The worm algorithm

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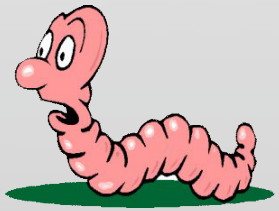
ETH Zürich



Outline

- Path integral representation of world lines
- The worm algorithm
  - What is a worm?
  - Local updates
  - Ergodicity
  - Non-local interactions
- Comparison with SSE
- Summary

Path integral representation

Interaction representation

off-diagonal term

$$H = H_0 + V$$

diagonal term

Partition function

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \mathrm{Tr}\left(e^{-\beta H_0}\mathrm{T}e^{-\int_0^\beta d\tau V(\tau)}\right)$$

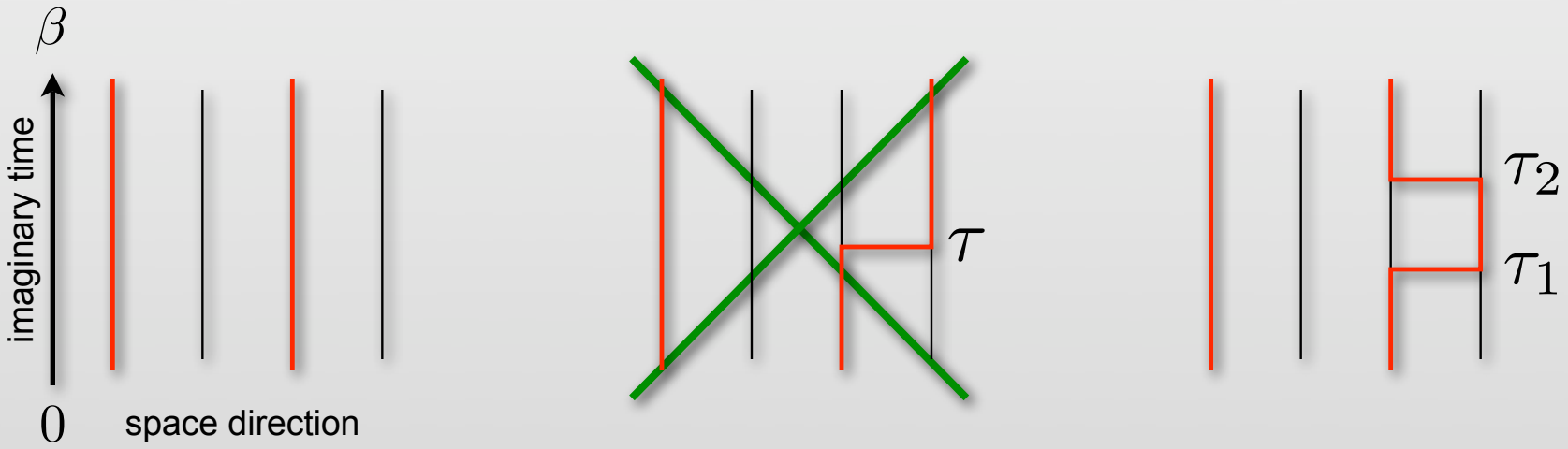
$$Z = \mathrm{Tr}\left(e^{-\beta H_0}\left[1 - \int_0^\beta d\tau V(\tau) + \int_0^\beta d\tau_1 V(\tau)\int_{\tau_1}^\beta d\tau_2 V(\tau_2)V(\tau_1) + \ldots\right]\right)$$

Advantage: diagonal terms are treated exactly.

Path integral representation

$$Z = \mathrm{Tr}\left(e^{-\beta H_0} \left[1 - \int_0^\beta d\tau V(\tau) + \int_0^\beta d\tau_1 V(\tau) \int_{\tau_1}^\beta d\tau_2 V(\tau_2) V(\tau_1) + \ldots \right] \right)$$

Each term represented by a world line configuration



Disadvantage: keeping track of times can be computational expensive.

Continuous time representation

What **data structures** are used to represent a world line configuration in continuous time?

Answer: **kinks** and **kink lists**.

