CLASSICAL AND QUANTUM WORM ALGORITHMS

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Collaborators on major algorithm developments

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National Science Foundation
WHERE DISCOVERIES BEGIN
DARPA DSO DEFENSE SCIENCES OFFICE
OLE OPTICAL LATTICE EMULATOR

Trieste, July 2012

Why bother with algorithms?

Efficiency

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

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

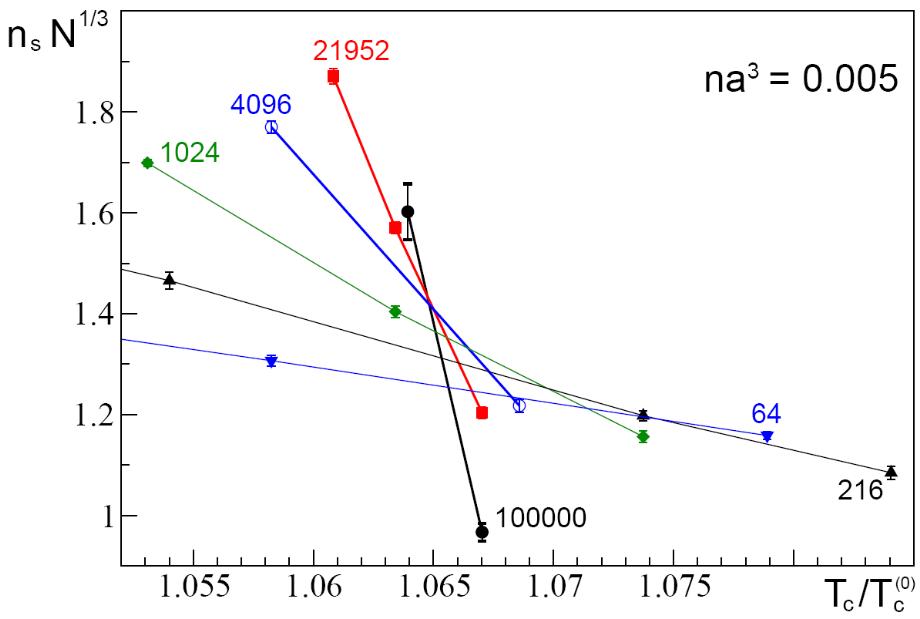
New physics

Applications: classical and quantum critical phenomena, latttice spin systems, cold atoms, liquid & solid Helium-4 , Feynman diagrams for fermions & frustrated magnetism

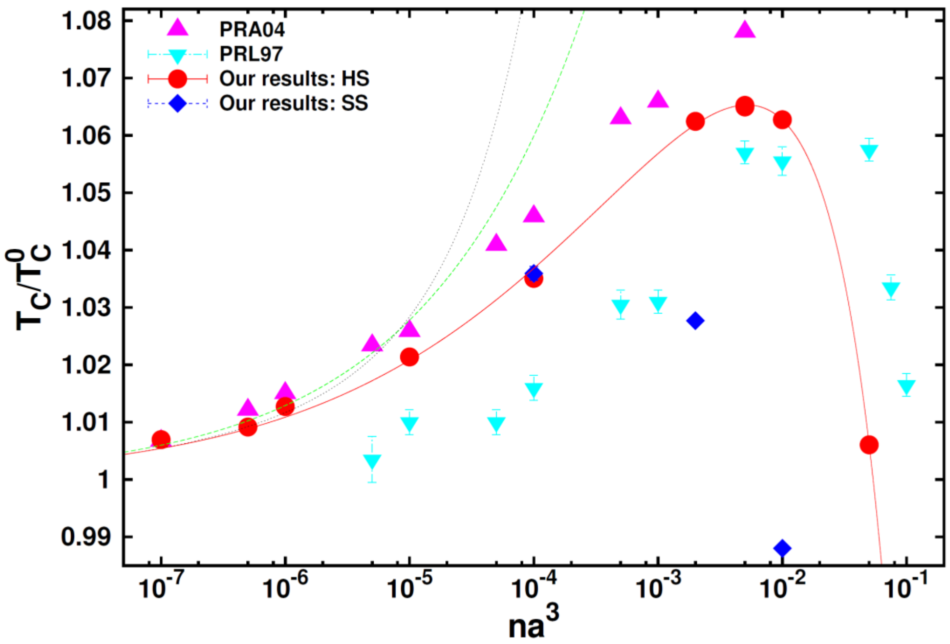
Weakly interacting Bose gas example: $T_C(a_S)$

Pilati, Giorgini, NP '08

from previous standard of $N \leq 216$ **to** $N \leq 100,000$



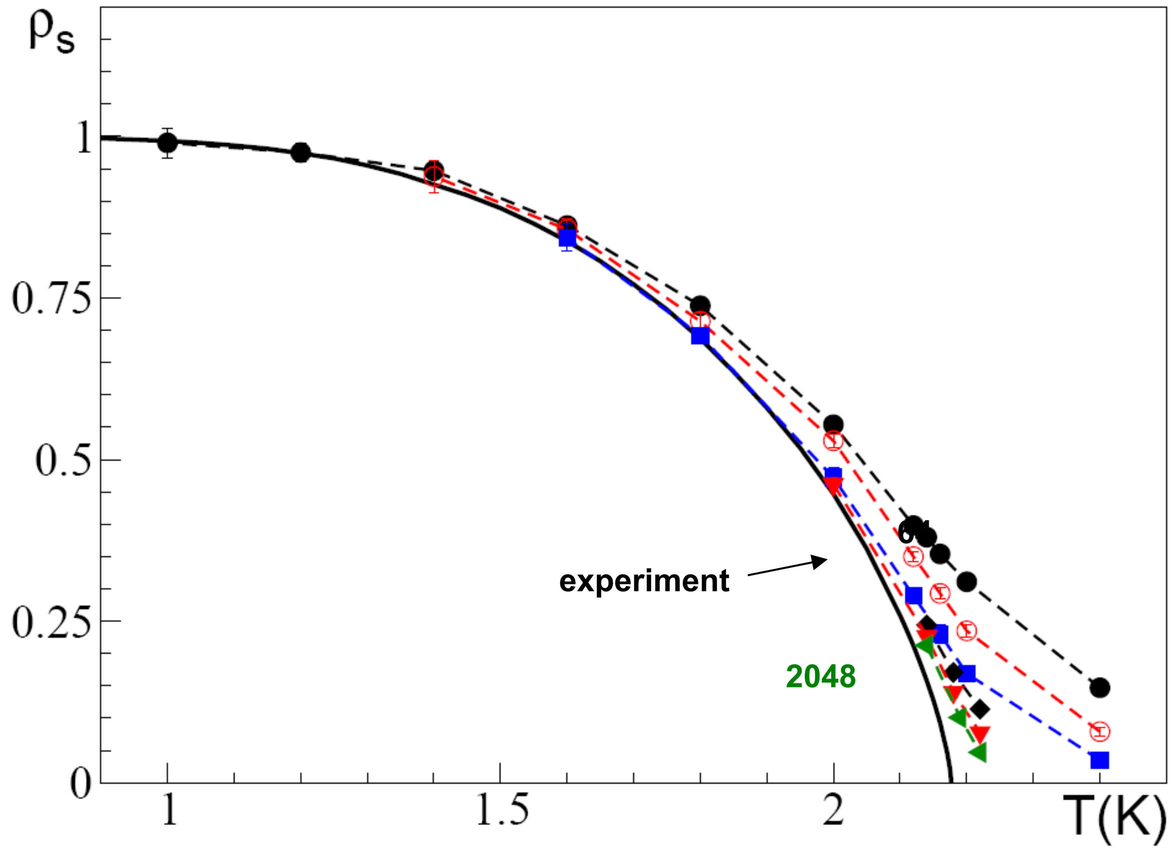
Finite-size scaling for superfluid density

