The Abdus Salam
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Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry

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Worm algorithm

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WORM ALGORITHM FOR CLASSICAL AND QUANTUM STATISTICAL MODELS

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National Science Foundation
WHERE DISCOVERIES BEGIN

DARPA DSO DEFENSE SCIENCES OFFICE

OLE OPTICAL LATTICE EMULATOR

NASA

Trieste, January 2008

Why bother with algorithms?

Efficiency

PhD while still young

PhD while still young
Better accuracy
Large system size
More complex systems
Finite-size scaling
Critical phenomena
Phase diagrams

Reliably!

New quantities, more theoretical tools to address physics

Grand canonical ensemble $N(\mu)$
Off-diagonal correlations $G(r,\tau)$
"Single-particle" and/or
condensate wave functions $\varphi(r)$
Winding numbers and ρ_S

New physics

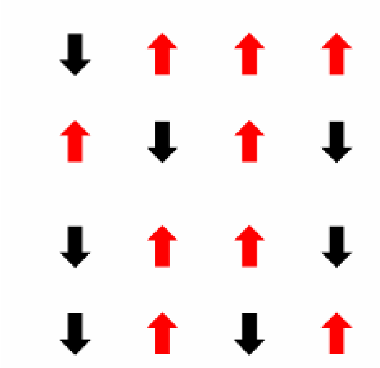
Applications: **classical and quantum critical phenomena,**
latttice spin systems, cold atoms (bosons & fermions),
liquid&solid Helium-4 ...

Worm algorithm idea

Standard Monte Carlo setup:

- configuration space =

(depends on the model and it's representation)



arbitrary closed loops
(more or less anything you can draw without loose ends)

- each cnf. has a weight factor W_{cnf}

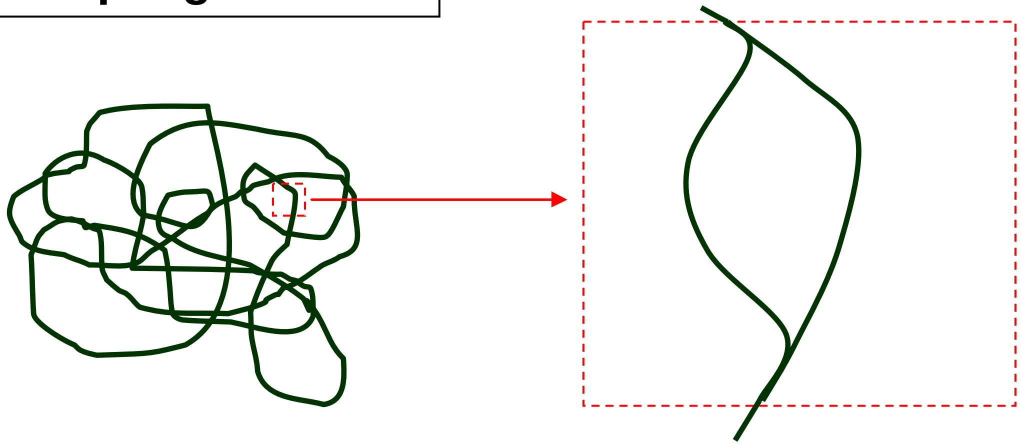
$$e^{-E_{cnf}/T}$$

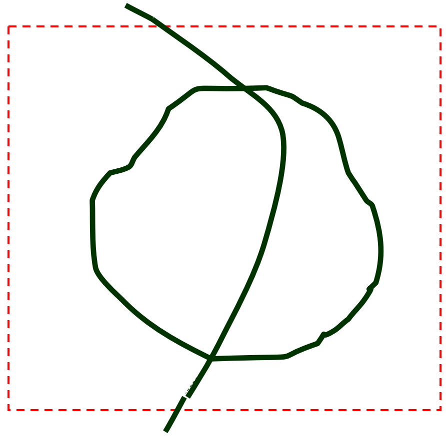
- quantity of interest $A_{cnf} \longrightarrow \langle A \rangle = \frac{\sum_{cnf} A_{cnf} W_{cnf}}{\sum_{cnf} W_{cnf}}$

“conventional” sampling scheme:

local shape change

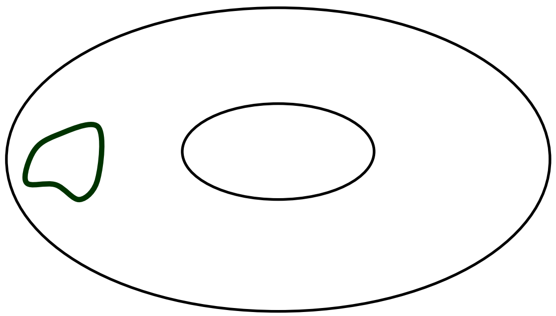
Add/delete small loops



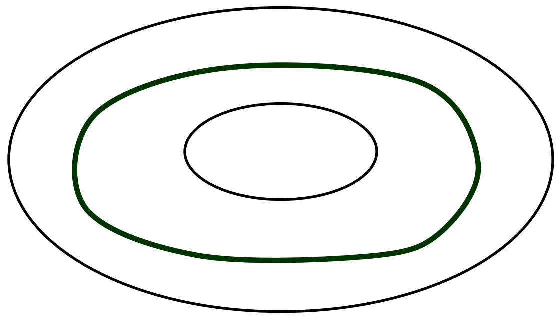


No sampling of topological classes

(non-ergodic)



can not evolve to



Critical slowing down

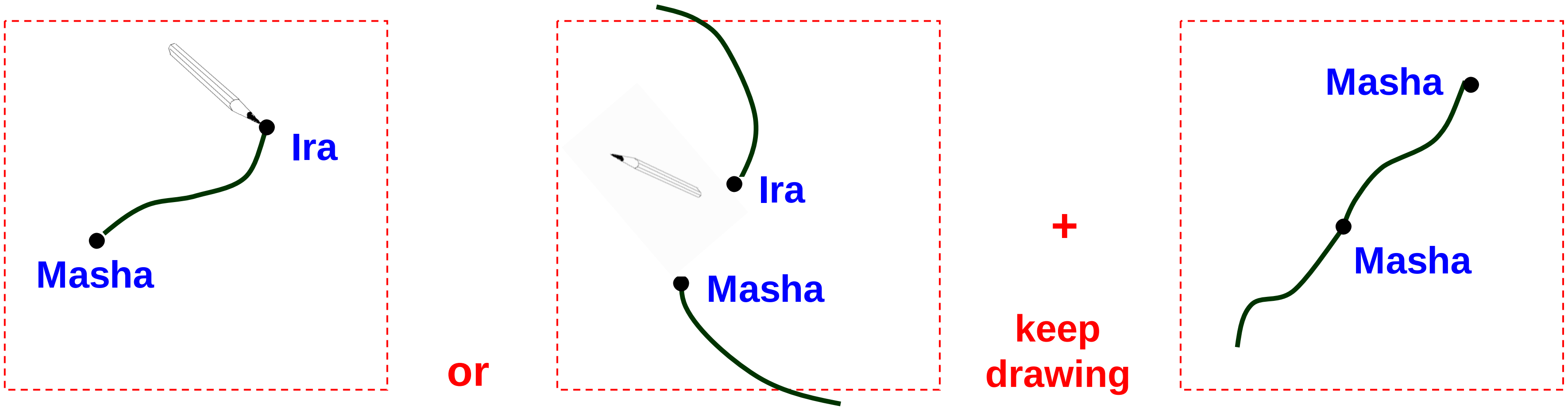
(large loops are related to critical modes)

$$\left(\frac{N_{\textbf{updates}}}{L^d} \right) \sim L^z$$

dynamical critical exponent
$z \approx 2$ **in many cases**

Worm algorithm idea

draw and erase:



- Topological classes are sampled efficiently (whatever you can draw!)

- No critical slowing down in most cases

Disconnected loops relate to important physics (correlation functions) and are not merely an algorithm trick!

High-T expansion for the Ising model

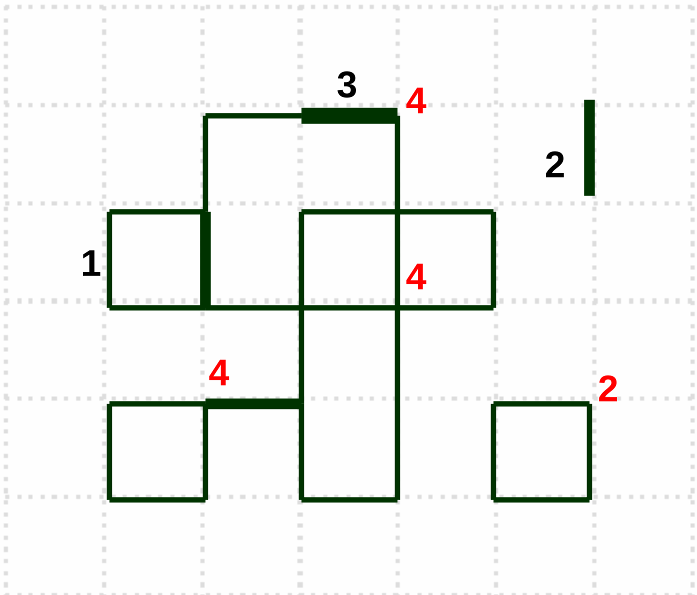
$$-\frac{H}{T} = K \sum_{<ij>} \sigma_i \sigma_j \qquad (\sigma = \pm 1)$$

$$Z = \sum_{\{\sigma_i\}} e^{\sum_{<ij>} K\sigma_i\sigma_j} = \sum_{\{\sigma_i\}} \left(\prod_{b=<ij>} e^{K\sigma_i\sigma_j} \right) \equiv \sum_{\{\sigma_i\}} \left(\prod_{b=<ij>} \sum_{N_b=0}^{\infty} \frac{K^{N_b}}{N_b!} (\sigma_i\sigma_j)^{N_b} \right)$$

$$\equiv \sum_{\{N_b\}} \left(\prod_{b=<ij>} \frac{K^{N_b}}{N_b!} \right) \prod_i \left(\sum_{\sigma_i=\pm 1} \sigma_i^{M_i} \right)$$

where $M_i = \sum_{<ij>} N_{b=<ij>} = even$

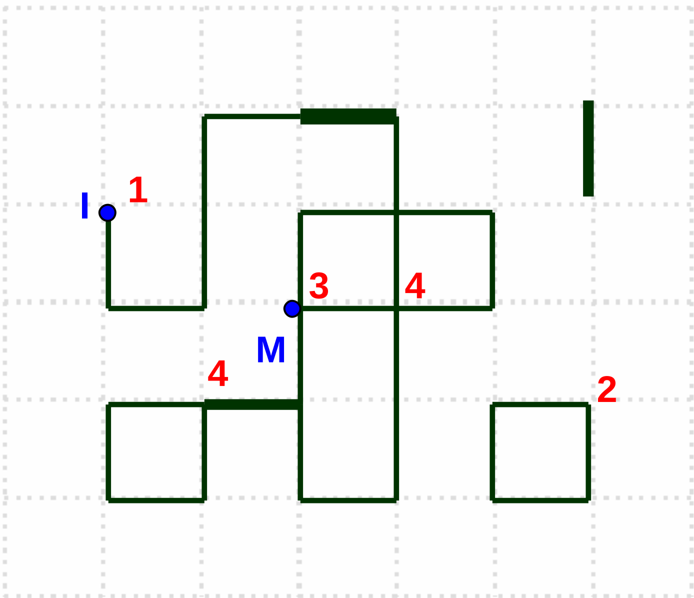
$$\equiv 2^N \sum_{\{N_b\}=loops} \left(\prod_{b=<ij>} \frac{K^{N_b}}{N_b!} \right)$$