new state

$0 : (\tau_4, 1) \quad (\tau_6, 0)$

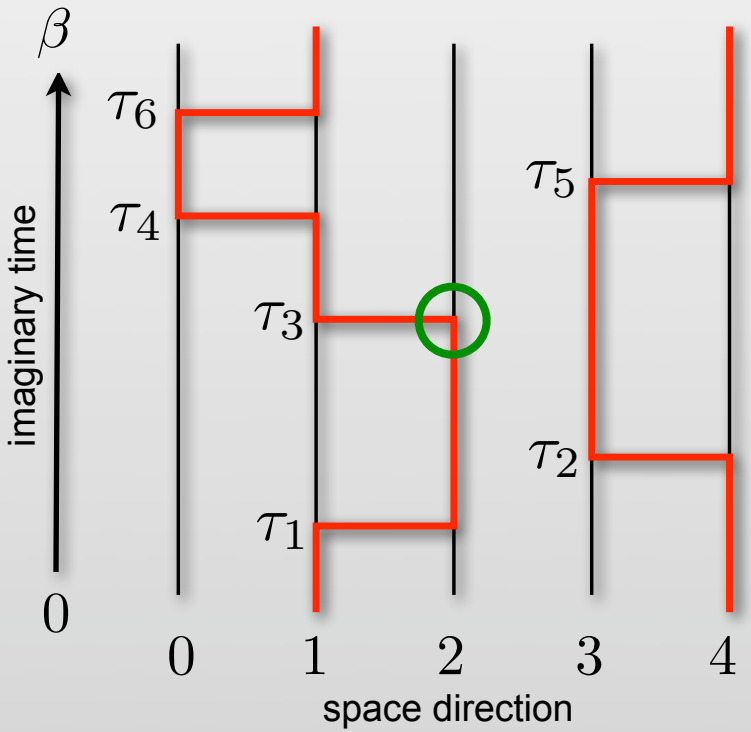
kink time

$1 : (\tau_1, 0) \quad (\tau_3, 1) \quad (\tau_4, 0) \quad (\tau_6, 1)$

$2 : (\tau_1, 1) \quad (\tau_3, 0)$

$3 : (\tau_2, 1) \quad (\tau_5, 0)$

$4 : (\tau_2, 0) \quad (\tau_5, 1)$



Local updates in continuous time

Shift kink

Insert / remove two kinks

$P = 1$ $\qquad$ $P = (\Delta\tau J/2)^2 \to 0$

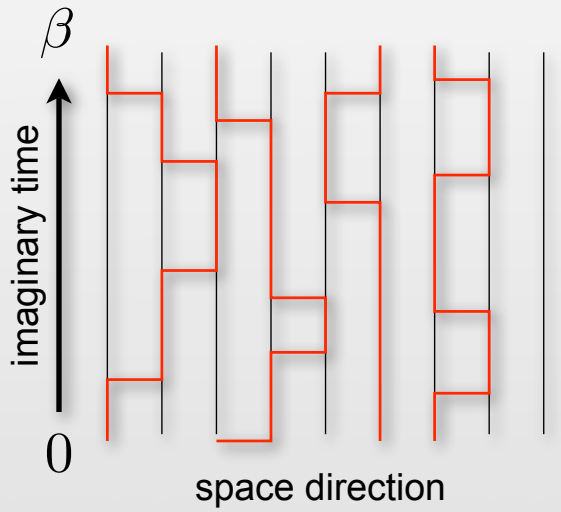
Vanishing acceptance rate $\qquad P_{\to} = \min\left[1, (\Delta\tau J/2)^2\right] \to 0$

Solution: **Integrate** over al possible insertions in a **time window**

$$P_{\to} = \int_0^{\Lambda}\int_{\tau_1}^{\Lambda} (J/2)^2 d\tau_2 d\tau_1 \to \frac{\Lambda^2 J^2}{8} \neq 0$$

Path integral vs. SSE representation

World lines in path integral



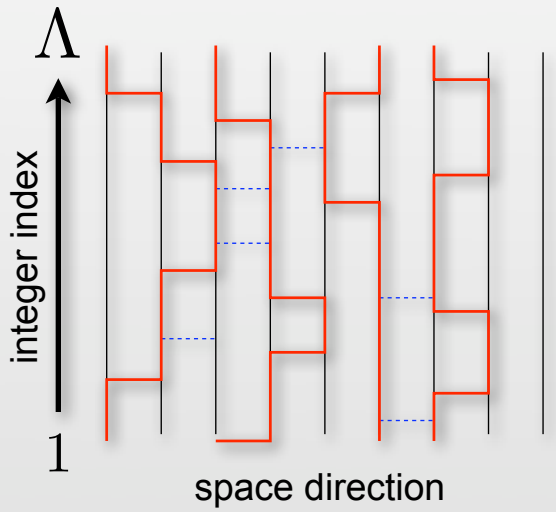
Advantage

diagonal terms treated exactly

Disadvantage

continuous imaginary time

World lines in SSE



Disadvantage

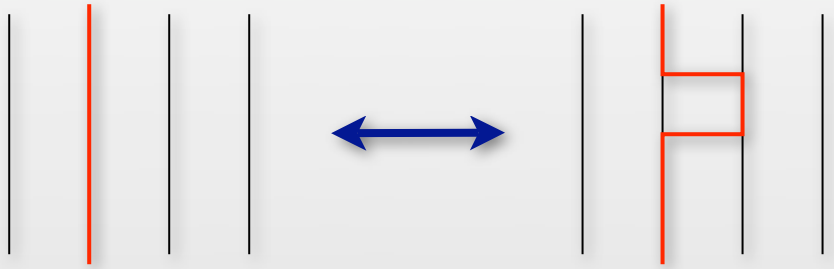
perturbation also in diagonal terms

Advantage

integer index instead of time

Local updates

Local changes using Metropolis updates



Problems

Restricted to canonical ensemble

No change of magnetization, particle number, winding number

Critical slowing down

Autocorrelation times grow fast

Solutions

Classical problem: cluster updates

Quantum problem: **worm algorithm**

The worm algorithm

N.V. Prokof'ev, B.V. Svistunov, and I.S. Tupitsyn (1998)