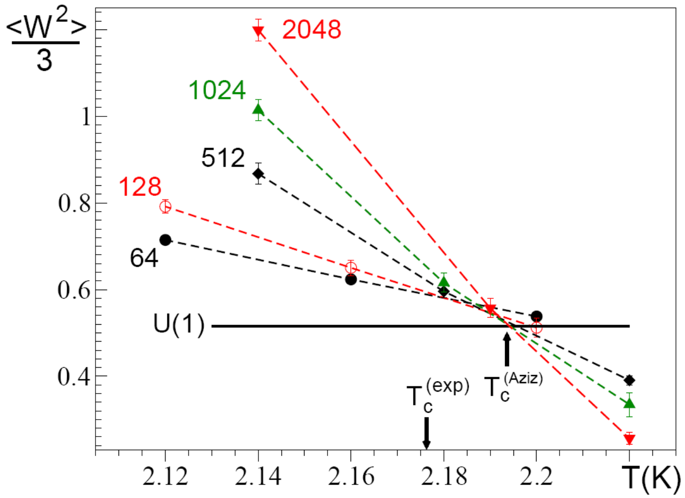


Critical temperature dependence on interaction

Problem to overcome: crossover from Gaussian to generic U(1) universality

3D He-4 at P=0 superfluid density & critical temperature





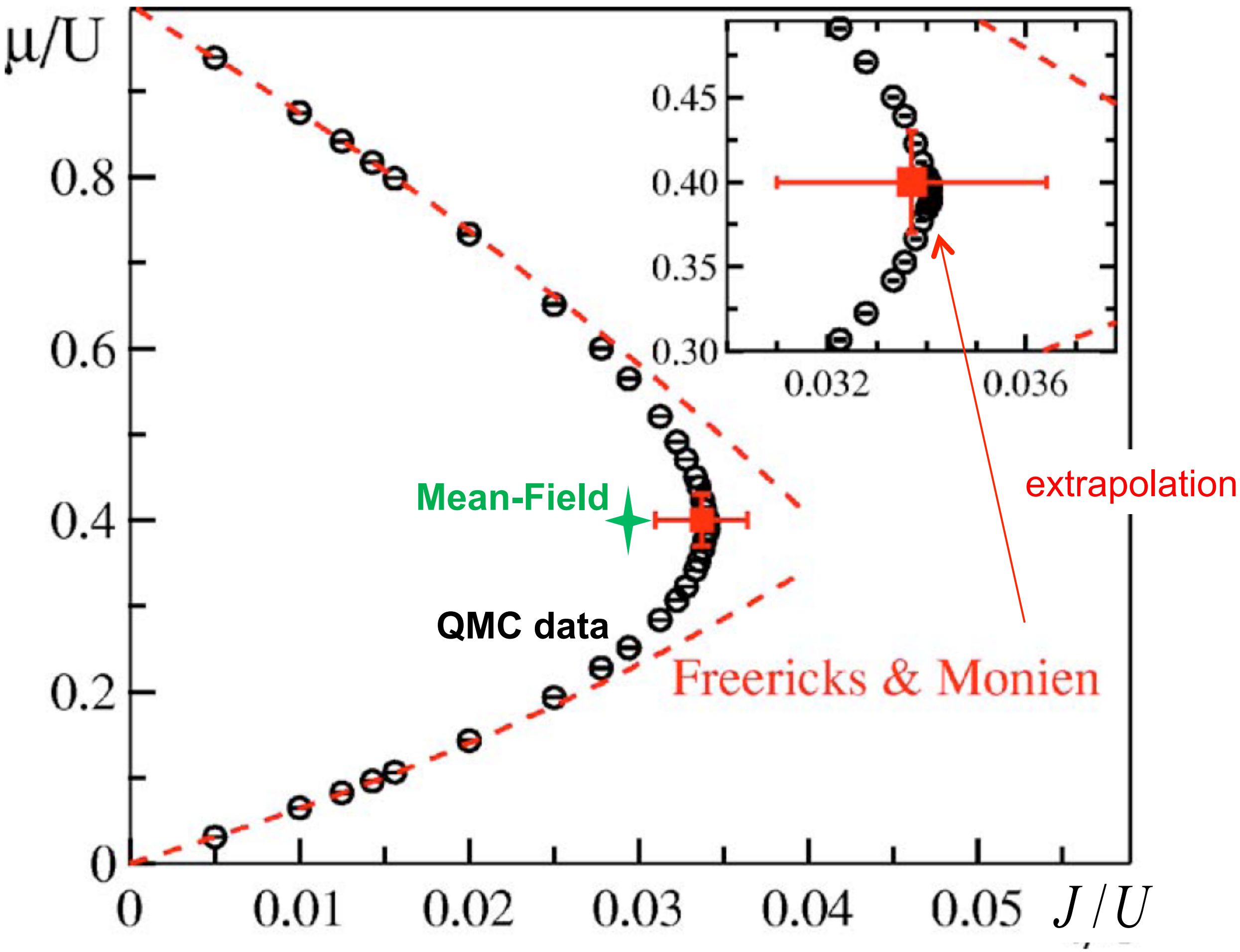
$T_C^{Aziz} = 2.193$ **vs** $T_C^{\exp} = 2.177$

Boninsegni, NP ,Svistunov '06

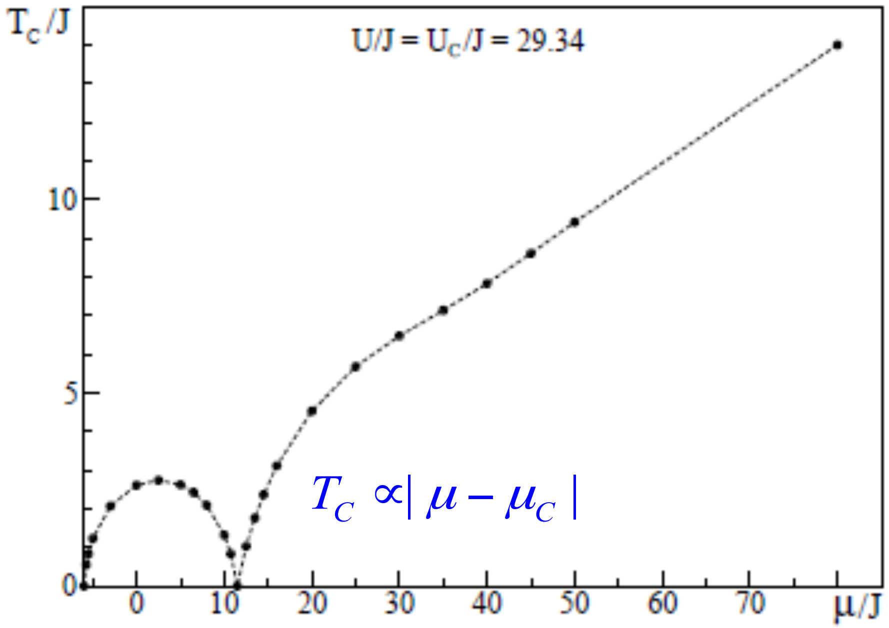
Interatomic potential was never optimized to fit $T_C^{\exp}$

Bose-Hubbard model (up to 5,000,000 bosons @ exper. temperature)