$N_b =$ **number of lines;**
enter/exit rule $\rightarrow M_i = even$

Spin-spin correlation function: $g_{IM} = \dfrac{G_{IM}}{Z}$, $G = \sum_{\{\sigma_i\}} e^{-H/T} \sigma_I \sigma_M$

$$G \equiv \underbrace{\sum_{\{N_b\}} \left(\prod_{b=<ij>} \frac{K^{N_b}}{N_b!} \right) \prod_i \left(\sum_{\sigma_i = \pm 1} \sigma_i^{M_i + \delta_{iI} + \delta_{iM}} \right)}_{\text{same as before}} \equiv 2^N \sum_{\substack{\{N_b\} = \text{ loops } + \\ \text{Ira}-\text{Masha worm}}} \left(\prod_{b=<ij>} \frac{K^{N_b}}{N_b!} \right)$$



Worm algorithm cnf. space = $Z \bigcup G$

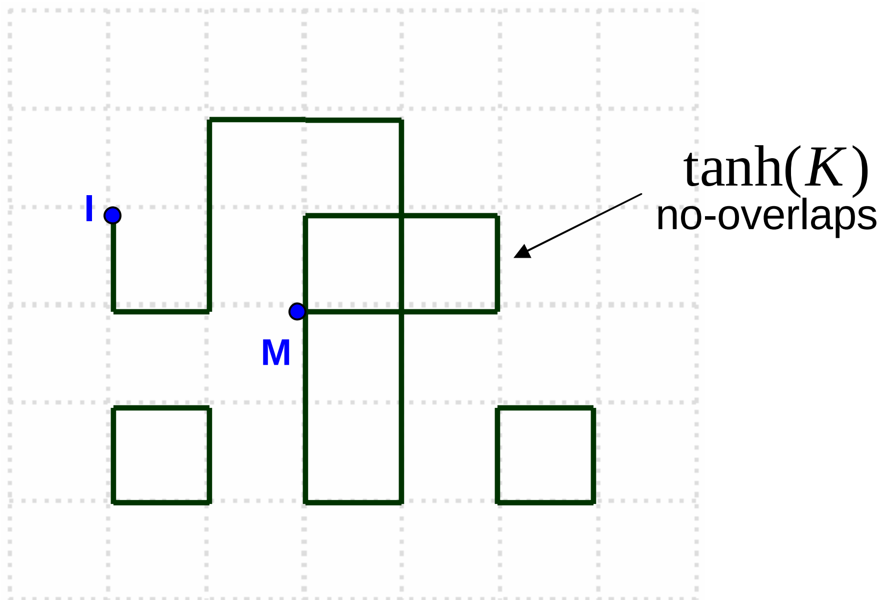
Same as for generalized partition

$$Z_W = Z + \kappa G$$

Getting more practical: **since** $e^{K\sigma_1\sigma_2} = \cosh^N(K)\left[1+\tanh(K)\sigma_1\sigma_2\right]$

$$Z = \cosh^{dN}(K) \sum_{\{N_b=0,1\}}^{loops} \left(\prod_b \tanh^{N_b}(K) \right)$$

Complete algorithm :



- If $I = M$, select a new site for them at random

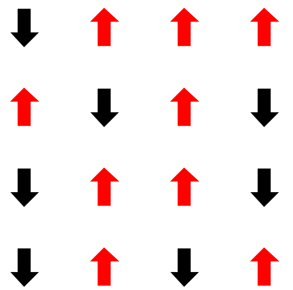
- select direction to move M, let it be bond b

- If $N_b = \begin{cases} 0 \\ 1 \end{cases}$ accept $N_b \to \begin{cases} 1 \\ 0 \end{cases}$ with prob. $R = \begin{cases} \min(1, \tanh(K)) \\ \min(1, \tanh^{-1}(K)) \end{cases}$

Solving the critical slowing down problem:

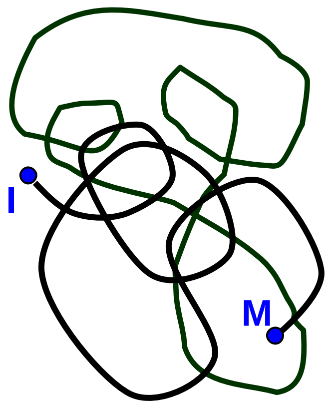
Question: What are the signatures of the phase transition (critical modes)?

spin representation

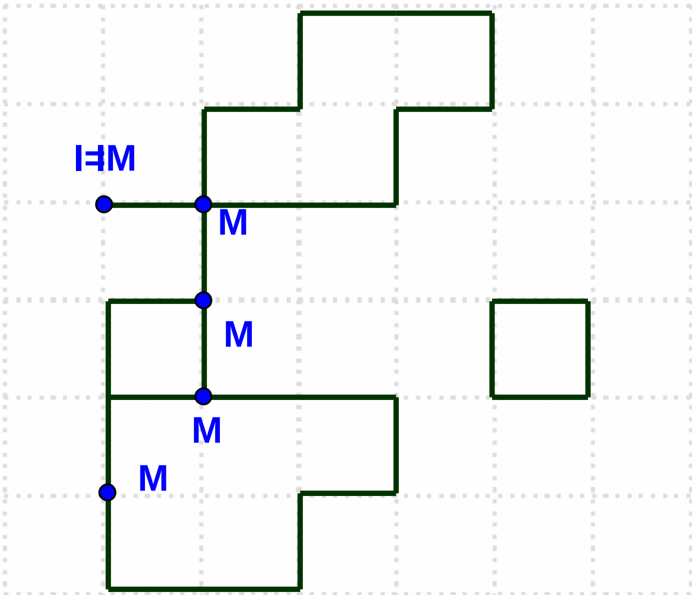


large domains of similarly oriented spins of linear size ~ L → **single-spin flips are not efficient in updating them!**

loop representation



large loops of linear size ~ L (long-range correlations between spins = large distance between I and M) → **draw large loops!**



$$G(I-M) = G(I-M) + 1$$

$$Z = Z + \delta_{I,M}$$

$$N_{links} = N_{links} + \left(\sum_b N_b \right)$$

Correlation function: $g(i) = G(i)/Z$

Magnetization fluctuations: $\left\langle M^2 \right\rangle = \left\langle \left(\sum \sigma_i \right)^2 \right\rangle = \sum_{ij} \left\langle \sigma_i \sigma_j \right\rangle = N \sum g(i)$

Energy: either $E = -JNd \left\langle \sigma_1 \sigma_2 \right\rangle = -JNdg(1)$

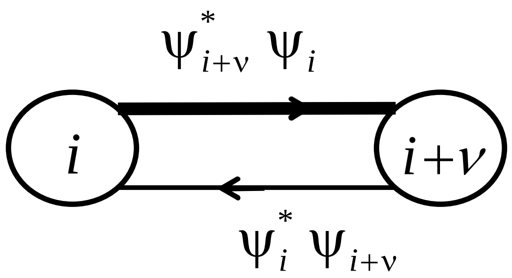
or $E = -J \tanh(K) \left[dN + \left\langle N_{links} \right\rangle \sinh^2(K) \right]$

Ising $\longrightarrow |\psi_i|^4$ lattice-field theory

$$-\frac{H}{T} = t\sum_{i\,\nu=\pm(x,y,z)} \psi^*_{i+\nu}\,\psi_i + \mu\sum_i|\psi_i|^2 - U\sum_i|\psi_i|^4$$

(XY-model in the $\mu = 2U \to \infty$ **limit)**

Start as before



$$Z = \prod_i \int d\psi_i\ e^{-H/T}$$

expand on each bond

$$e^{t\,\psi^*_{i+\nu}\,\psi_i} = \sum_{N=0}^{\infty} \frac{t^{N_{i\nu}}\,(\psi^*_{i+\nu}\psi_i)^{N_{i\nu}}}{N_{i\nu}!}$$

Integrate over phases

$$\psi_i = xe^{i\varphi}$$

$$Z = \sum_{N_{i\nu}}\left(\prod_{i\nu}\frac{t^{N_{i\nu}}}{N_{i\nu}!}\right)\underbrace{\prod_i\left(\int d\psi_i\ \underbrace{\psi_i^{M_{1i}}\left(\psi^*_i\right)^{M_{2i}}}_{e^{i\varphi(M_{1i}-M_{2i})}\ \to\ M_{1i}=M_{2i}=M_i}\ e^{\mu|\psi_i|^2-U|\psi_i|^4}\right)}_{\prod_i Q(M_i)}$$

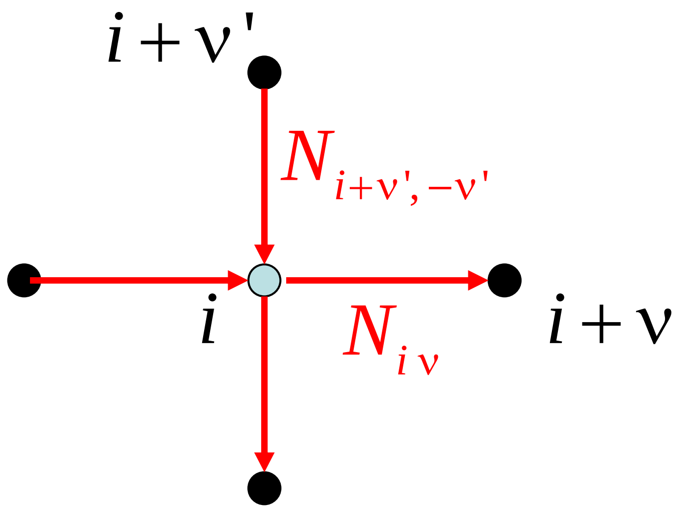
where
$$Q(M) = \begin{cases} 0 & \text{if } M_1 \neq M_2 \\ \pi\int_0^\infty dx\ x^M e^{\mu x - Ux^2} & \end{cases}$$

$\longrightarrow$ **closed oriented loops**

$=$ **tabulated numbers**

$$\psi_i^{\sum_\nu N_{i\nu}} \left(\psi^*_i\right)^{\sum_\nu N_{i+\nu,-\nu}}$$

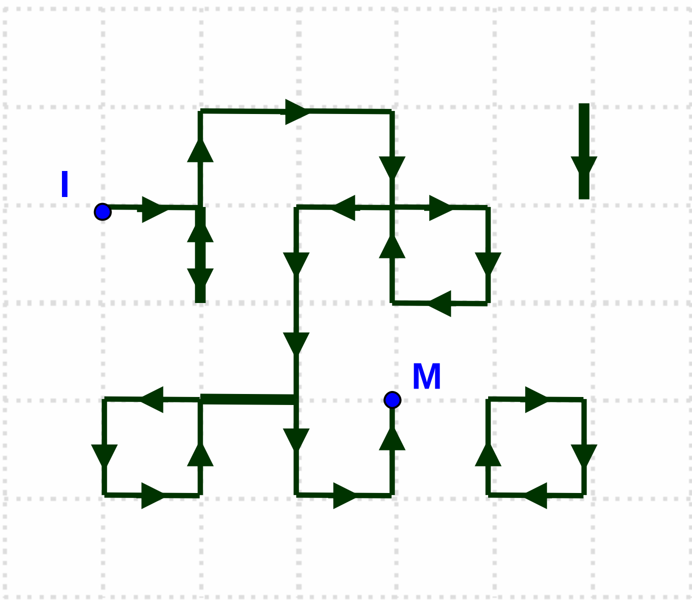
Flux in = Flux out $\Rightarrow$ closed oriented loops of integer N-currents



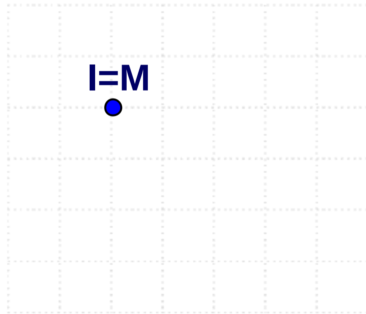
$$g(I-M) = \frac{G(I-M)}{Z} = \left\langle \psi_I \psi^*_M \right\rangle$$