JOURNAL OF EXPERIMENTAL AND THEORETICAL PHYSICS VOLUME 87, NUMBER 2 AUGUST 1998

Exact, complete, and universal continuous-time worldline Monte Carlo approach to the statistics of discrete quantum systems

N. V. Prokof'ev,*) B. V. Svistunov, and I. S. Tupitsyn

Kurchatov Institute, 123182 Moscow, Russia
(Submitted 20 November 1997)
Zh. Éksp. Teor. Fiz. **114**, 570–590 (August 1998)

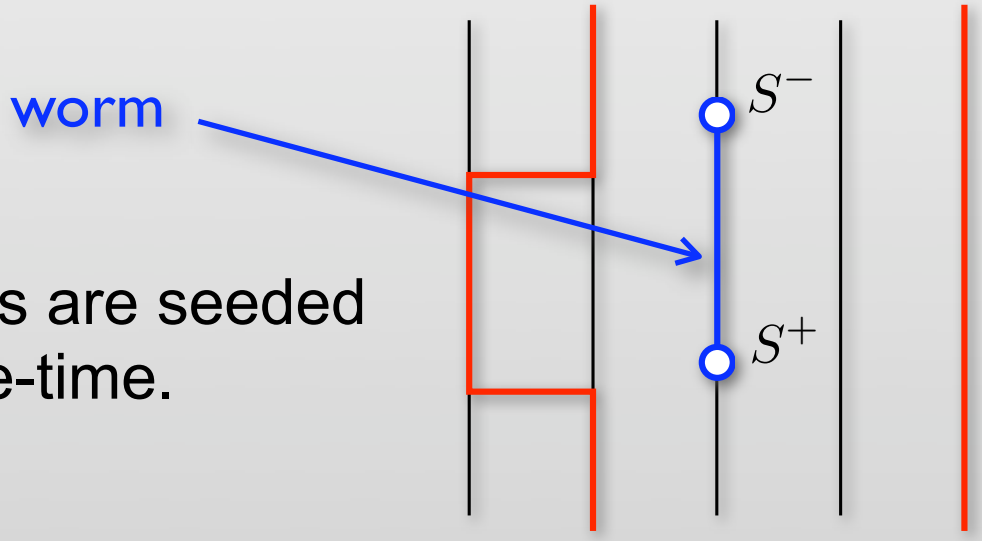
We show how the worldline quantum Monte Carlo procedure, which usually relies on an artificial time discretization, can be formulated directly in continuous time, rendering the scheme exact. For an arbitrary system with discrete Hilbert space, none of the configuration update procedures contain small parameters. We find that the most effective update strategy involves the motion of worldline discontinuities (both in space and time), i.e., the evaluation of the Green's function. Being based on local updates only, our method nevertheless allows one to work with the grand canonical ensemble and nonzero winding numbers, and to calculate any dynamical correlation function as easily as expectation values of, e.g., total energy. The principles found for the update in continuous time generalize to any continuous variables in the space of discrete virtual transitions, and in principle also make it possible to simulate continuous systems exactly. [S1063-7761(98)01508-X]

The worm algorithm

N.V. Prokof'ev, B.V. Svistunov, and I.S. Tupitsyn (1998)

Extend world line configuration space of closed world lines by an **open world line fragment**, the "worm".

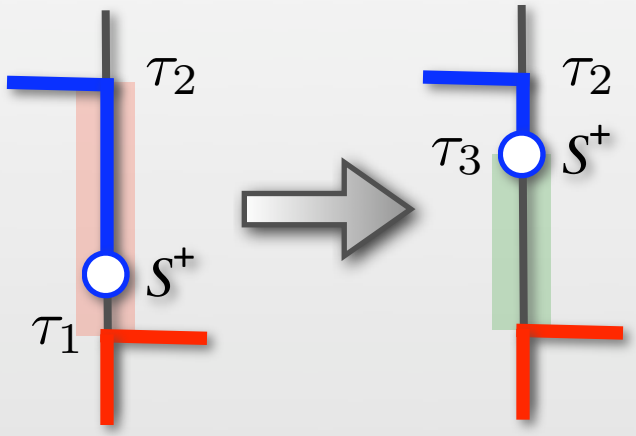
$$H_{\mathrm{worm}} = H - \eta \sum_i \left(S_i^+ + S_i^- \right)$$



Additional world lines are seeded at any point in space-time.

