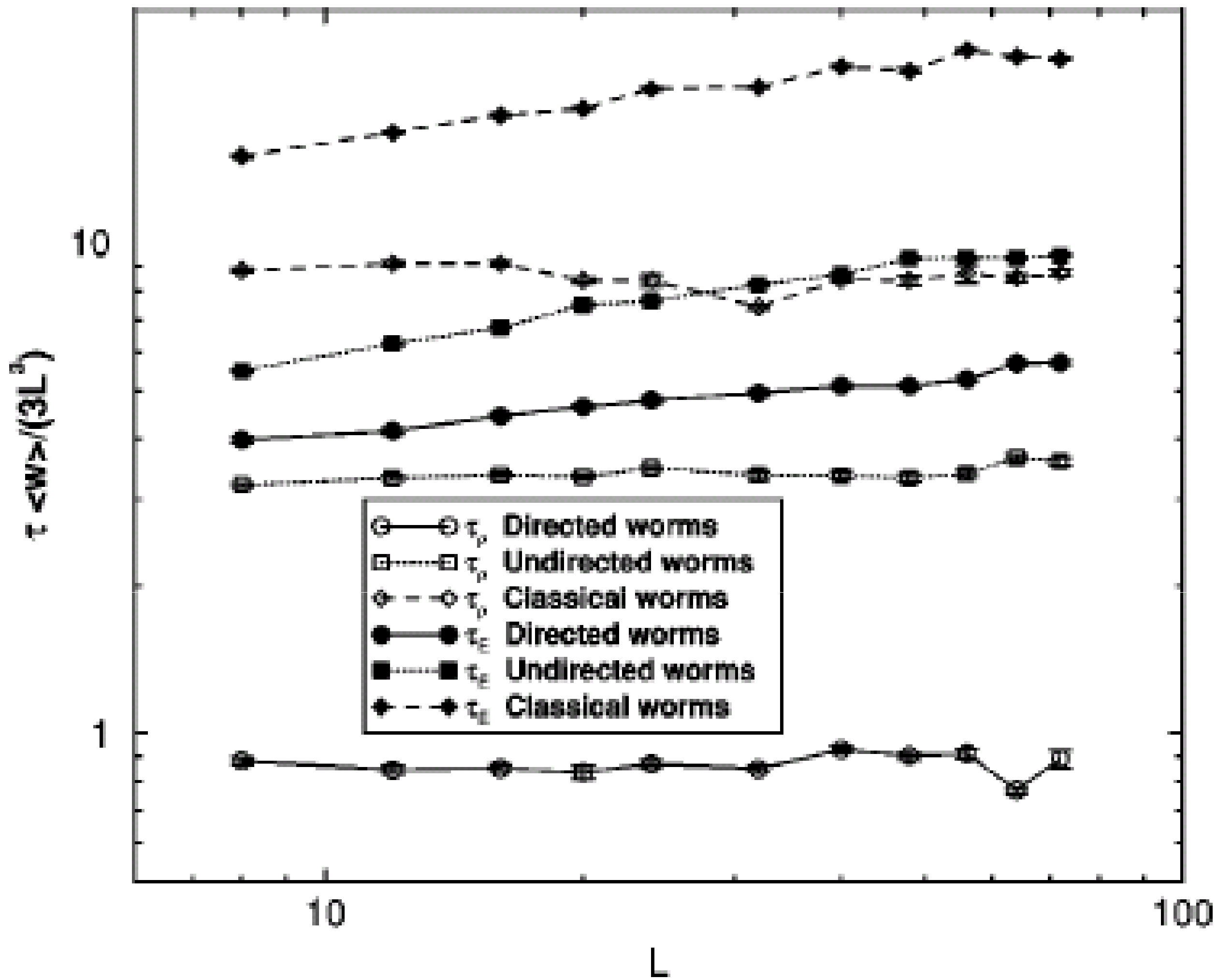


FIG. 6. Autocorrelation times of stiffness ρ and energy E for the three presented algorithms vs lattice size L. These autocorrelation times are *rescaled* autocorrelation times where the computational effort is taken into account.