(one open loop)

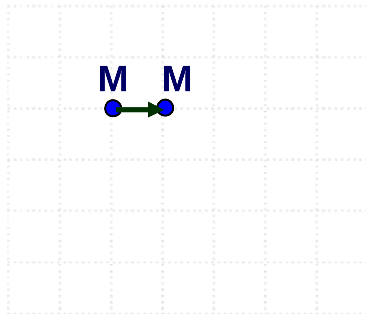
Z-configurations have $I = M$



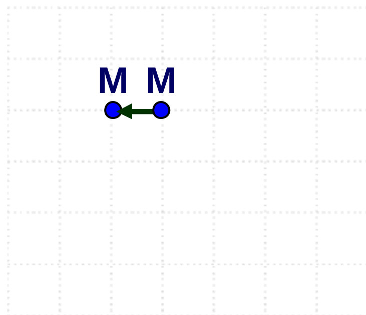
Same algorithm:



- $Z \leftrightarrow G$ **sectors, prob. to accept** $R_{Z\to G} = \min\left[1, \dfrac{Q(M_I+1)}{Q(M_I)}\right]$



- $N_{M\,\nu} \to N_{M\,\nu}+1$ **draw** $R = \min\left[1, \dfrac{t\,Q(M_{M'}+1)}{(N_{M\,\nu}+1)Q(M_{M'})}\right]$



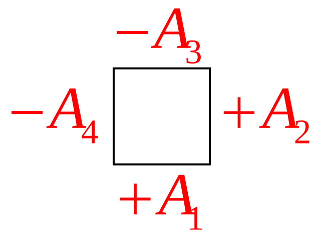
- $N_{M+\nu,-\nu} \to N_{M+\nu,-\nu}-1$ **erase** $R = \min\left[1, \dfrac{(N_{M+\nu,-\nu})\,Q(M_M-1)}{t\,Q(M_M)}\right]$

Keep drawing/erasing …

Multi-component gauge field-theory:

$$-\frac{H}{T} = t\sum_{a;i\nu} \psi^{*}_{a,i+\nu}\psi_{a,i}\, e^{iA_\nu(i)} + \mu \sum_{a;i} \left|\psi_{a,i}\right|^2 - \sum_{ab;i} U_{ab} \left|\psi_{a,i}\right|^2 \left|\psi_{b,i}\right|^2 - \kappa \sum_{\square} [\nabla \times A_\nu(i)]^2$$

plaquette sum



solid-liquid transitions, deconfined criticality,
XY-VBS and Neel-VBS quantum phase transitions, etc.

… and finite-T quantum models

Interacting particles on a lattice:

$$H = H_0 + H_1 = \sum_{ij} U_{ij} n_i n_j - \sum_i \mu_i n_i \quad - \sum_{<ij>} t(n_i, n_j)\, b_j^+ b_i$$

diagonal

off-diagonal

$$Z = \mathrm{Tr}\, e^{-\beta H} \equiv \mathrm{Tr}\, e^{-\beta H_0}\, e^{-\int_0^\beta H_1(\tau)\, d\tau}$$

$$H_1(\tau) = e^{\beta H_0} H_1\, e^{-\beta H_0}$$

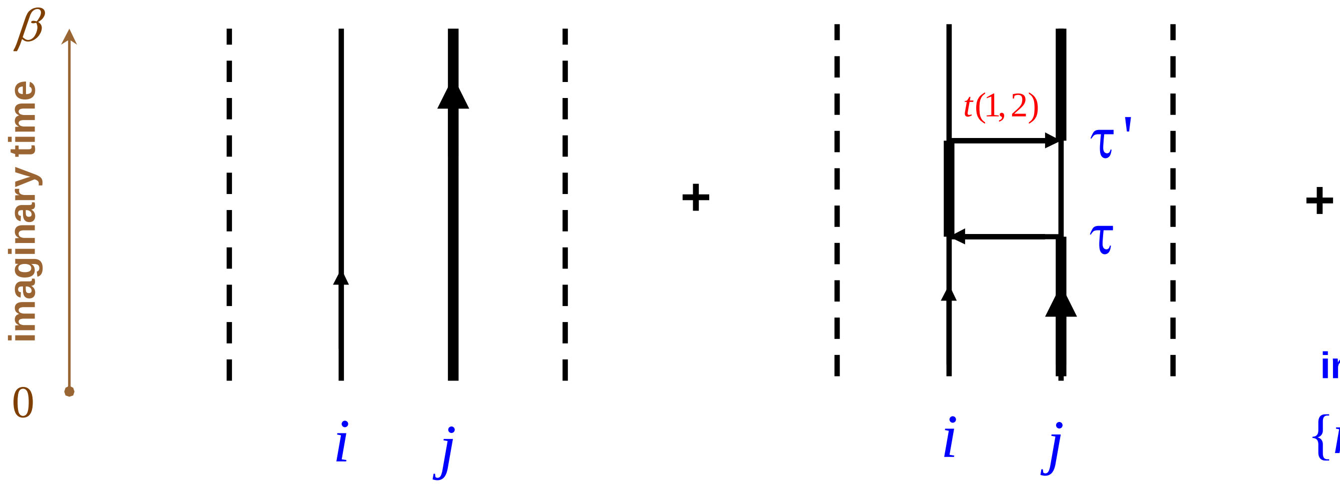
$$= \mathrm{Tr}\, e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau)\, d\tau + \int_{\tau'}^{\beta}\int_0^{\beta} H_1(\tau)\, H_1(\tau')\; d\tau\, d\tau' + \ldots \right\}$$

In the diagonal basis set (occupation number representation): $\langle \{n_i\} | = \langle \{n_1, n_2, n_3, \ldots\} |$

$$Z = \sum_{\{n_i\}} \left\langle \{n_i\} \right| \; e^{-\beta H_0} - \int_0^\beta e^{-(\beta-\tau) H_0} H_1 e^{-\tau H_0}\; d\tau + \int_{\tau'}^{\beta}\int_0^{\beta} e^{-(\beta-\tau) H_0} H_1\, e^{-(\tau-\tau') H_0} H_1\, e^{-\tau' H_0}\; d\tau\, d\tau' + \ldots \left| \{n_i\} \right\rangle$$

Each term describes a particular evolution of $\{n_i\}$ as imaginary "time" increases

0-order term **one of the 2-order terms**



in this example

$\{n_i\} = 0, 1, 2, 0$

$$Z = \sum_{\{n_i(\tau)\}} e^{-\int_0^\beta U(\{n_i(\tau)\})d\tau} \prod_{k=1}^{K} \langle \{n_i(\tau_k + 0)\} \,|\, (-H_1\, d\tau_k) \,|\, \{n_i(\tau_k - 0)\} \rangle$$

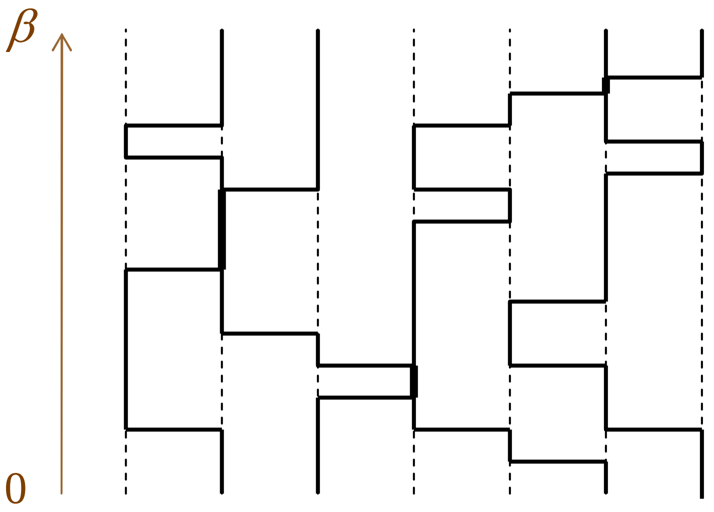
all possible trajectories for N particles with K hopping transitions

potential energy contribution

off-diagonal matrix elements for the trajectory with K kinks at times $\beta > \tau_K > \ldots > \tau_2 > \tau_1 > 0$ (ordered sequence on the β-cylinder)

in this example, for K=2, it equals
$t\sqrt{2} \times t\sqrt{2}$ **for bosons**

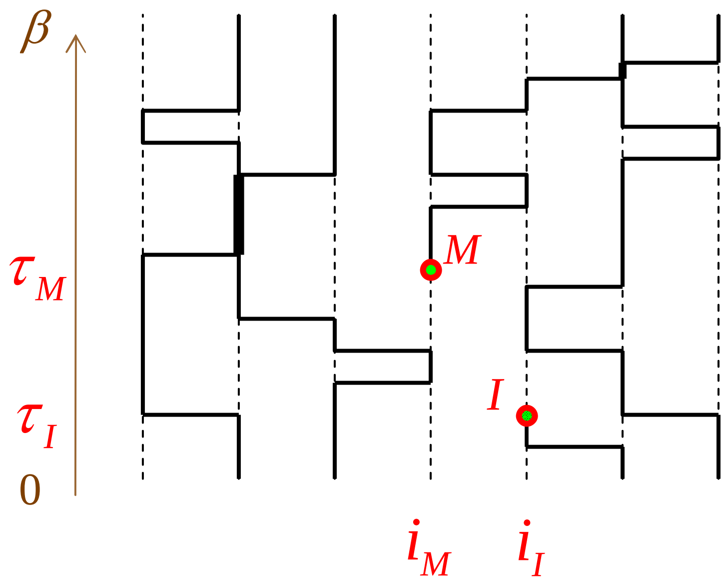
high-order term for $Z = \mathrm{Tr}\, e^{-\beta H}$



Similar expansion in hopping terms for

$$G_{IM} = \mathrm{Tr}\, b_M^{\dagger}(i_M, \tau_M)\, b_I(i_I, \tau_I)\, e^{-\beta H}$$

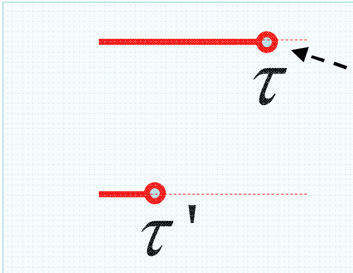
+ two special points for Ira and Masha



The rest is worm algorithm in this $Z \cup G_{IM}$ **configuration space:**
draw and erase lines using exclusively Ira and Masha

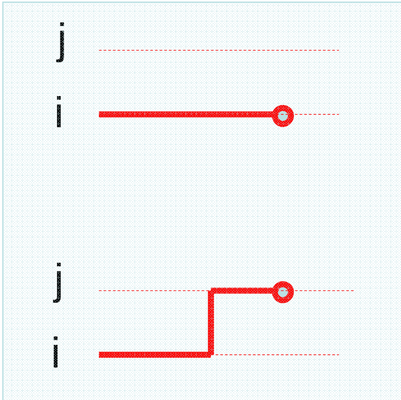
ergodic set of local updates

time shift:

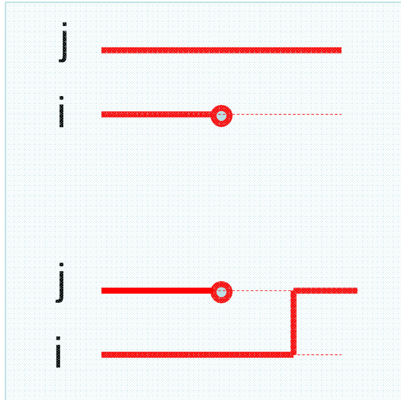


Ira or Masha

space shift ("particle" type):

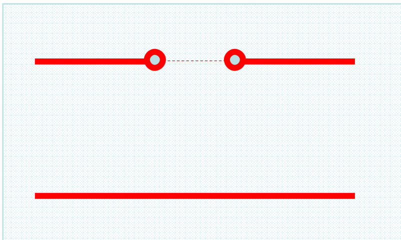


space shift ("hole" type):