Worm updates

Time shift



$$\lambda = -\beta \Delta E < 0$$

$$\text{integrated weight} = \int_0^{\Delta\tau} d\tau e^{\lambda\tau} = \frac{1}{\lambda}\left(e^{\lambda\Delta\tau} - 1\right)$$

$$\text{partial weight} = \int_{\Delta\tau'}^{\Delta\tau} d\tau e^{\lambda\tau} = \frac{1}{\lambda}\left(e^{\lambda\Delta\tau} - e^{\lambda\Delta\tau'}\right)$$

$\Delta\tau = \tau_2 - \tau_1$ $\Delta\tau' = \tau_3 - \tau_1$

random number

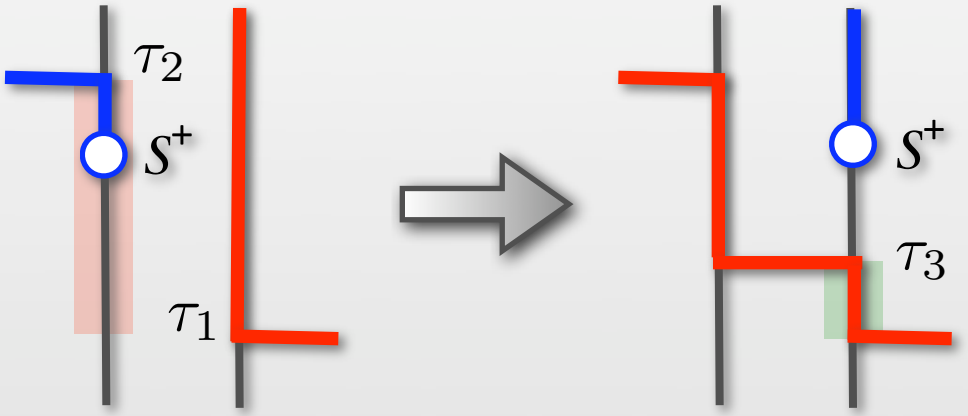
$$p = \frac{\text{partial weight}}{\text{integrated weight}}$$

$0 \le p \le 1$

shifted time $\tau_3 = \tau_1 + \frac{1}{\lambda} \ln\left[e^{\lambda\Delta\tau} + p \cdot \left(1 - e^{\lambda\Delta\tau}\right)\right]$

Worm updates

Jump of worm head



$$\lambda = -\beta\left(\Delta E_1 + \Delta E_2\right) < 0$$

$\Delta\tau = \tau_2 - \tau_1$

$\Delta\tau' = \tau_3 - \tau_1$

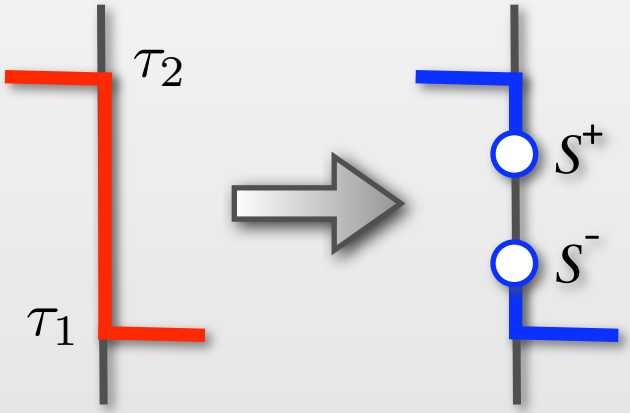
$$p = \frac{\text{partial weight}}{\text{integrated weight}} = \frac{e^{\lambda\Delta\tau} - e^{\lambda\Delta\tau'}}{e^{\lambda\Delta\tau} - 1}$$

jump time $$\tau_3 = \tau_1 + \frac{1}{\lambda}\ln\left[e^{\lambda\Delta\tau} + p\cdot\left(1 - e^{\lambda\Delta\tau}\right)\right]$$