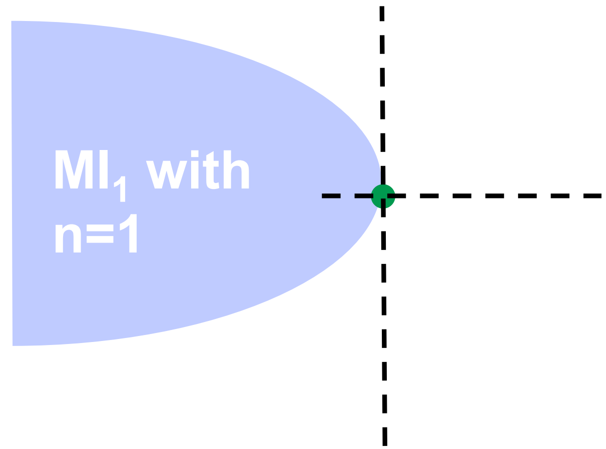
The first insulating lobe/gap in 3D



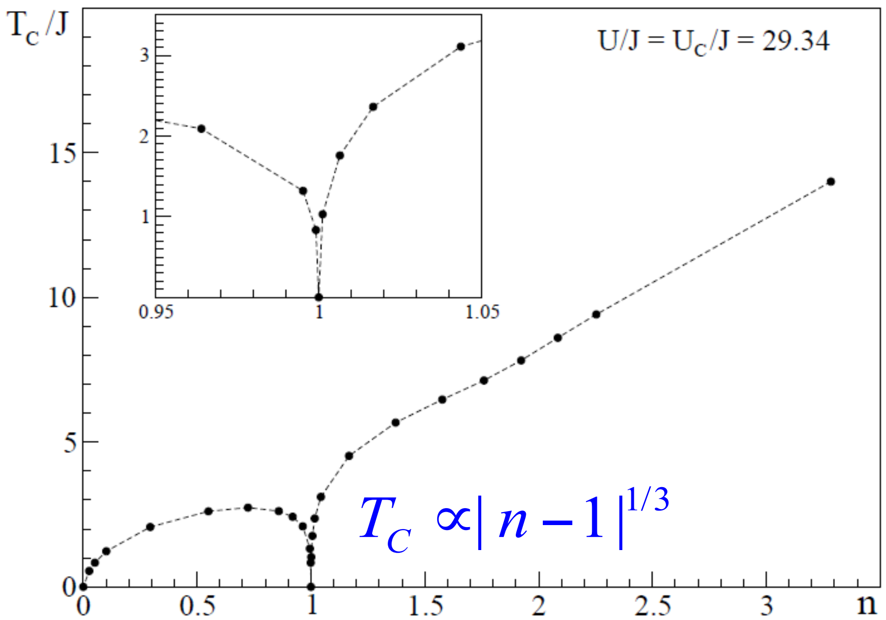
Capogrosso-Sansone, NP, Svistunov '07



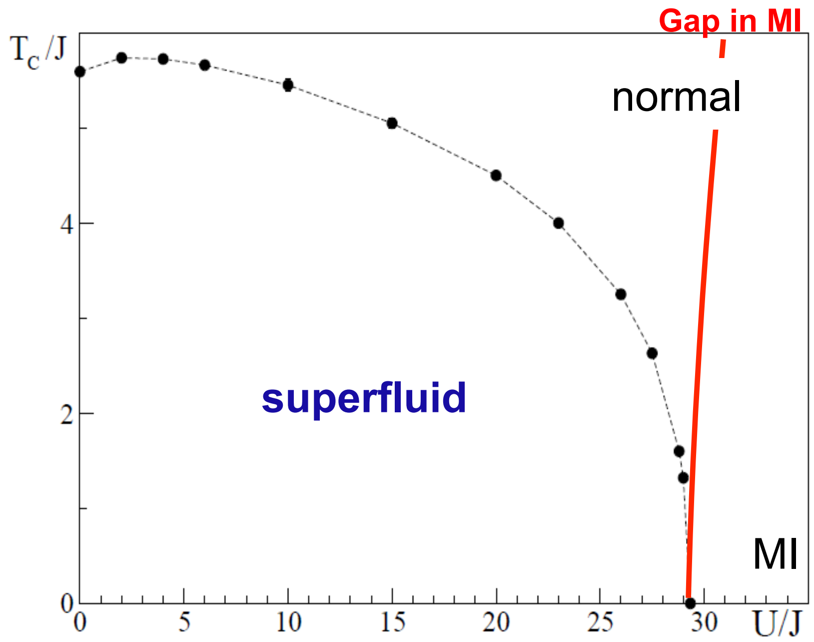
U/J = U_C/J = 29.34
T_C/J
μ/J
$T_C \propto |\mu - \mu_C|$



MI_1 with
n=1

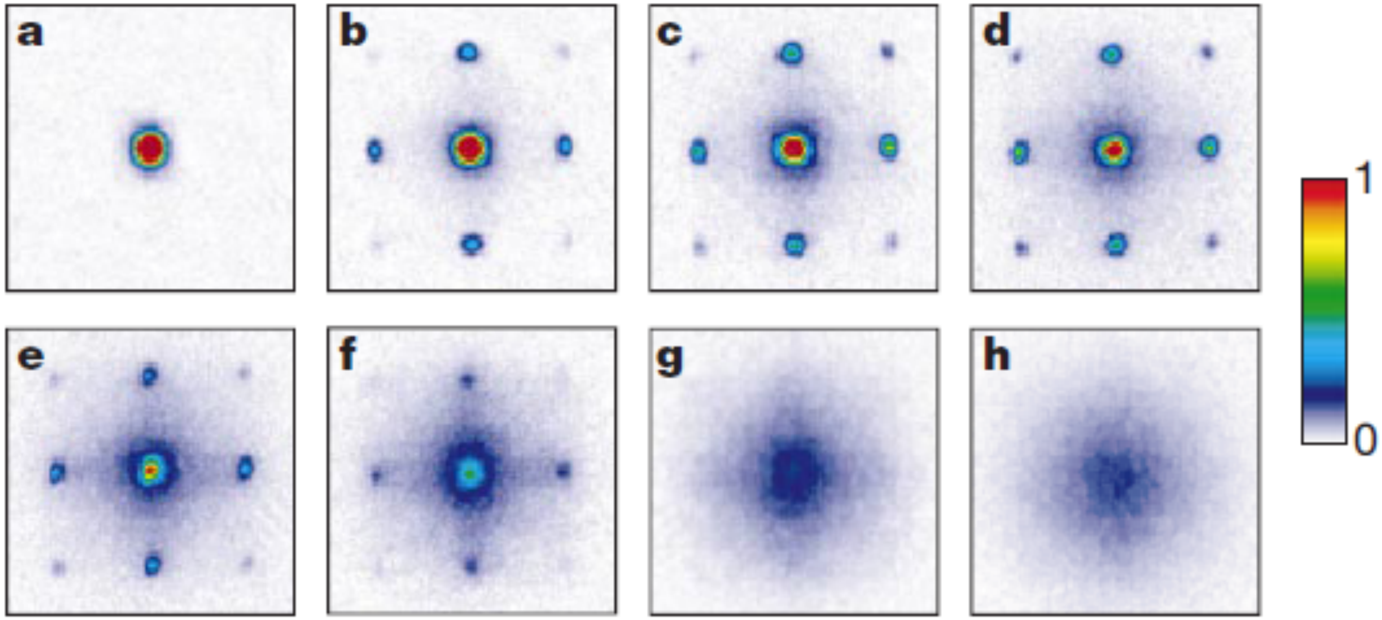


U/J = U_C/J = 29.34
T_C/J
n
$T_C \propto |n-1|^{1/3}$



Gap in MI
normal
superfluid
MI
T_C/J
U/J

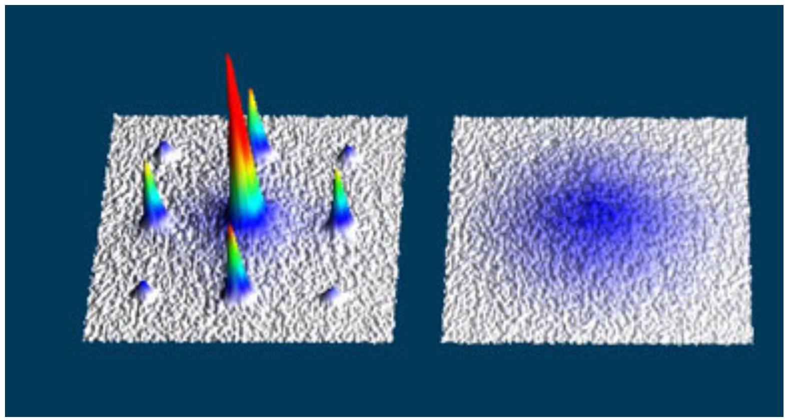
M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch, and I. Bloch ’02