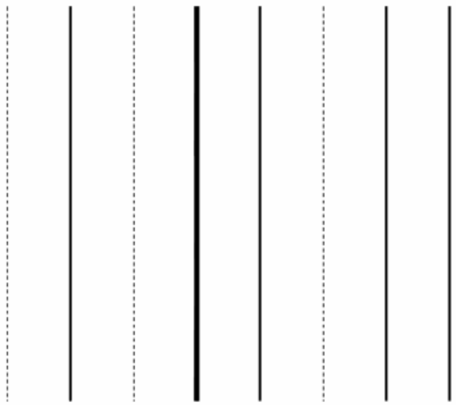


Insert/delete Ira and Masha:

$Z \leftrightarrow G$



connects Z and G configuration spaces



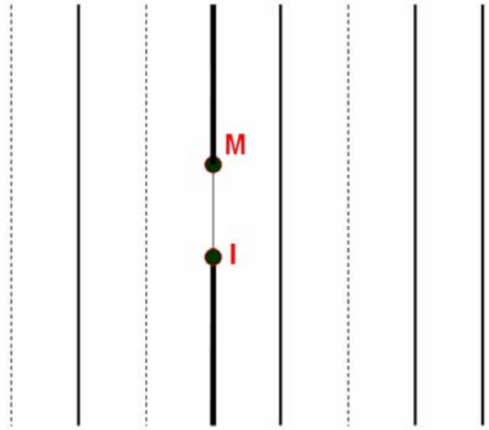


Fig.1

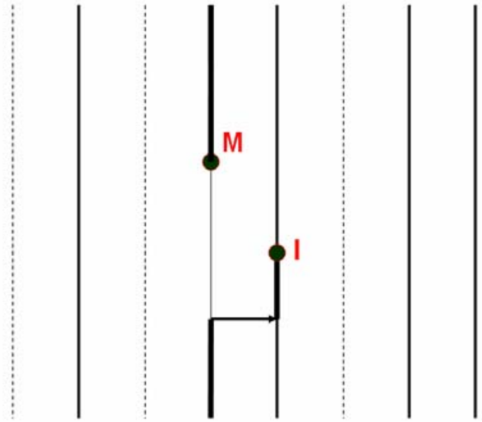


Fig.2

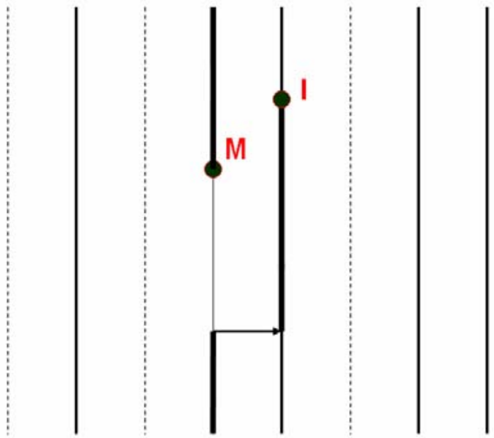


Fig.3

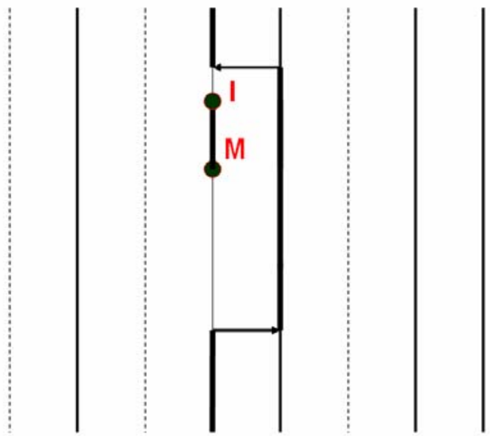


Fig.4

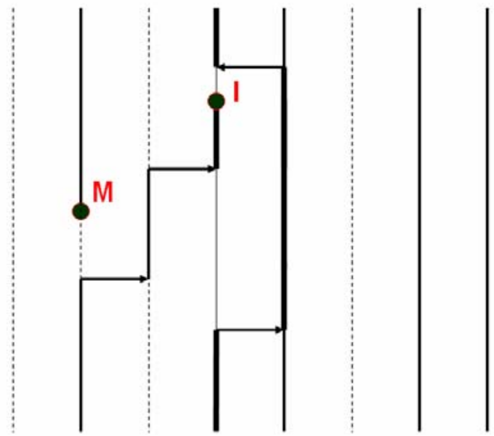
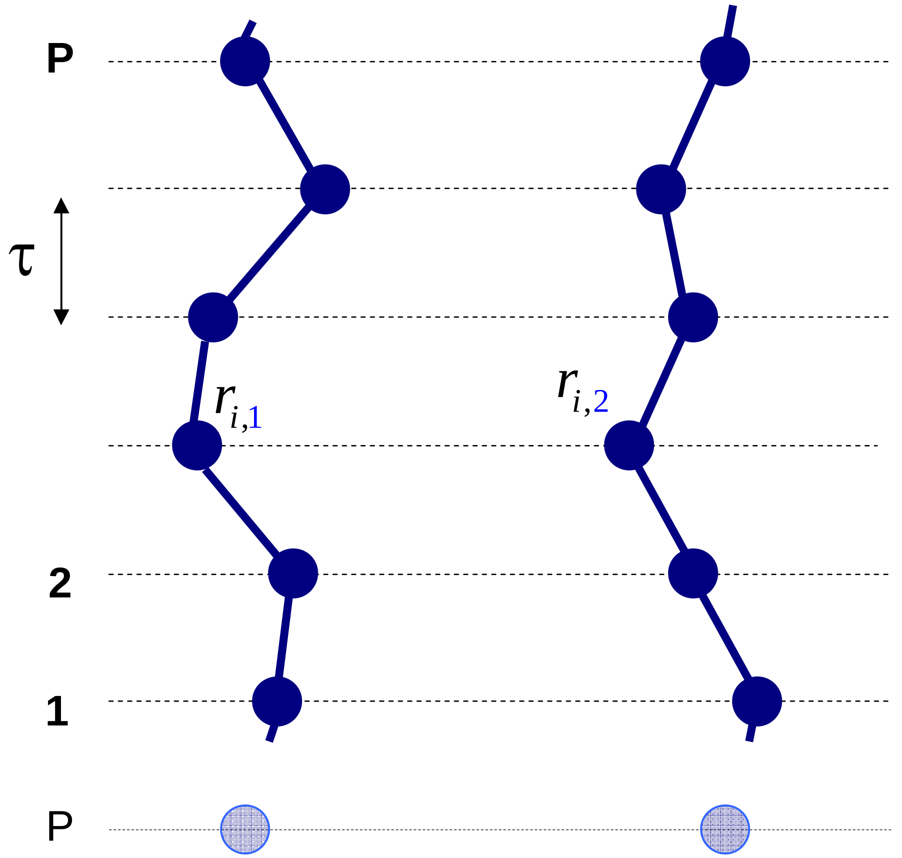