random number

Worm updates

Creation of a worm



$$\lambda = -\beta \Delta E < 0$$

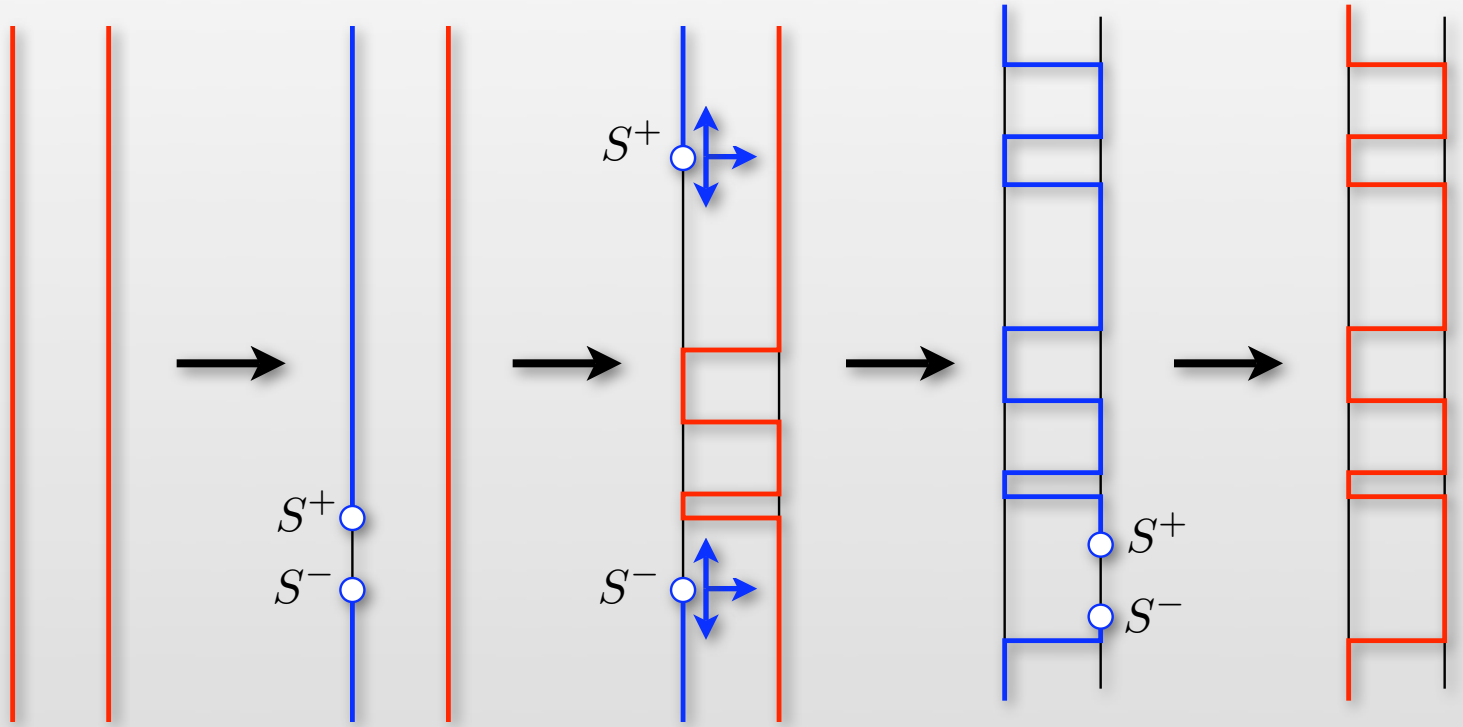
$$\text{creation probability} = \int_{\tau_1}^{\tau_2} d\tau_4 \int_{\tau_1}^{\tau_4} d\tau_3 \, e^{\lambda(\tau_3 - \tau_4)}$$

$$= \frac{1}{\lambda^2} \left(\lambda \Delta\tau + e^{-\lambda \Delta\tau} - 1 \right)$$

$\Delta\tau = \tau_2 - \tau_1$ $\qquad$ τ_3, τ_4 $\qquad$ creation probability $\propto \Delta\tau^2$

1) randomly choose $\tau_3 \in [0, \beta]$
2) calculate creation probability for respective time interval $[\tau_1, \tau_2]$
3) accept / reject move
4) randomly choose $\tau_4 \in [\tau_3, \tau_2]$ and then shift τ_4