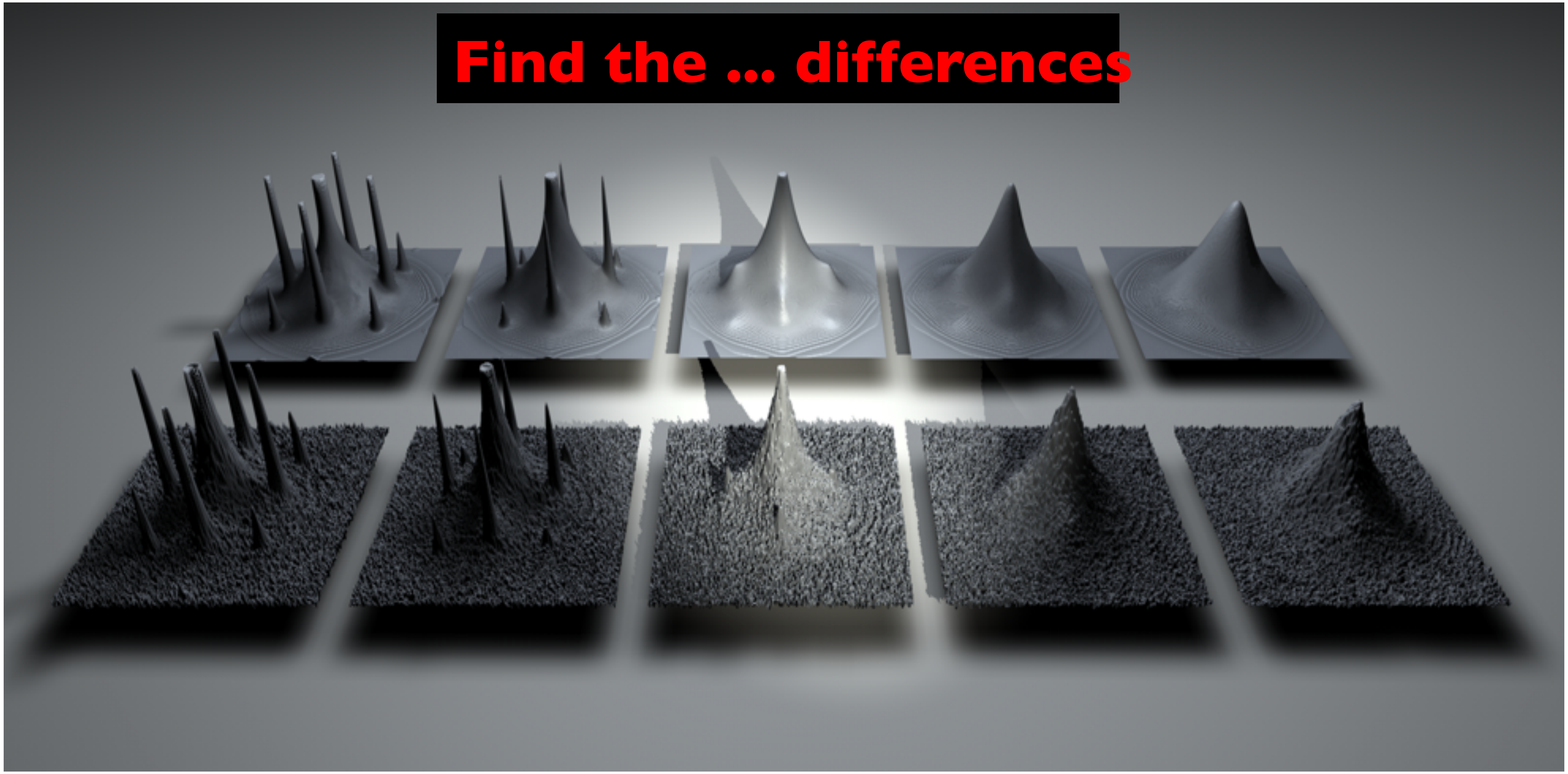


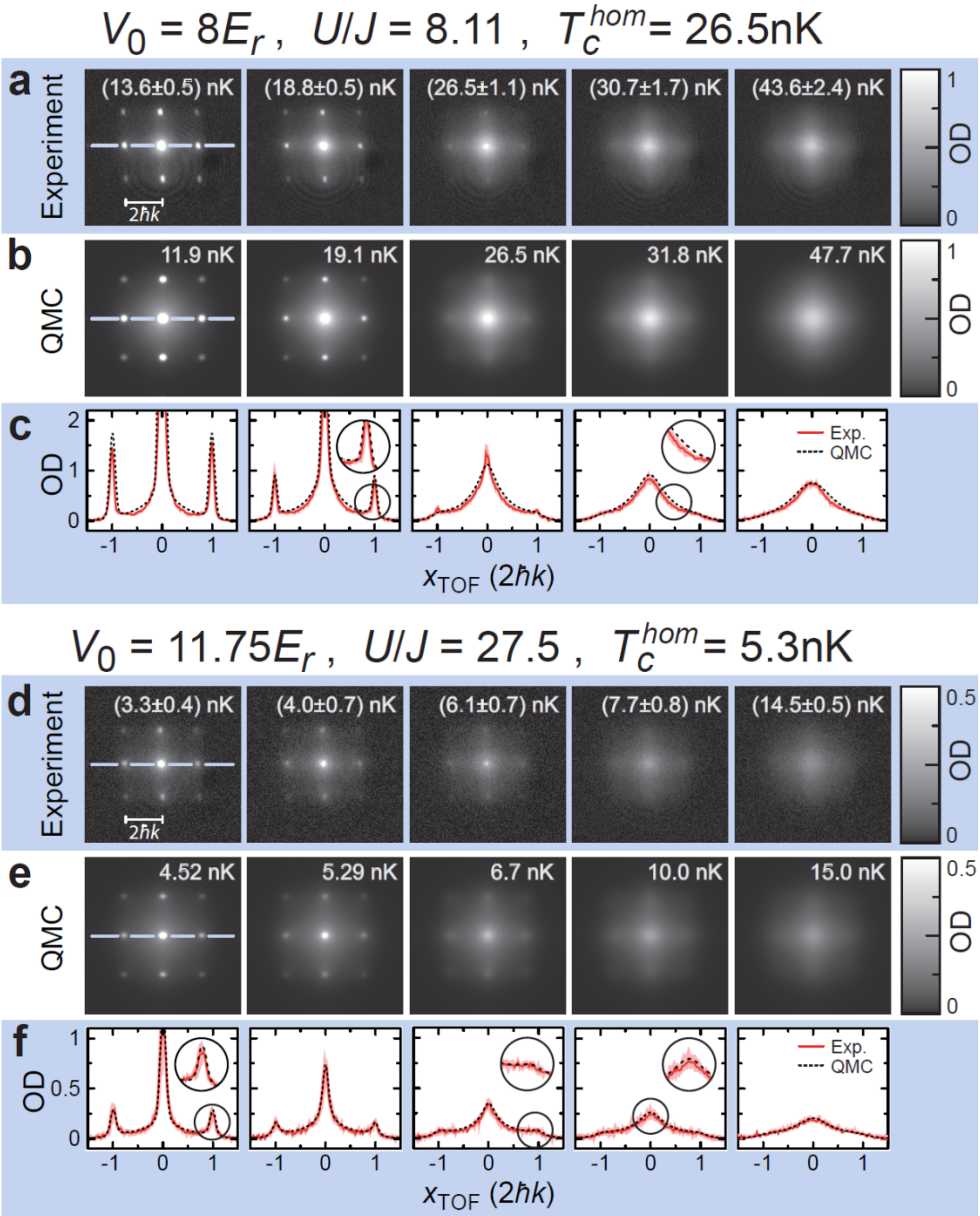
Superfluid

MI

Figure 2 Absorption images of multiple matter wave interference patterns. These were obtained after suddenly releasing the atoms from an optical lattice potential with different potential depths V_0 after a time of flight of 15 ms. Values of V_0 were: **a**, 0 E_r; **b**, 3 E_r; **c**, 7 E_r; **d**, 10 E_r; **e**, 13 E_r; **f**, 14 E_r; **g**, 16 E_r; and **h**, 20 E_r.