Continuous worm algorithm

- Boninsegni, Prokof'ev, Svistunov
  PRE **74**, 036701 2006
- No need to use discrete space lattices
  Worms can be continuous
- Worldlines with continuum position but discrete timesteps

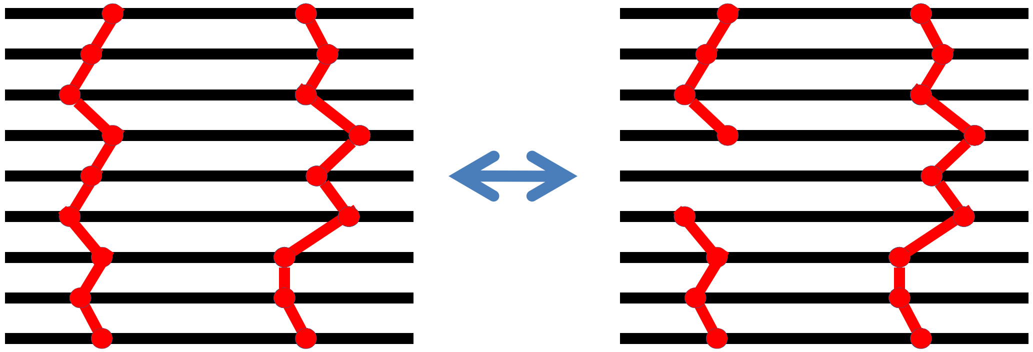
$$\hat{H} = -\lambda \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} v(|\mathbf{r}_i - \mathbf{r}_j|)$$

- 3 worm MC moves accepted with Metropolis

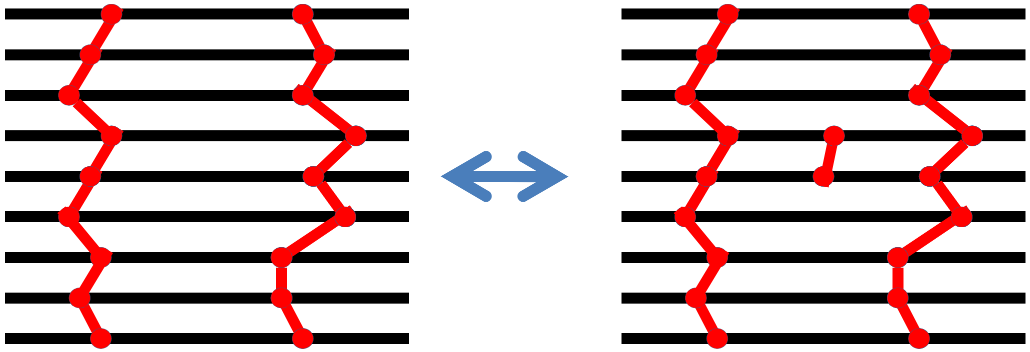
1. Open/close
2. Insert/remove
3. Advance/recede