Example of update sequence



closed world lines

worm creation

shift / jump worm heads

worm annihilation

closed world lines

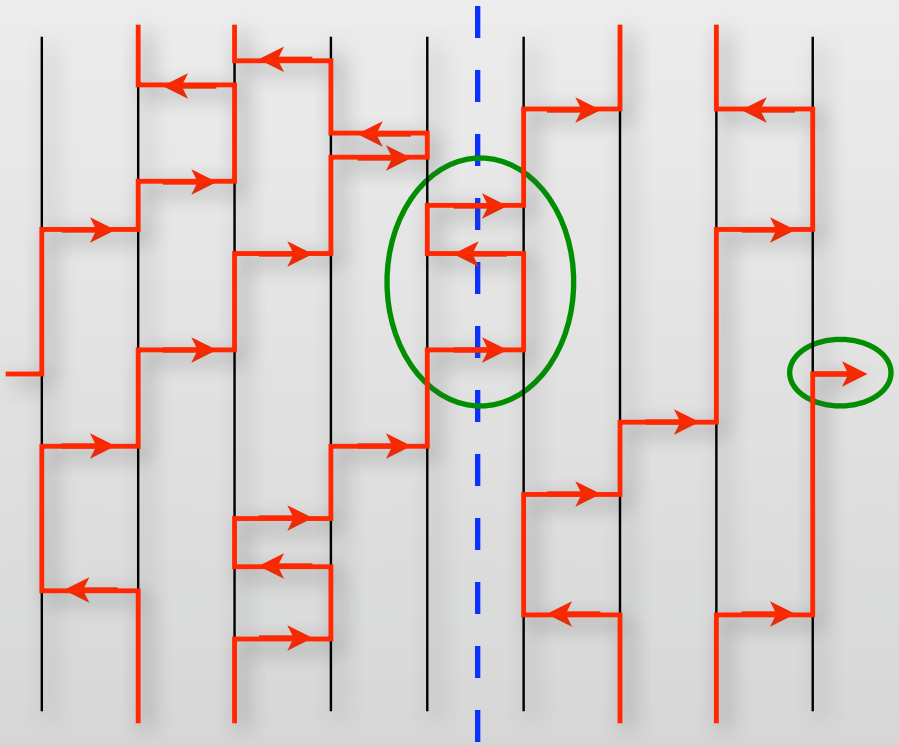
Ergodicity

Non-local updates in temporal and spatial directions.

The worm algorithm can simulate a **grand-canonical ensemble.**

We can study **winding-number fluctuations**, e.g. the stiffness.

Example:



$$N_x = +1$$

Non-local interactions

Can we include diagonal site-site interactions?

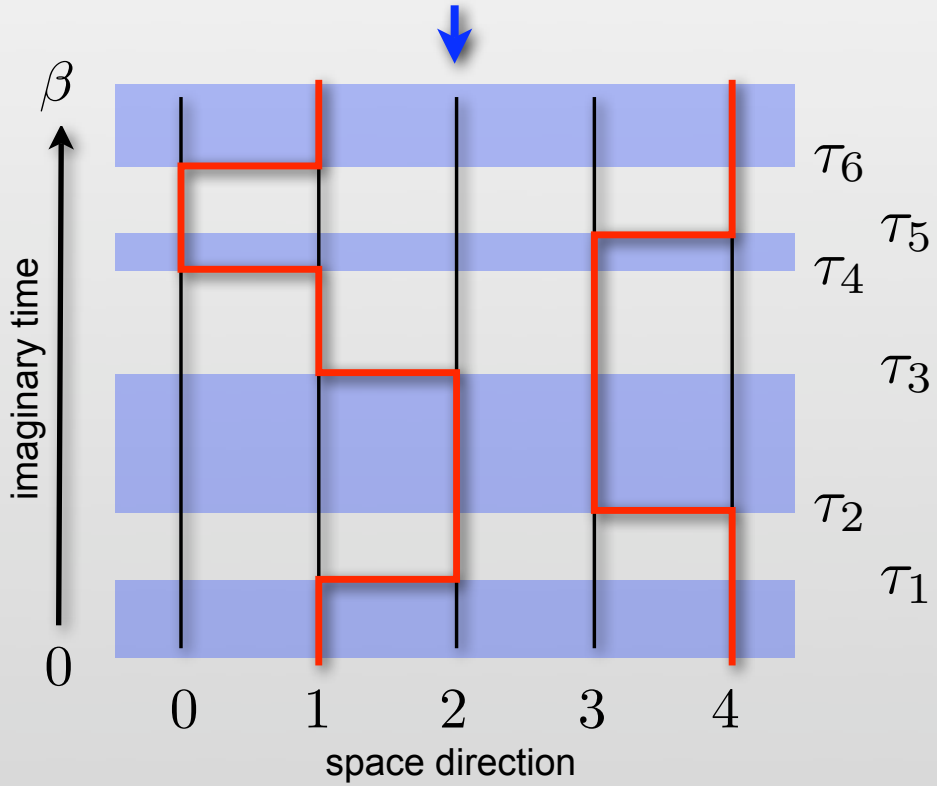
Example :

$$H' = H + V \sum_{\langle ij \rangle} n_i n_j$$

Answer: Yes, but ...