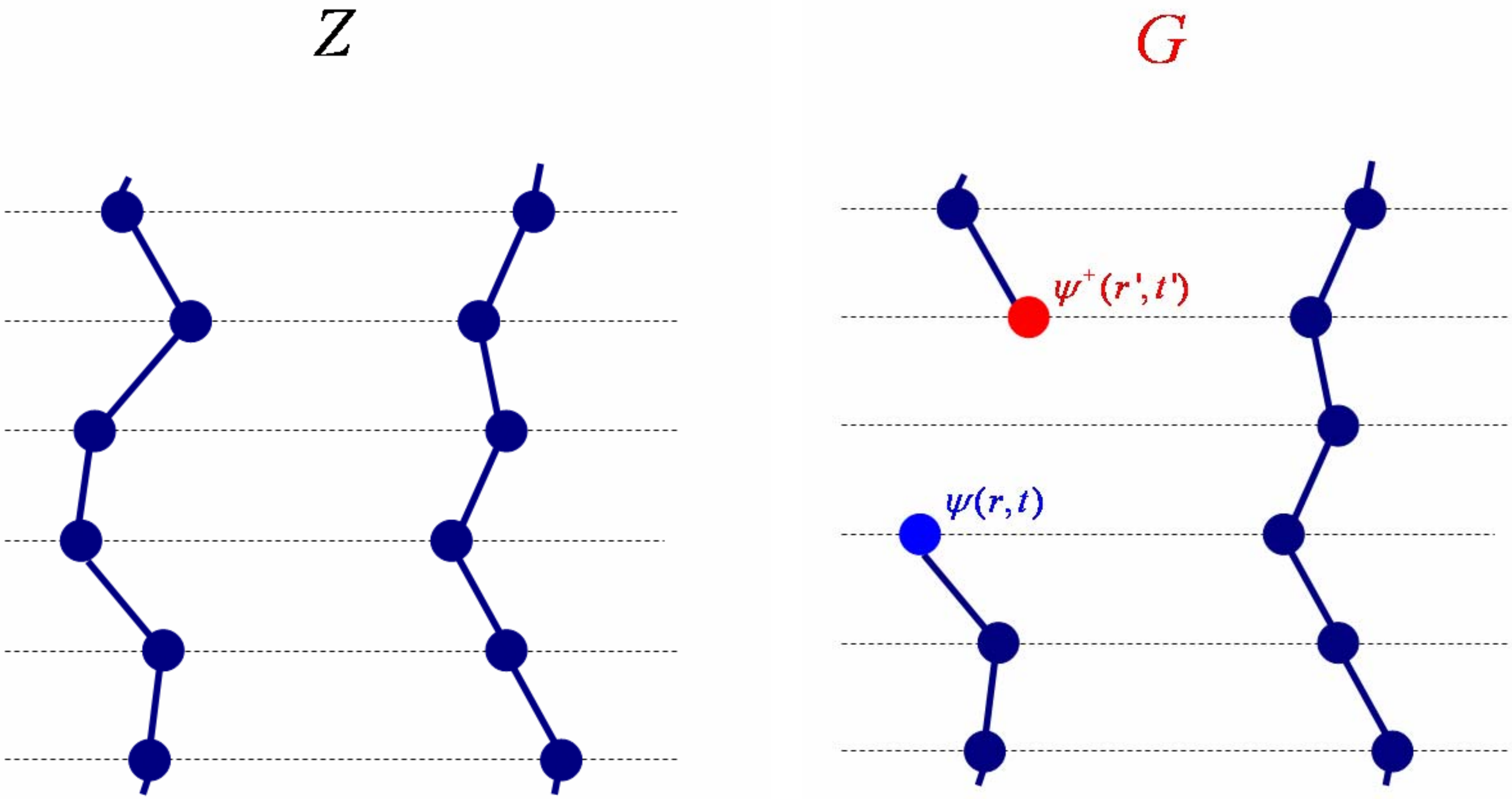
Fig.5

Path-integrals in continuous space

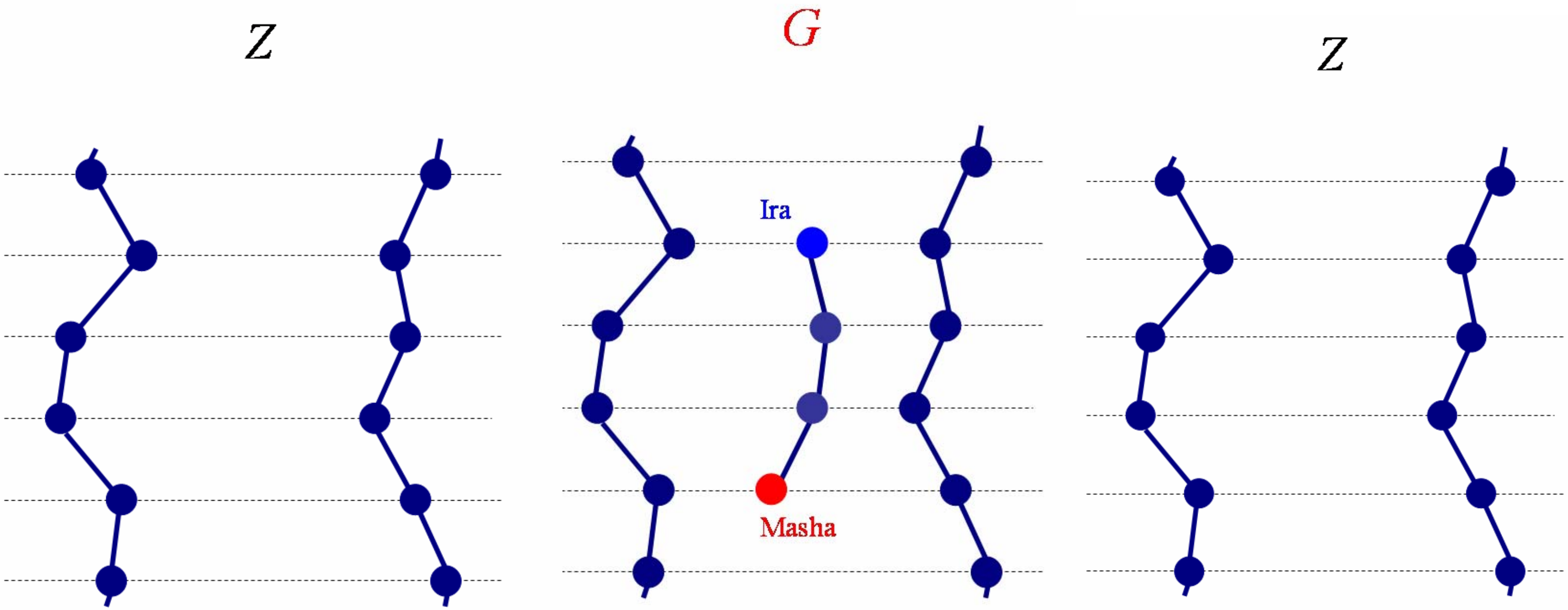
$$Z = \iiint dR_1 \ldots dR_P \exp\left\{ -\sum_{i=1}^{P=\beta/\tau} \left(\frac{m(R_{i+1} - R_i)^2}{2\tau} + U(R)\tau \right) \right\}$$



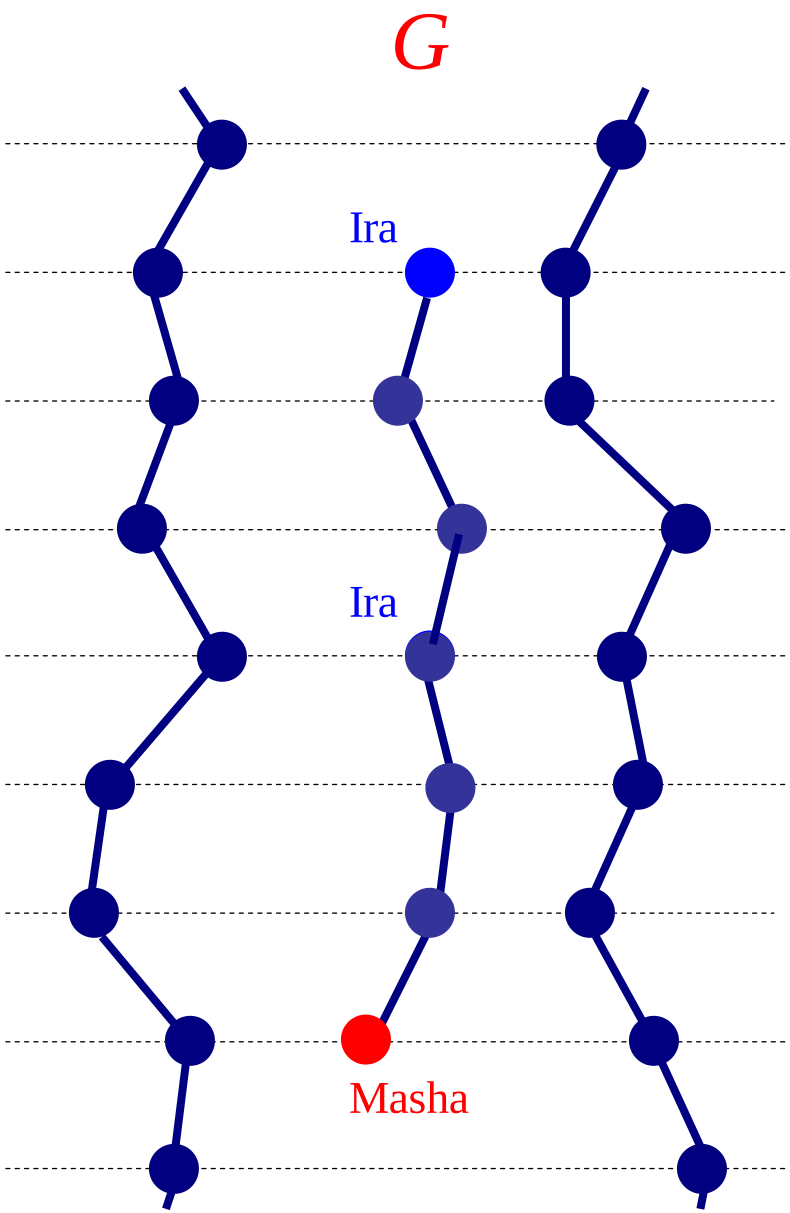
$$R_i = (r_{i,1}, r_{i,2}, \ldots, r_{i,N})$$



(open/close update)

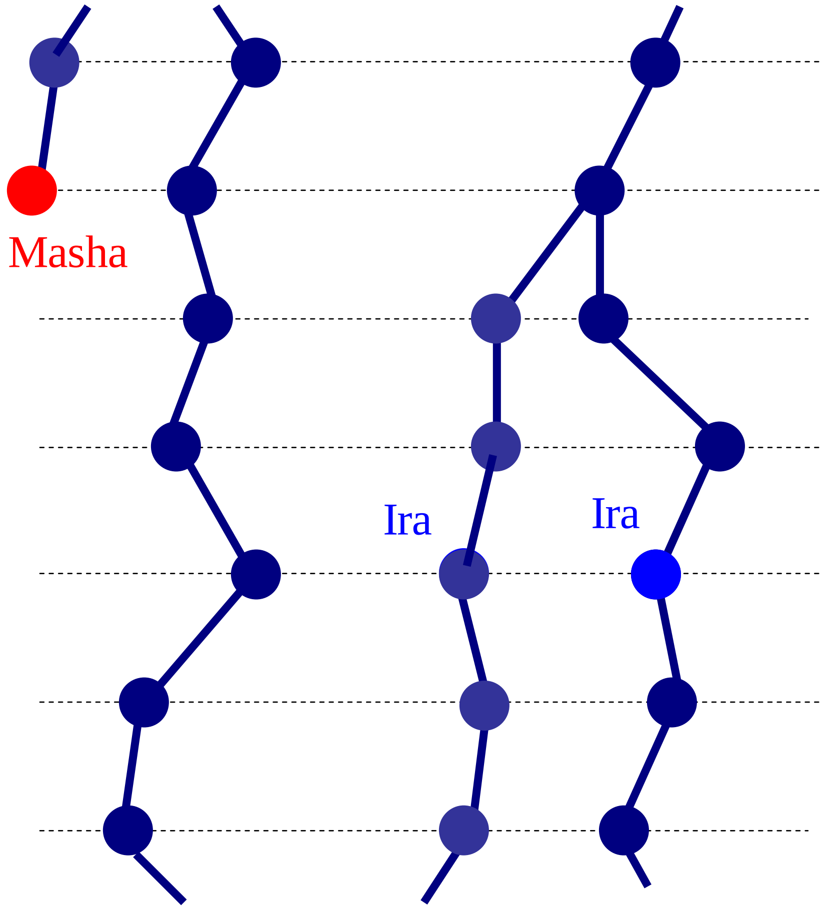


(insert/remove update)



(advance/recede update)

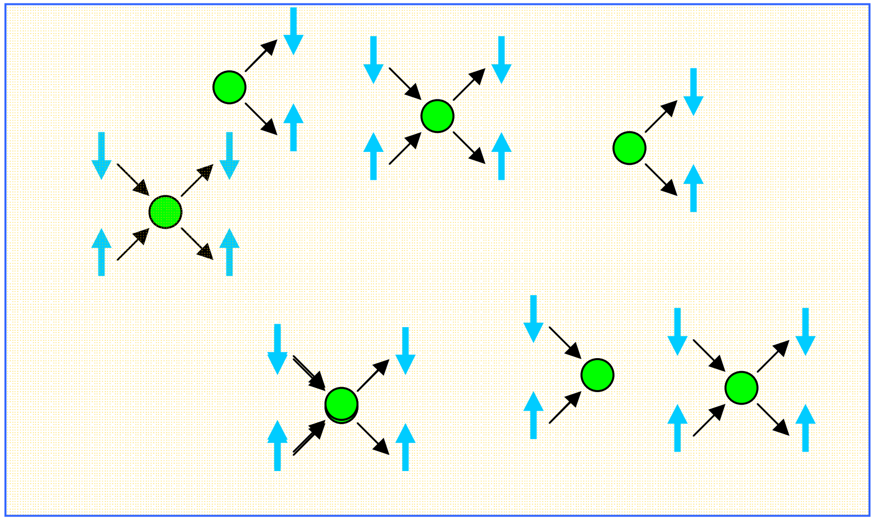
G



(swap update)

Not necessarily for closed loops!

Feynman (space-time) diagrams for fermions with contact interaction (attractive) $\bullet = -U$
(n=1 positive Hubbard model too)



Pair correlation function

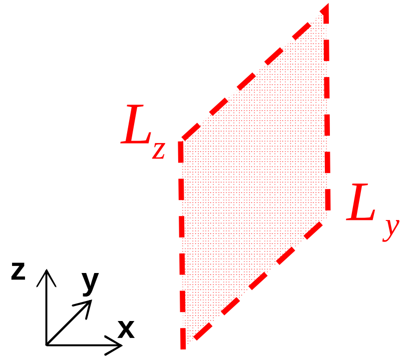
$$\left\langle a_\uparrow^{+}(r_1,\tau_1) a_\downarrow^{+}(r_1,\tau_1)\ a_\downarrow(r_2,\tau_2) a_\uparrow(r_2,\tau_2) \right\rangle$$