Find the ... differences



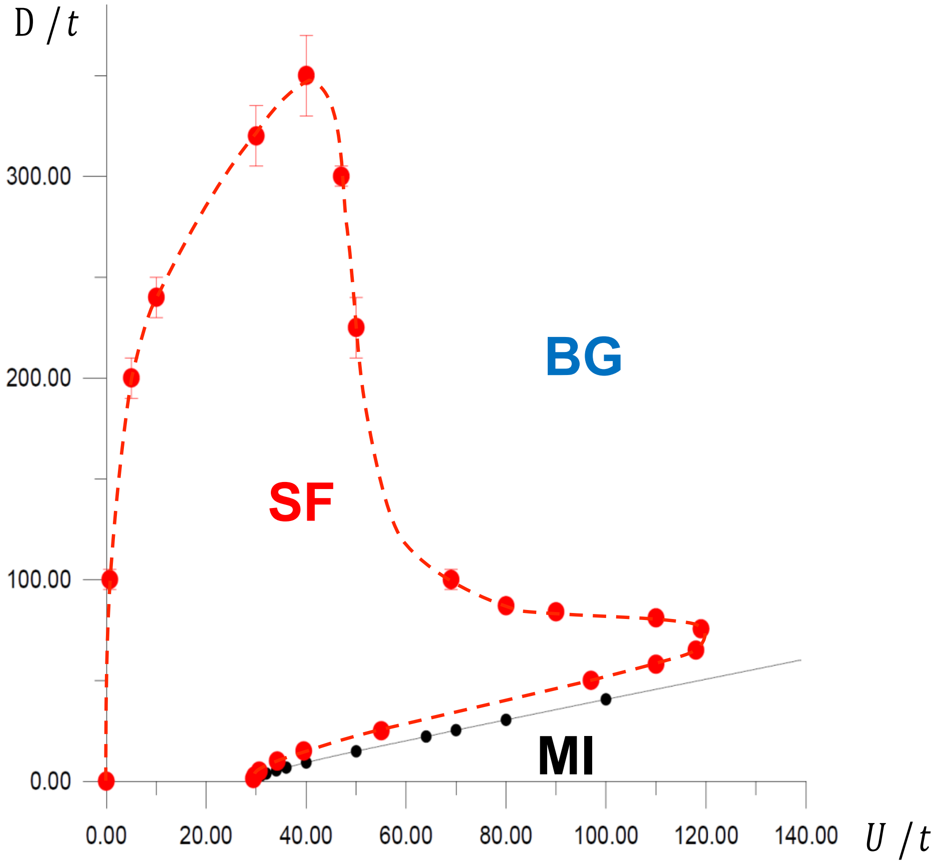
No fit comparison of time-of-flight images (momentum distributions)

$N \approx 300000$

S. Trotzky, L. Pollet, F. Gerbier,
U. Schnorrberger, I. Bloch, NP
B. Svistunov, M. Troyer, '10

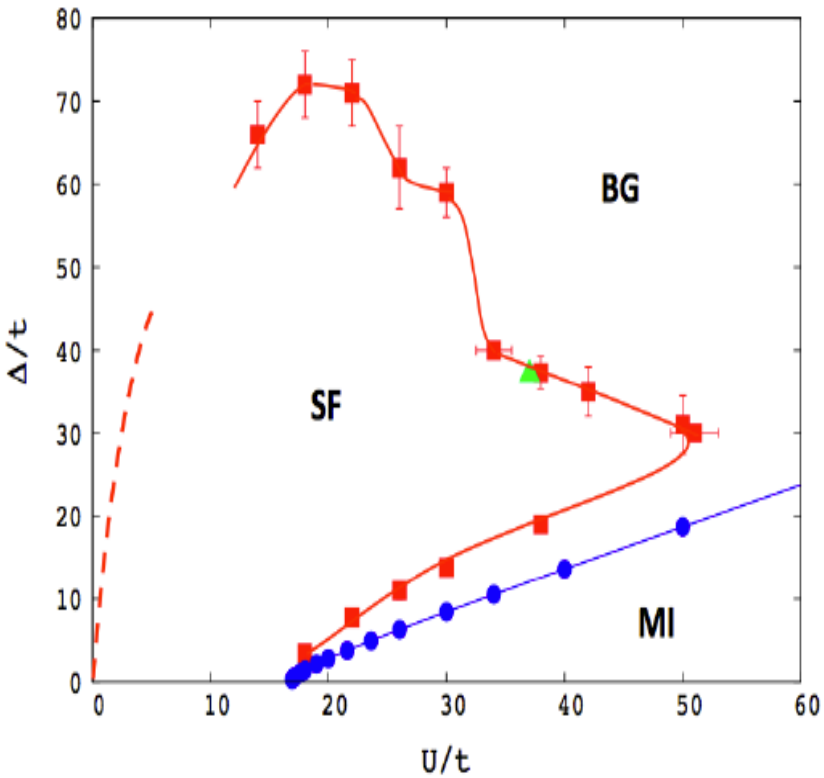
Disordered Bose-Hubbard model (ground state phase diagram)

3D



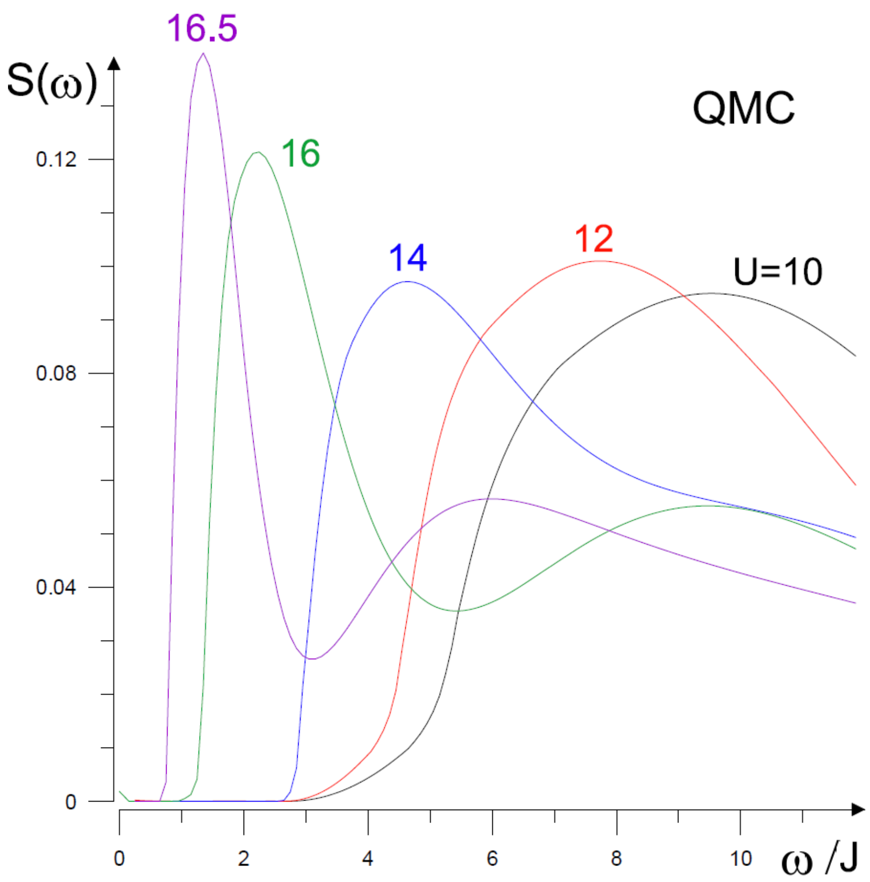
Gurarie, Pollet, NP, Svistunov, Troyer ‘09