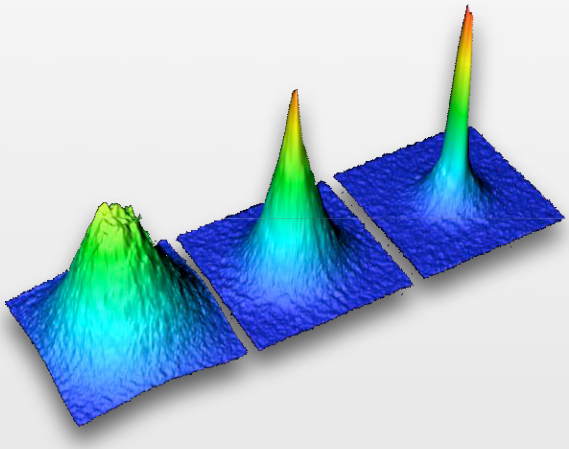
- tedious calculation of statistical weights for local worm updates
  ➡ implemented in ALPS

- high computational cost



An application of the worm code

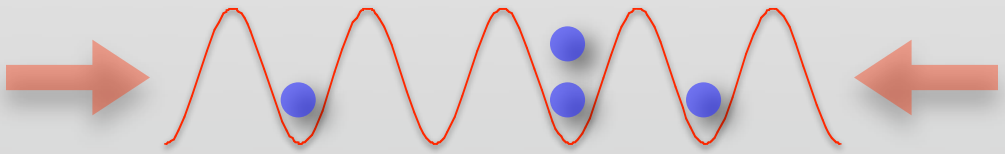
BEC in ultracold atomic gases



- Ultracold ^{87}Rb atoms form a Bose-Einstein condensate (BEC)
  - first observed in 1995

T. Esslinger, ETH Zürich

- Standing laser waves form an optical lattice



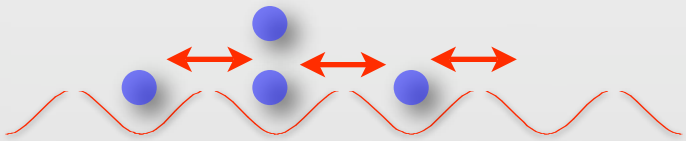
Realization of Bose-Hubbard model

$$H = -t \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + \text{h.c.} \right) + U \sum_i n_i (n_i - 1)/2 - \mu \sum_i n_i + V \sum_i r_i^2 n_i$$