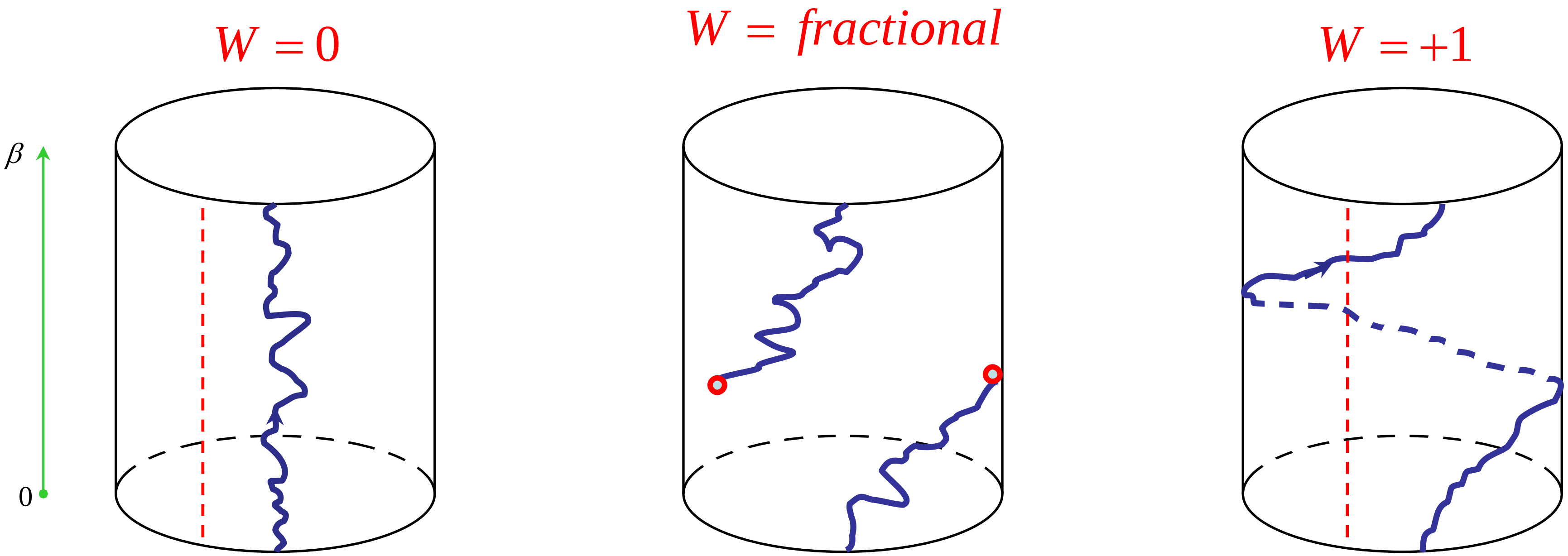
The rest is worm algorithm in this $Z \cup G_{IM}$ **configuration space:**
draw and erase interaction vertexes using exclusively Ira and Masha

More: winding numbers and superfluid density

$$W_\mu = \int_0^\beta \left[\text{particle number flux}\right]_\mu d\tau$$

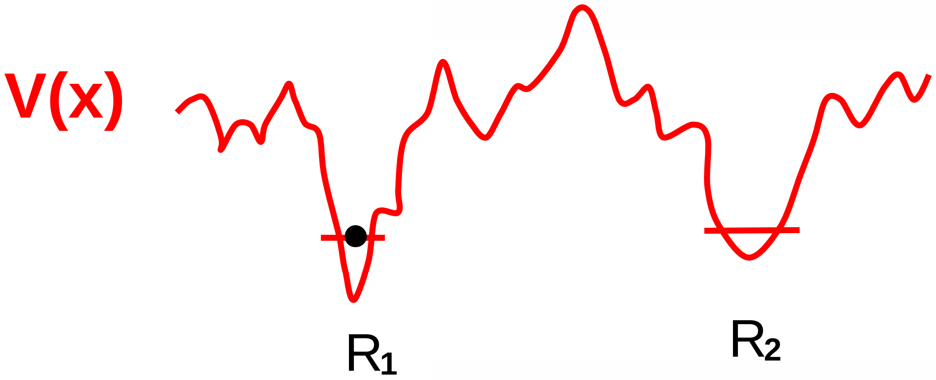
(cross-section independent in Z-sector)





$$\boxed{\rho_S = (m / \beta d L^{d-2}) \left\langle W^2 \right\rangle}$$

Grand canonical ensemble (a “must” for disorder problems!)



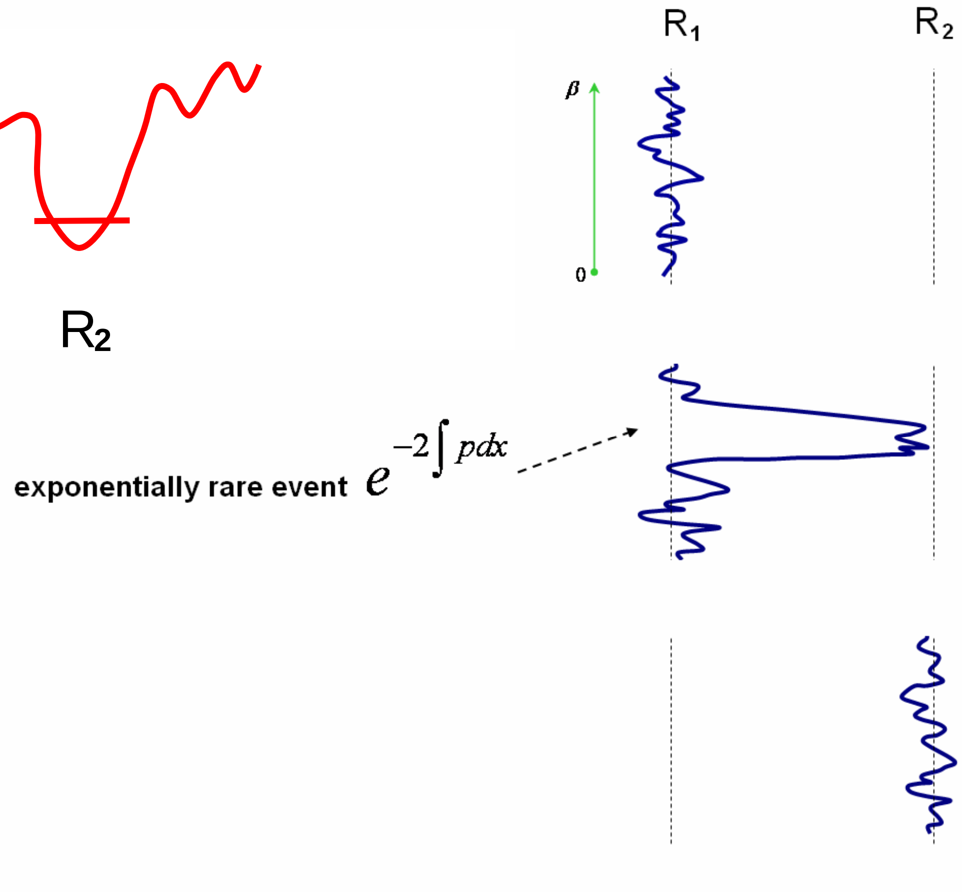


Fig.1

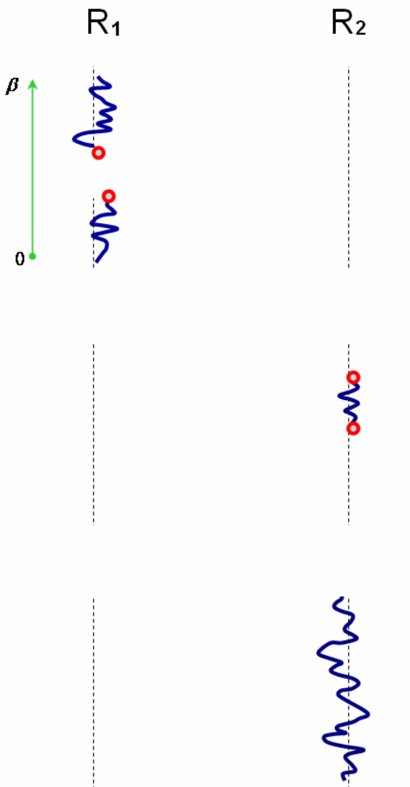


Fig.2

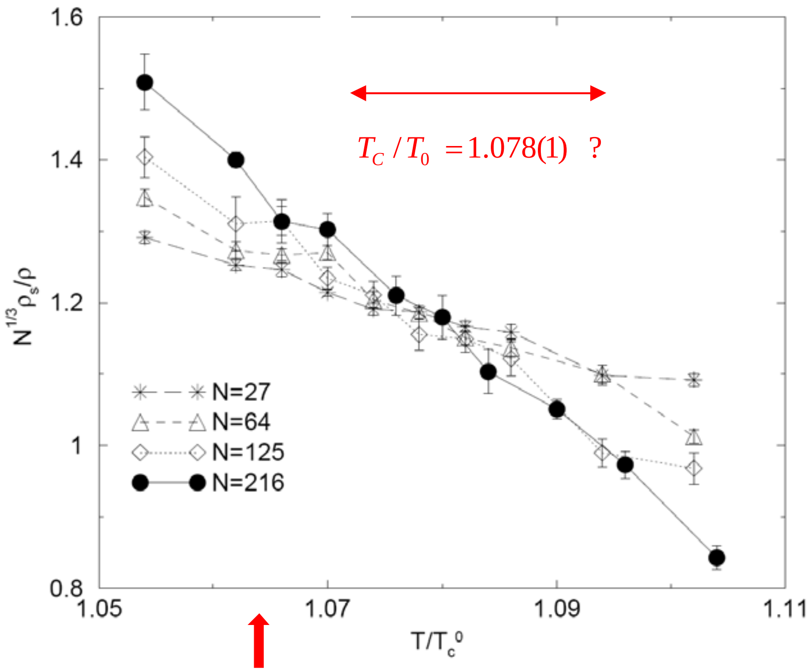
Some examples:

Weakly interacting Bose gas:

$$T_C(n^{1/3}a)/T_C^{(0)}$$

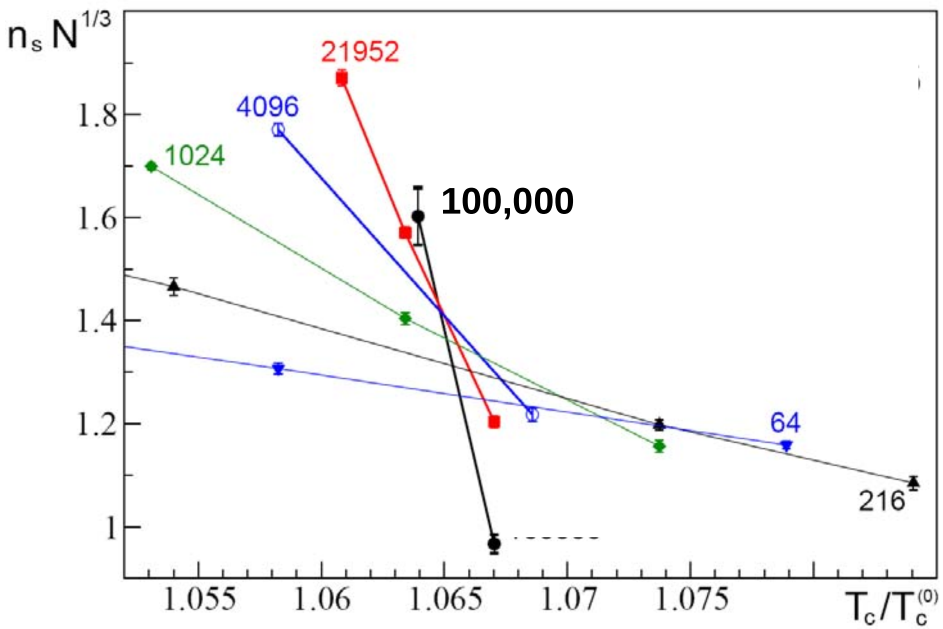
$na^3 = 5\times 10^{-3}$

Nho, Landau '04



correct value

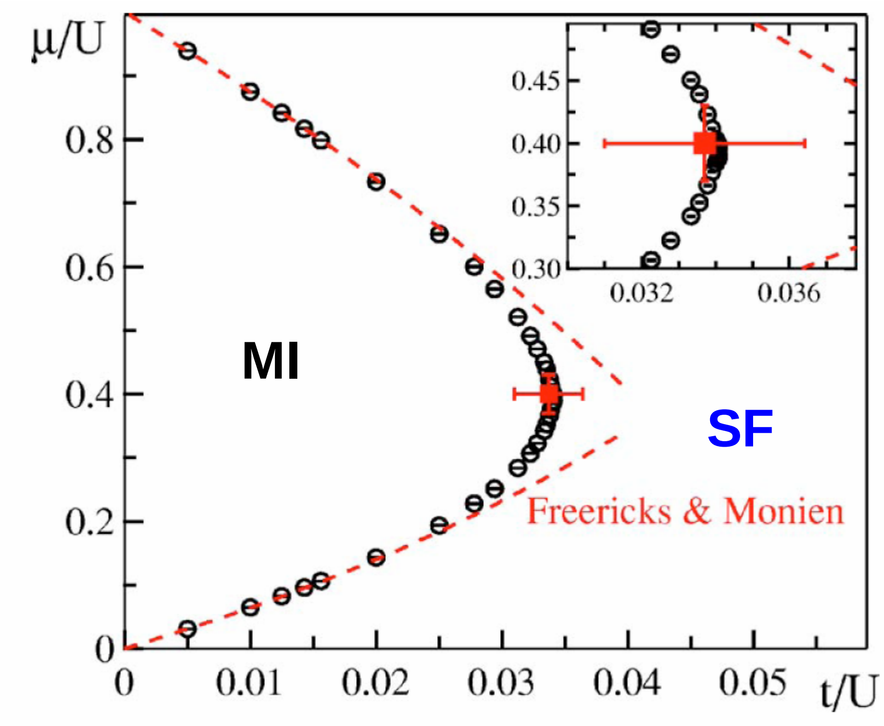
Worm algorithm: Pilati, Giorgini, NP



Imperfect crossing due to corrections to scaling

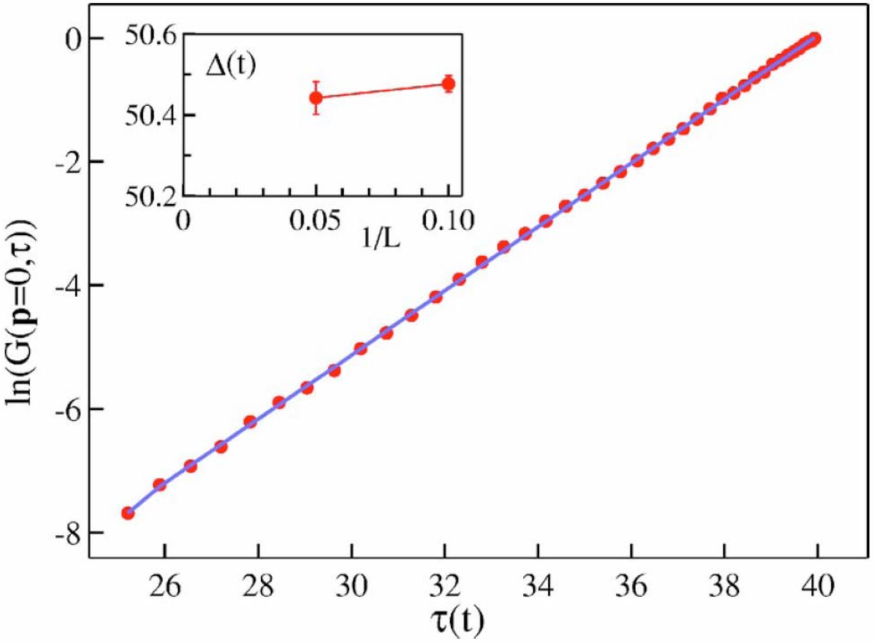
Mott insulator – superfluid T=0 phase diagram:

$(\mu/U,\ t/U)$ plane , 3D case



$(\mu/U)_{\pm}$ **determine gaps for adding/removing particles from the MI state with** $\langle n \rangle = 1$

gaps control the exponential decay of the Green's function $G(p=0,\tau)$ **in time**



Otherwise, good luck in calculating energy differences

$E(N\pm1)-E(N)$ for $N=L^3$ with $L=40$

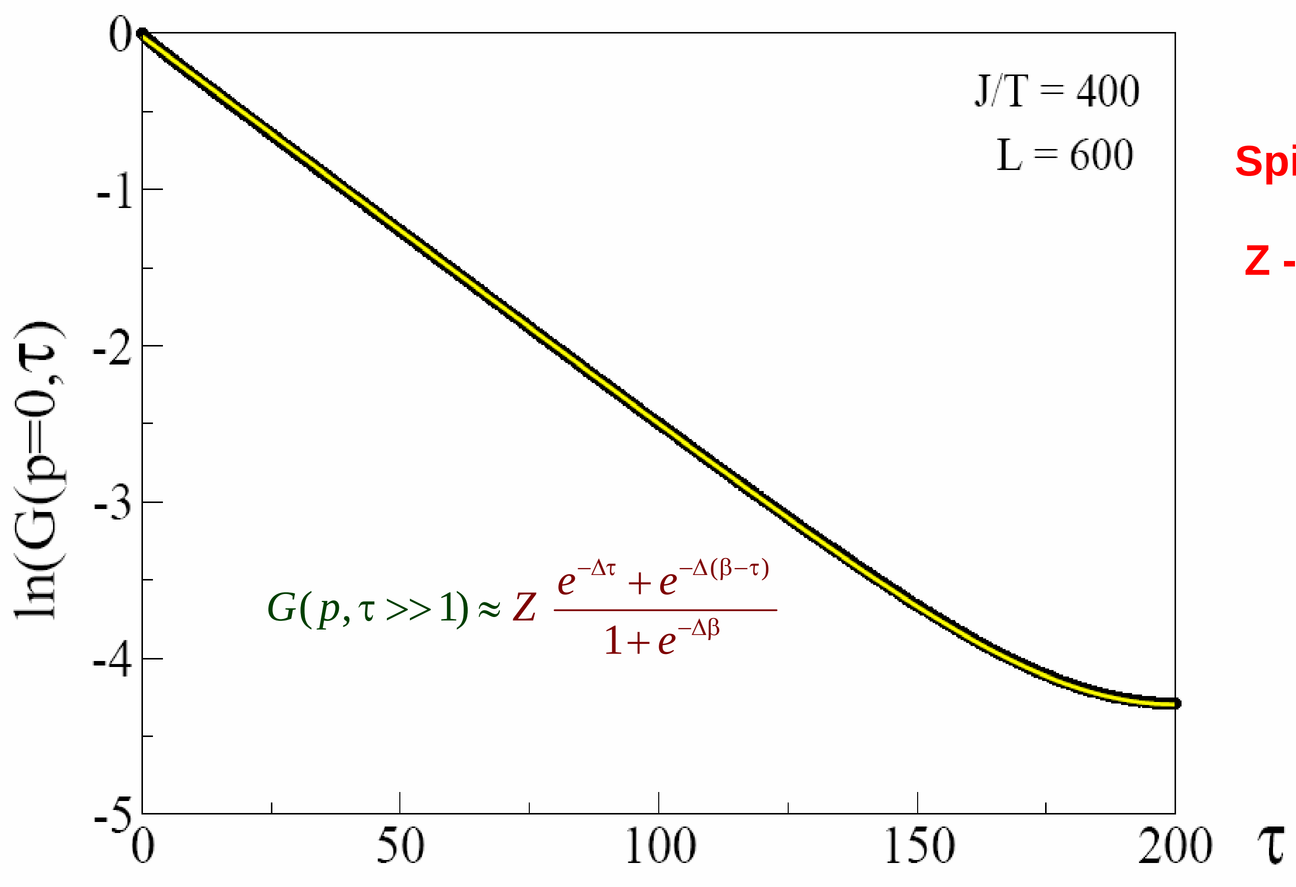
Current standard for simulations of bosons in optical lattices and in traps:

all experimental parameters “as is”, including particle number” $N \sim 10^6$

Quantum spin chains gaps, spin wave spectra, magnetization curves …

$$\mathbf{H} = -\sum_{<ij>} [J_x\,(S_{jx}S_{ix} + S_{jy}S_{iy}) + J_z\,S_{jz}S_{iz}] - H\sum_i S_{iz}$$