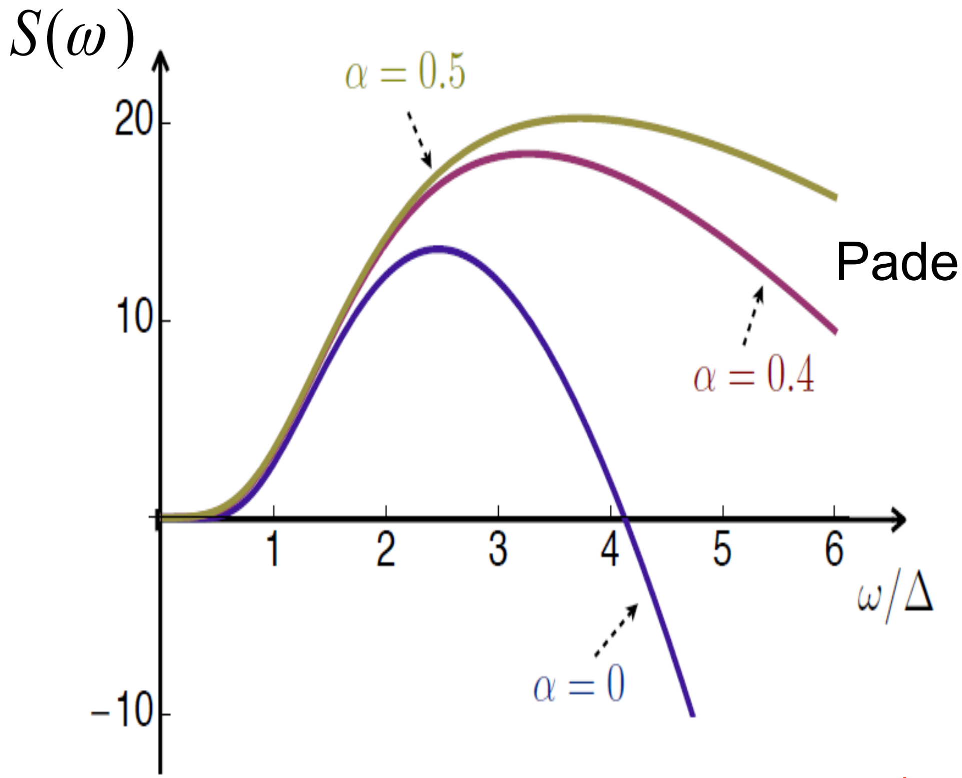
2D



Soyler, Kiselev, NP,, Svistunov, -11

Higgs amplitude mode in 2D





Sachdev, Podolsky ‘12

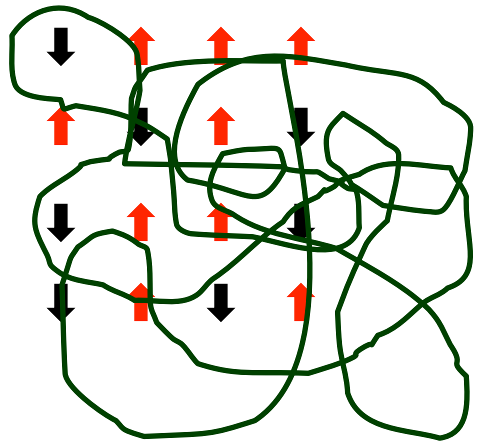
PI Monte Carlo: Pollet, NP ‘12

Field theory in 1/N + corrections (here N=2)


TIME TO CALL WORMS!

Worm algorithm idea

Standard Monte Carlo setup:



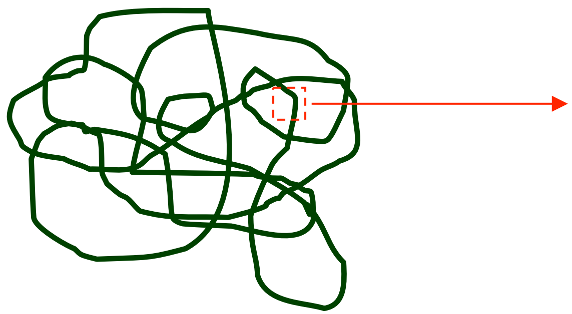
- configuration space = (depends on the model and it's representation)

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

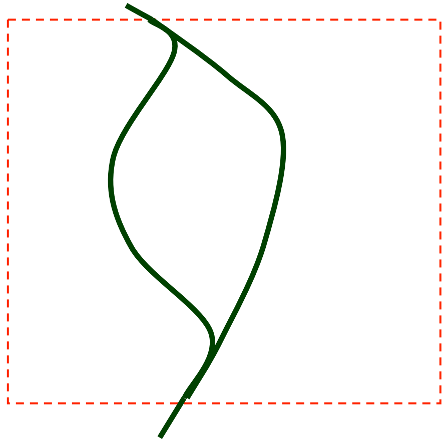
- each cnf. has a weight factor W_{cnf} $e^{-E_{cnf}/T}$

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

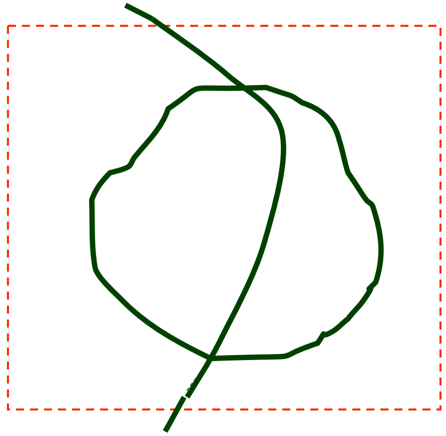
"conventional" sampling scheme:



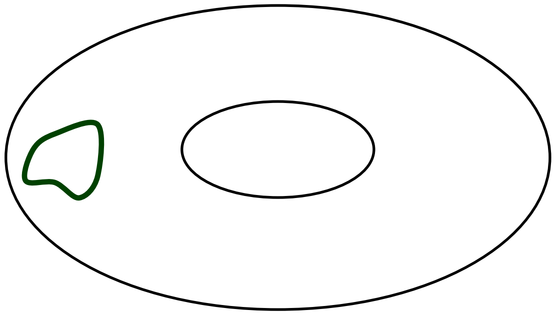
local shape change



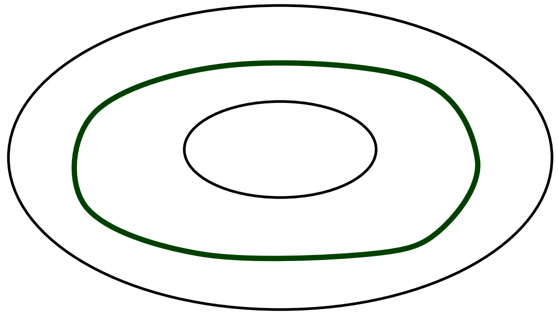
Add/delete small loops



No sampling of topological classes
(non-ergodic)



can not evolve to



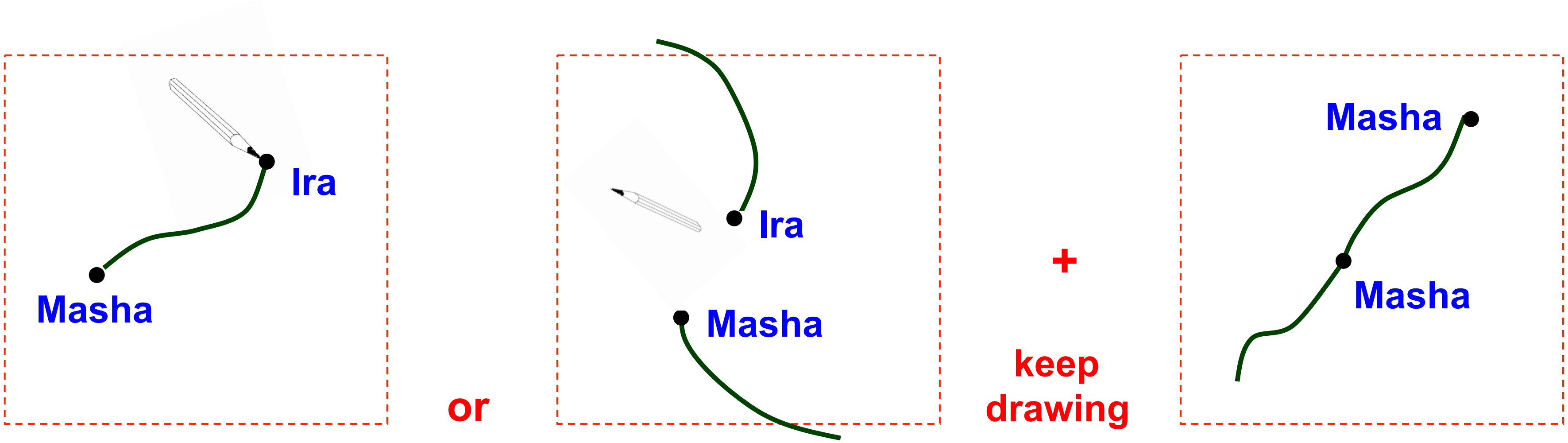
Critical slowing down
(large loops are related to critical modes)