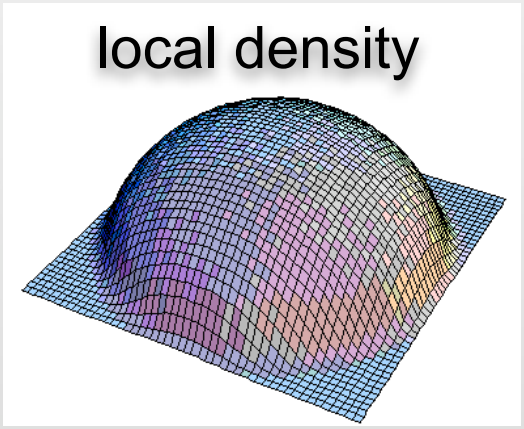
kinetic term

repulsion

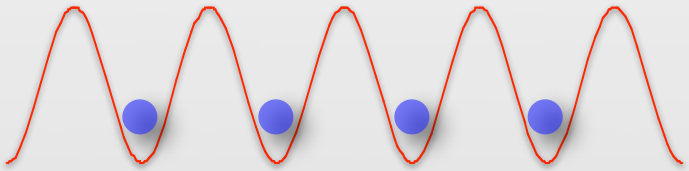
trap



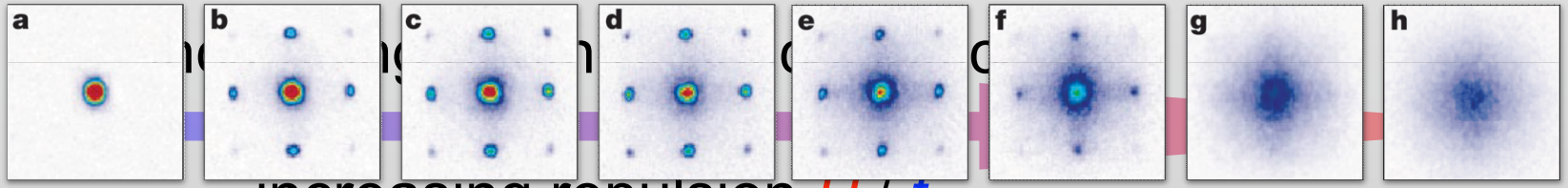
suprafluid
coherent BEC



S. Wessel, F. Alet, M. Troyer



Mott-isolator
incoherent



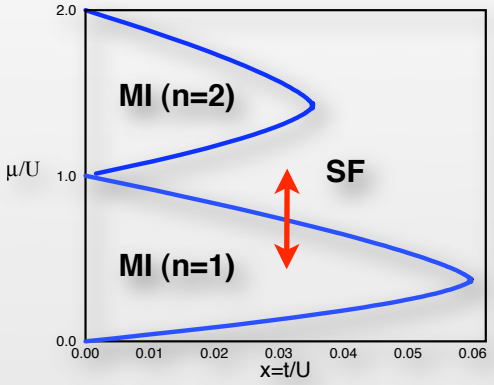
increasing repulsion U / t

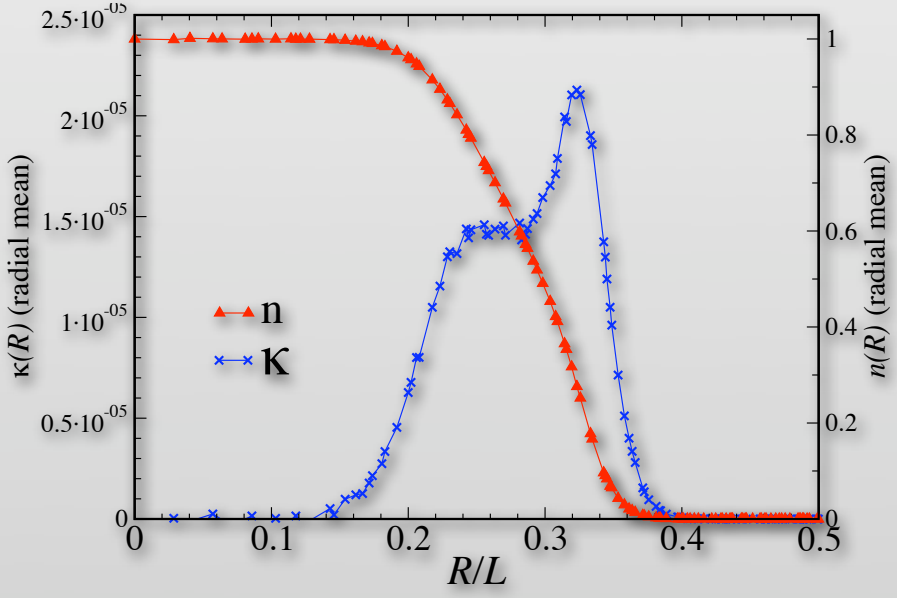
M. Greiner et al. Nature (2001)

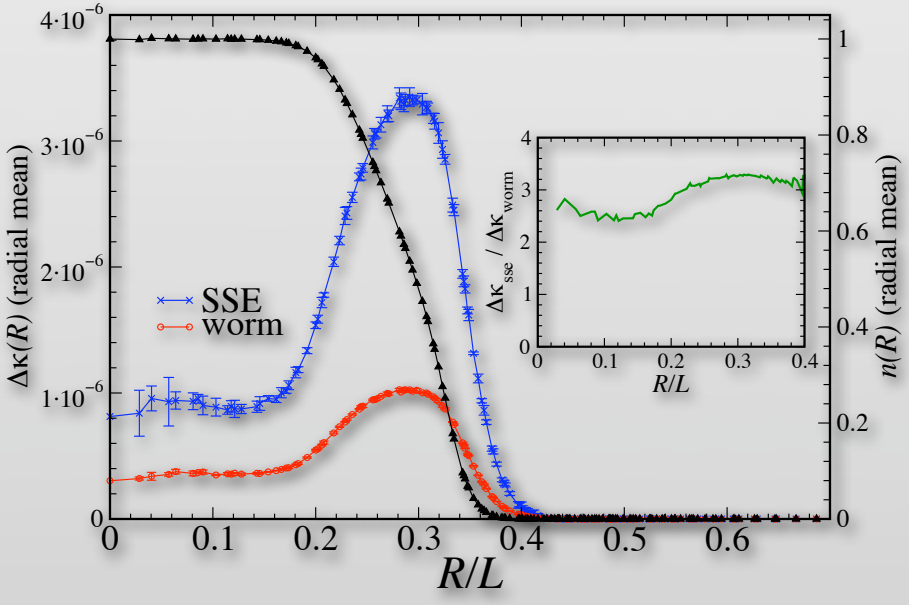
Simulations of trapped bosons

We are interested in the limit $t/U \ll 1$

Comparison: worms & SSE $t/U = 0.03$







Summary

The worm algorithm

Path integral representation in continuous time
➡ no error from time discretization.

Perturbation in off-diagonal terms only
➡ high acceptance rate for updates, also when

$$\frac{\text{off} - \text{diagonal terms}}{\text{diagonal terms}} \ll 1$$

Ergodicity in temporal and spatial directions
➡ grand-canonical ensembles, non-zero winding numbers

Non-local interactions
➡ high-computational cost

References

Worm algorithm

N.V. Prokof'ev, B.V. Svistunov, I.S. Tupitsyn,
Exact, Complete, and Universal Continuous-Time Worldline Monte Carlo Approach to the Statistics of Discrete Quantum Systems
Phys. Lett. A **238**, 253 (1998)
Sov. Phys. - JETP **87**, 310 (1998); eprint cond-mat/9703200

Non-local updates

M. Troyer, F. Alet, S. Trebst, S. Wessel
Non-local Updates for Quantum Monte Carlo Simulations
AIP Conference Proceedings **690**, 400 (2003)