Continuum worm MC moves

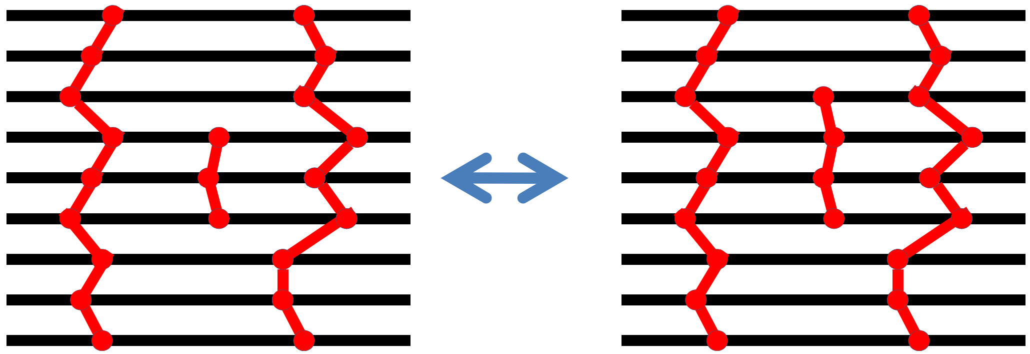
1. Open/close



2. Insert/remove



3. Advance/recede



Superfluid transition in liquid ^{4}He

BONINSEGNI, PROKOF'EV, AND SVISTUNOV PHYSICAL REVIEW E **74**, 036701 2006

PIMC: *Tc*=2.1936 Experiment *Tc*=2.177 K,

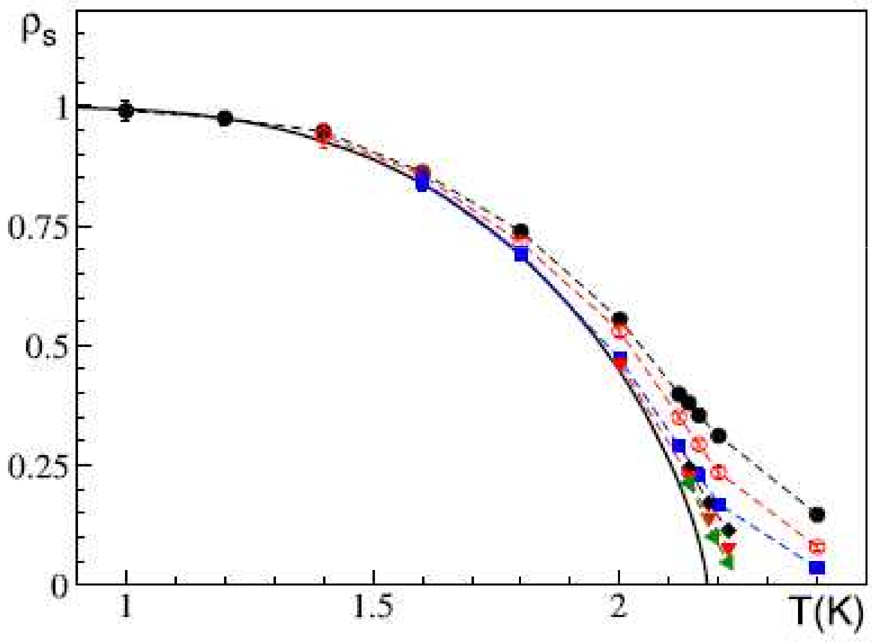


FIG. 9. (Color online). Superfluid fraction $\rho_s(T)$ as a function of temperature at SVP, computed for different system sizes, namely N=64 (filled circles), N=128 (open circles), N=256 (filled squares), N=512 (diamonds), N=1024 (triangles down), and N=2048 (triangles left). The solid line is the experimental curve.

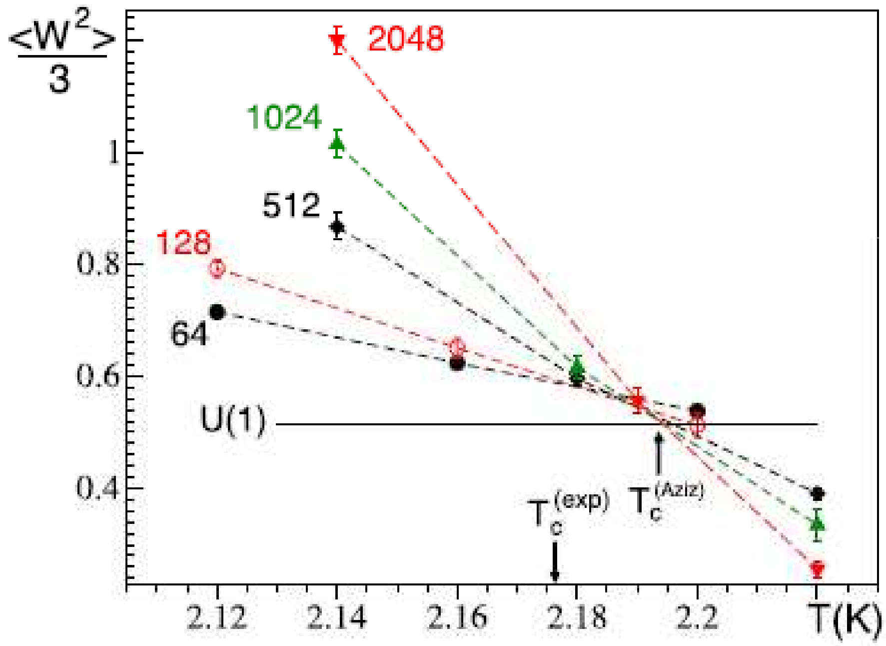


FIG. 10. (Color online) Finite-size scaling plot for $2\lambda n \rho_s L/T = \langle W^2 \rangle /3$ at SVP. The solid line is the U(1) universality class value of 0.516(1).