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

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

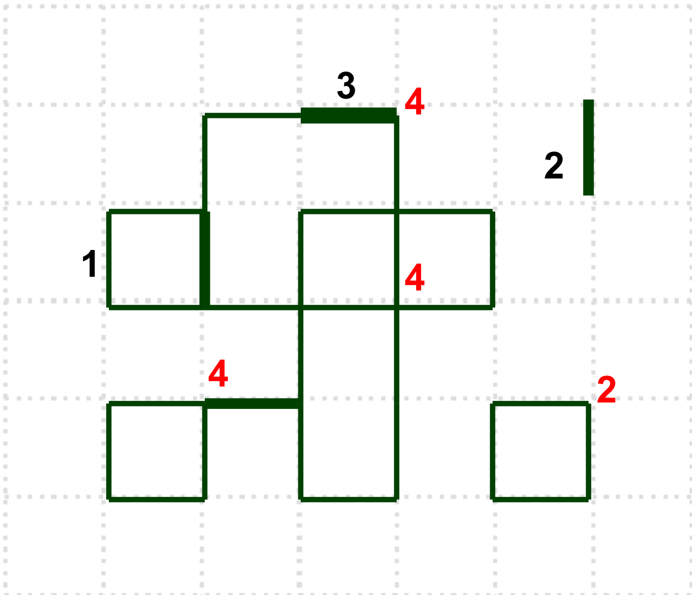
$$-\frac{H}{T} = K\sum_{<ij>}\sigma_i\sigma_j \qquad (\sigma = \pm 1)$$

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

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

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

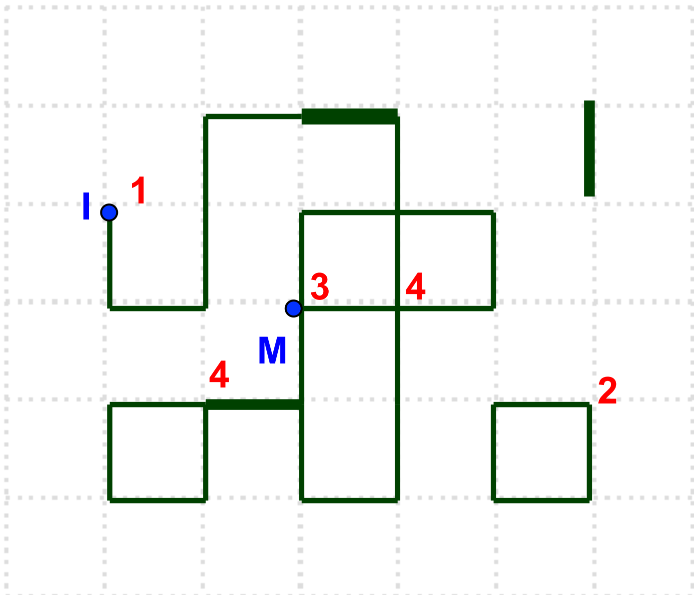
$$\equiv 2^N \sum_{\{N_b\}=loops}\left(\prod_{b=<ij>}\frac{K^{N_b}}{N_b!}\right)$$



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

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

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



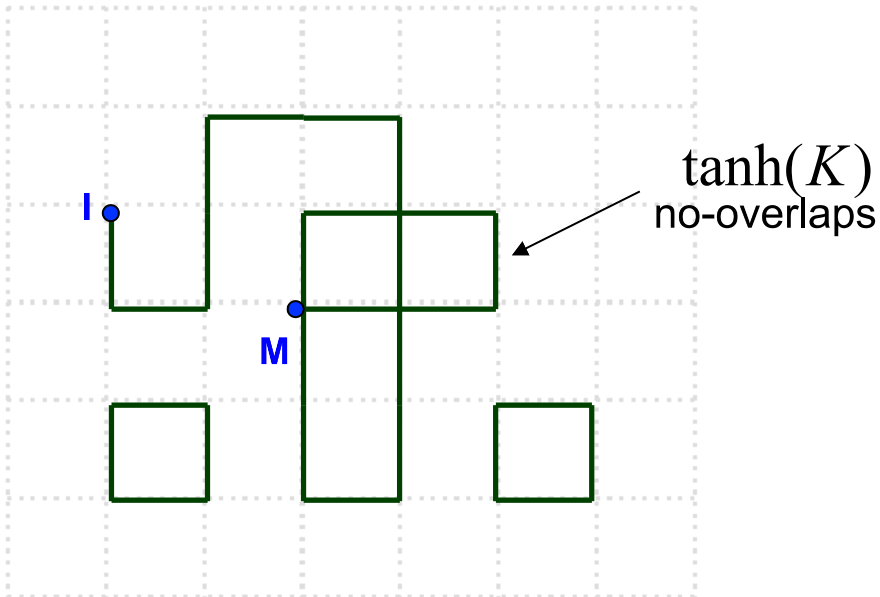
Worm algorithm cnf. space = $Z \cup G$

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 f

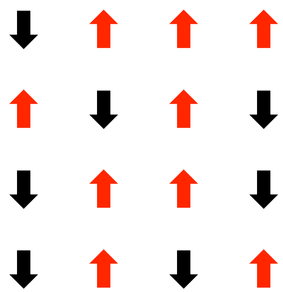
- select direction to move M, let it be bond b

- 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:

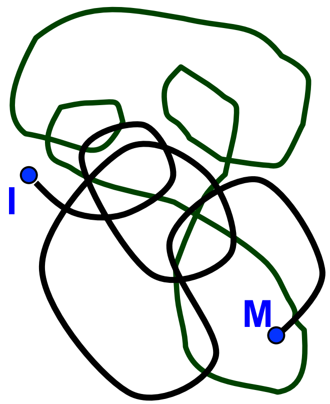
Question: What are the signatures of the phase transition (critical modes)?

spin representation

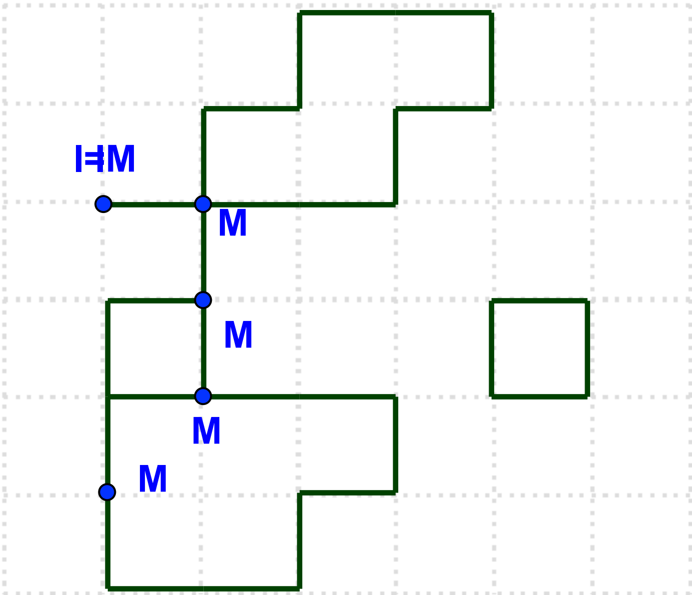


→ large domains of similarly oriented spins of linear size ~ L → single-spin flips are not efficient in updating them!