Energy gap: One dimensional S=1 chain with $J_z / J_x = 0.43$

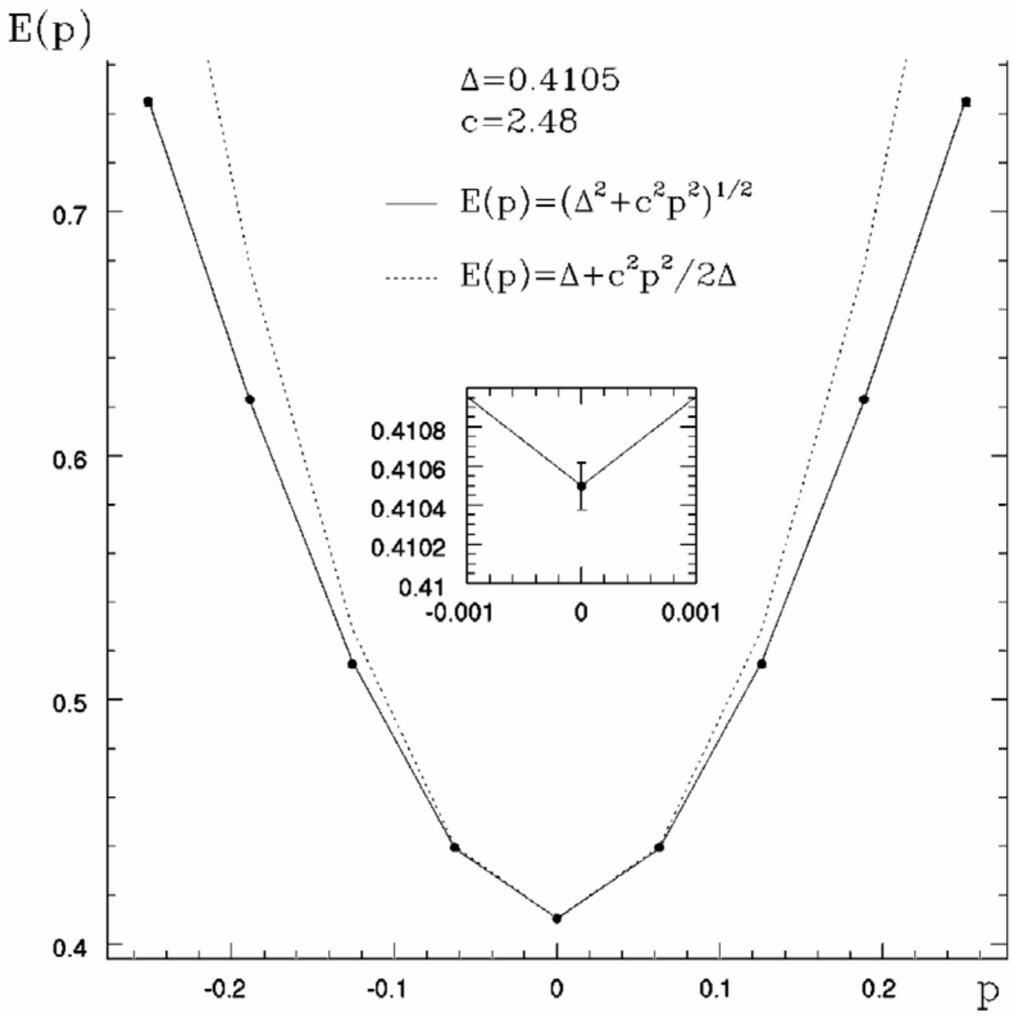


Spin gap $\Delta = 0.02486(5)$

Z -factor $Z = 0.980(5)$

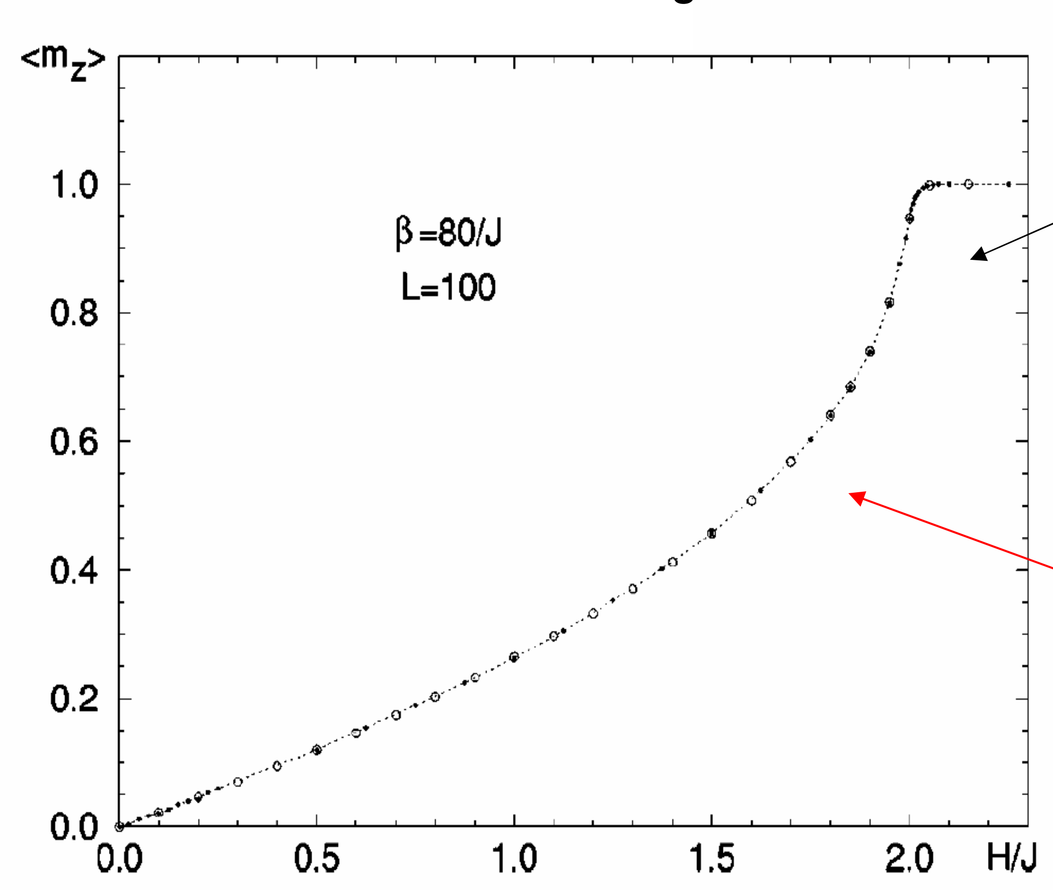
Spin waves spectrum:

One dimensional S=1 Heisenberg chain



magnetization curves

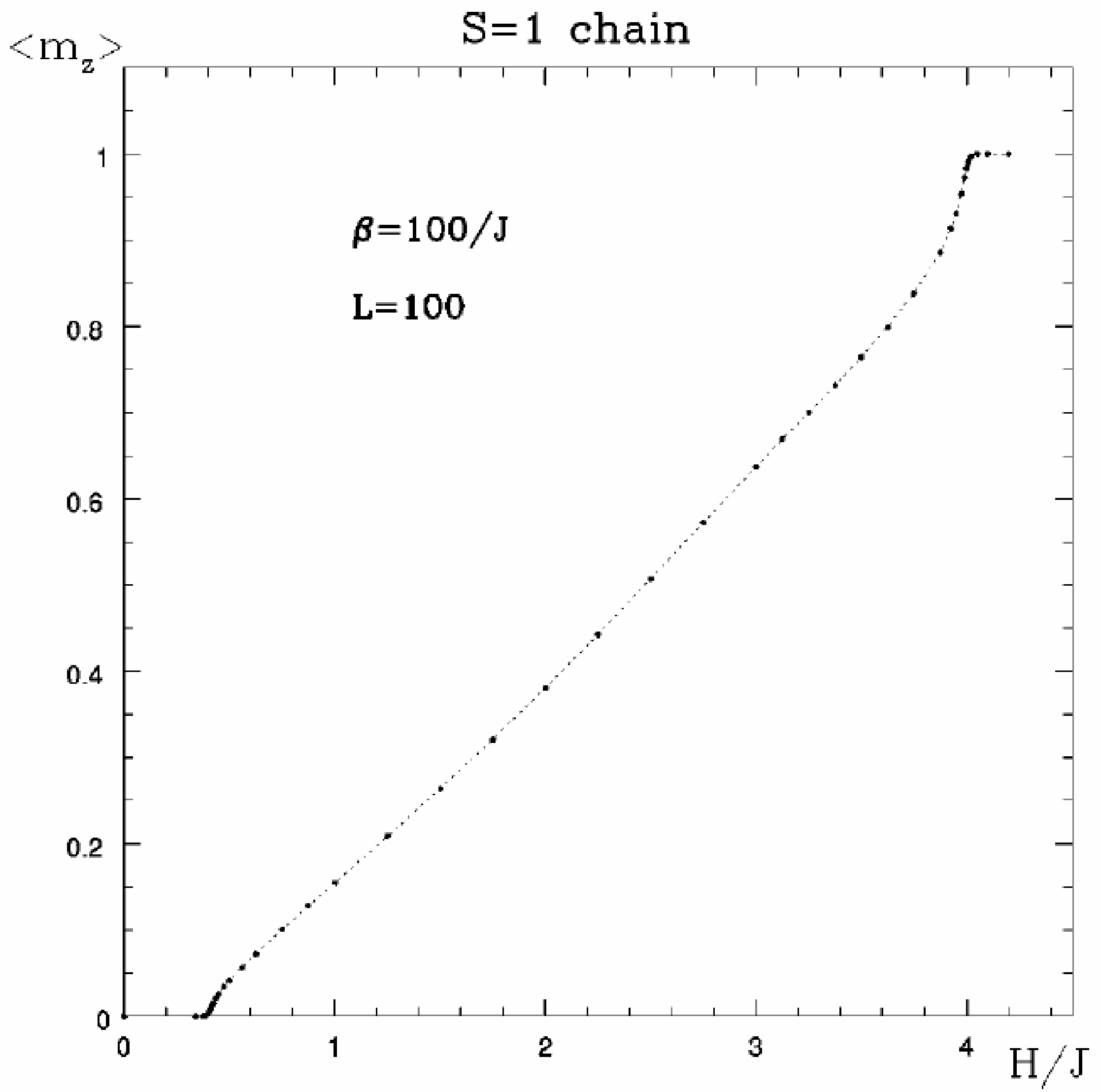
S=1/2 Heisenberg chain



MC data

Bethe ansatz

magnetization curves



More tools:

1. Density matrix $n(r',r)=\left\langle \psi^{\dagger}(r',\tau)\psi(r,\tau)\right\rangle$ (and the condensate fraction) is as cheap as energy

2. μ is an input parameter, and $\langle N\rangle_{\mu}$ is a simple diagonal property

3. But also compressibility $\kappa VT=\left\langle \left(N-\langle N\rangle\right)^{2}\right\rangle_{\mu}$

$$P_{\mu'}(N)=P_{\mu}(N)\,e^{(\mu'-\mu)N/T}$$

4. Added particle wavefunction:

$$G(\beta/2\to\infty,r,r')=\left\langle G_N\left|\psi^{\dagger}(r)\right|G_{N-1}\right\rangle\left\langle G_{N-1}\left|\psi(r')\right|G_N\right\rangle=\varphi(r)\varphi(r')$$

mobility thresholds, participation ratio, etc.

Why bother with algorithms?

Efficiency

PhD while still young

PhD while still young
Better accuracy
Large system size
More complex systems
Finite-size scaling
Critical phenomena
Phase diagrams

Reliably!

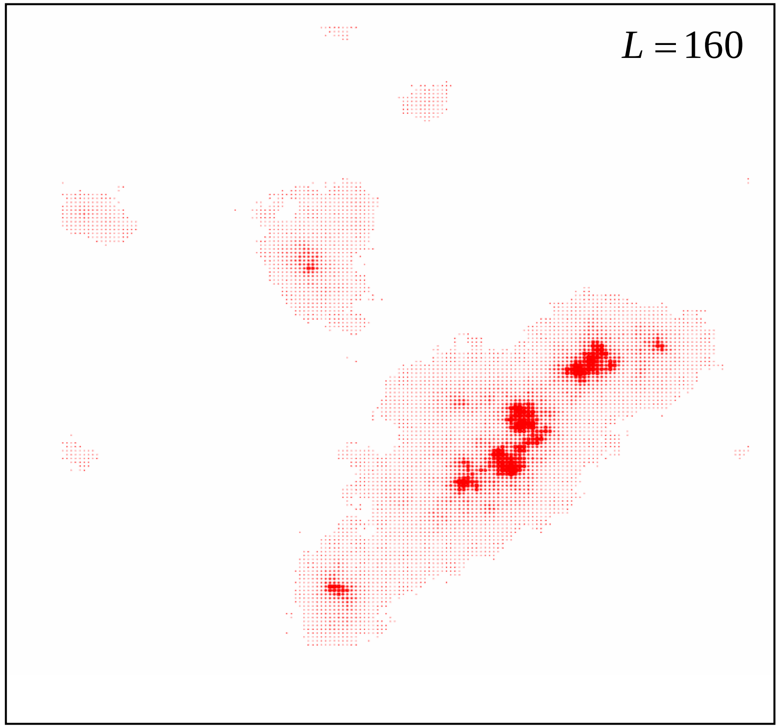
New physics

New quantities, more theoretical tools to address physics

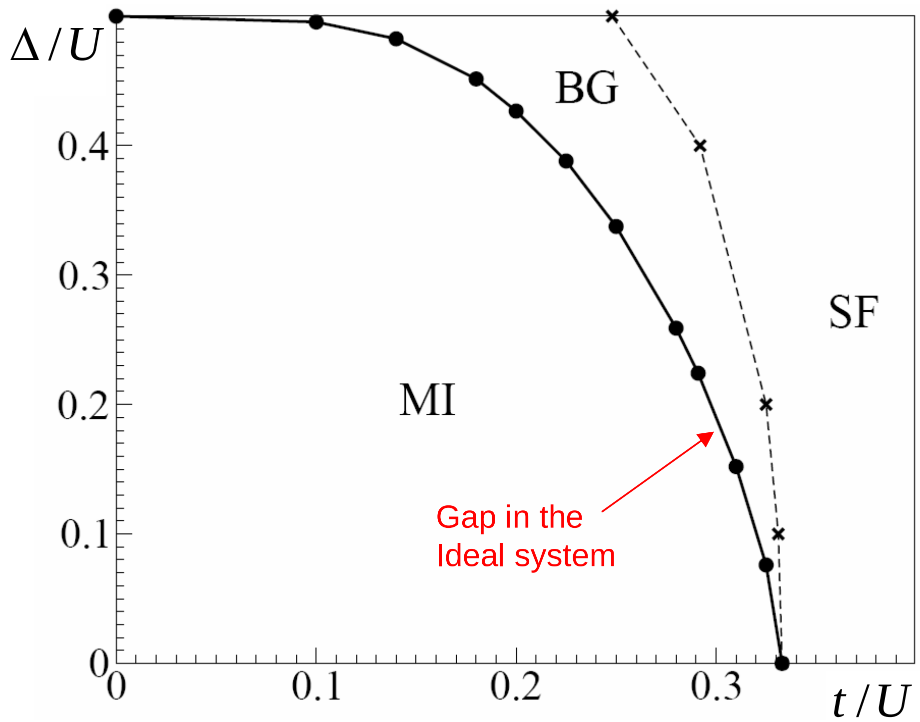
Grand canonical ensemble $N(\mu)$
Off-diagonal correlations $G(r,\tau)$
“Single-particle” and/or condensate wave functions $\varphi(r)$
Winding numbers and ρ_S

“Wave function” of the added particle

$$\phi_N(\mathbf{r}) = \langle \Psi_G(N) | b^\dagger_{\mathbf{r}} | \Psi_G(N-1) \rangle$$



Complete phase diagram



It is a theorem that for $\Delta > E_{GAP}$
the compressibility is finite