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

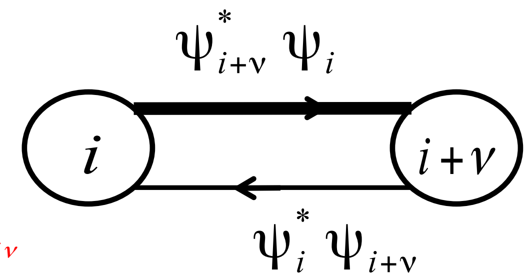
Energy: either $E = -JNd \left\langle \sigma_1 \sigma_2 \right\rangle = -JNdg(1)$

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 $\mu = 2U \rightarrow \infty$ **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

$\psi_i = x e^{i\varphi}$

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

$e^{i\varphi(M_{1i}-M_{2i})} \rightarrow M_{1i} = M_{2i} = M_i$

$$\prod_i Q(M_i)$$

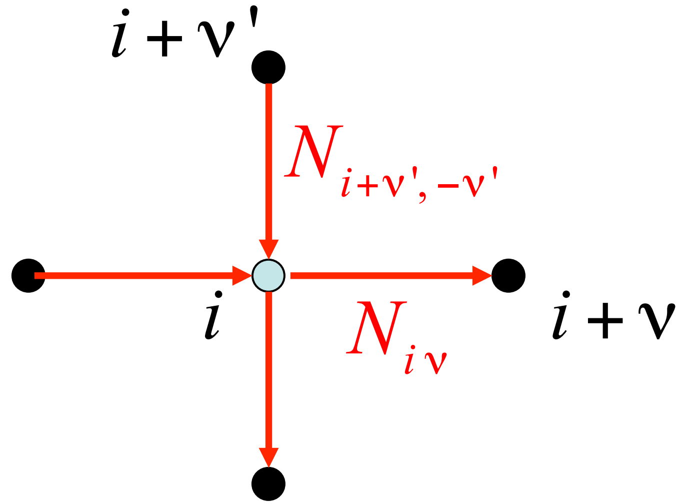
where $Q(M) = \begin{cases} 0 & \text{if } M_1 \neq M_2 \\ \pi \int_0^\infty dx \; x^M e^{\mu x - U x^2} \end{cases}$

$\longrightarrow$ **closed oriented loops**

$=$ **tabulated numbers**

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

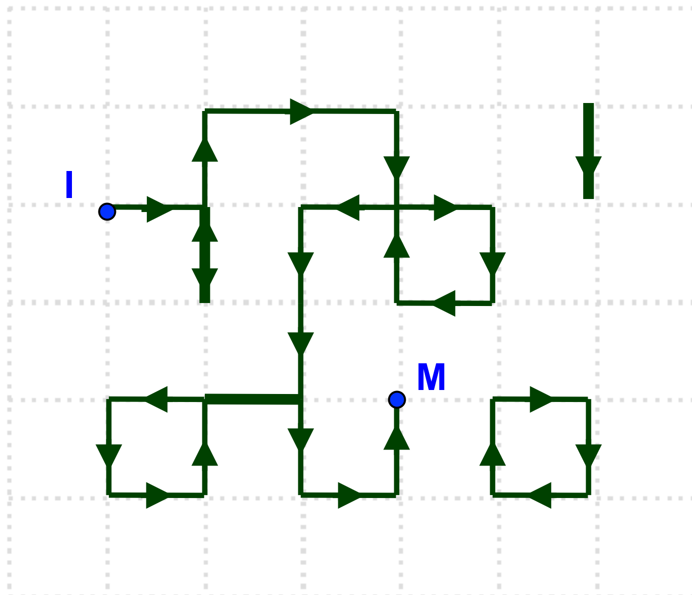
Flux in = Flux out ⇨ closed oriented loops of integer N-currents



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

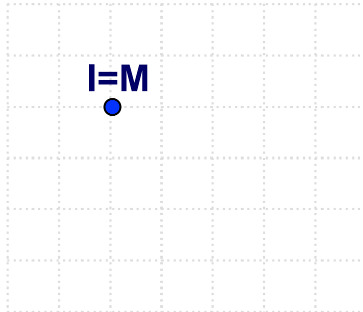
(one open loop)

Z-configurations have $I = M$

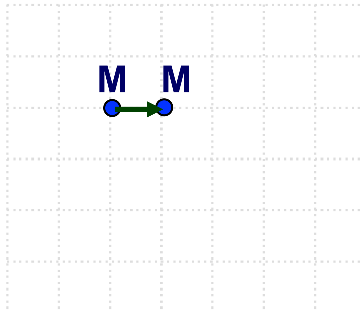


Same algorithm:

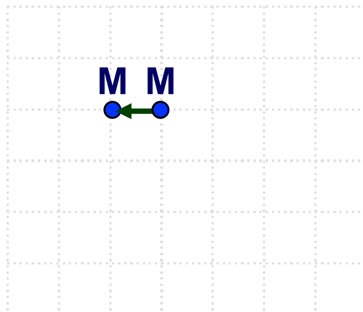
- $Z \leftrightarrow G$ **sectors, prob. to accept** $R_{Z \to G} = \min\left[1, \frac{Q(M_I + 1)}{Q(M_I)}\right]$



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



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

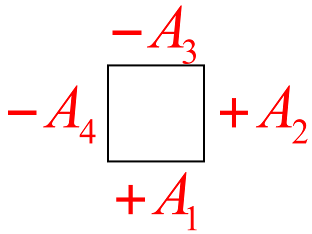


Keep drawing/erasing …

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

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

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

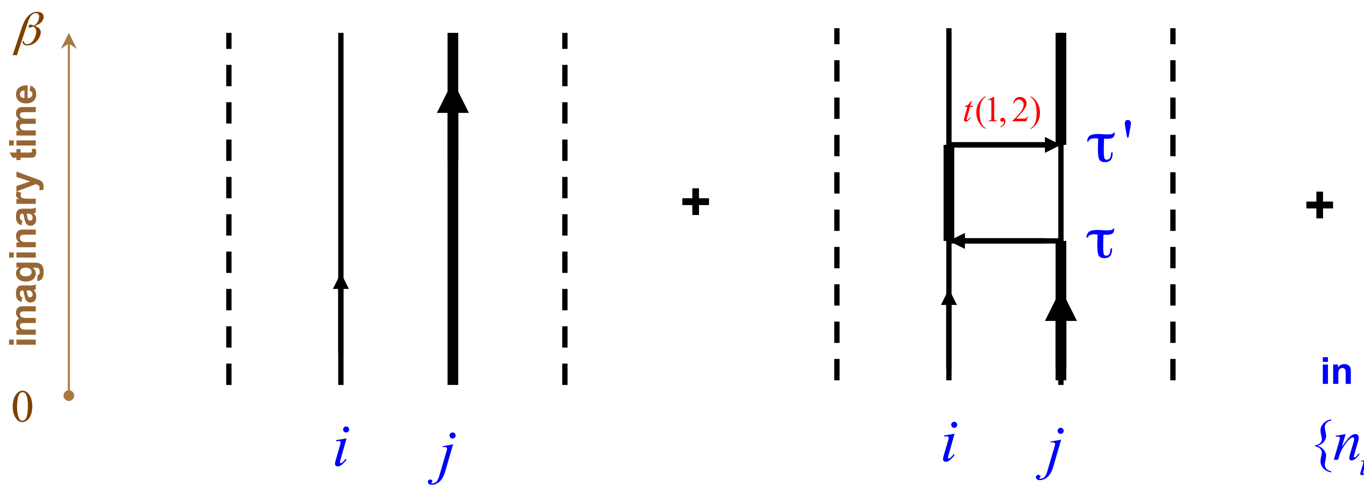
$$= \mathrm{Tr}\, e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau)\, d\tau + \int_{\tau'}^\beta \int_0^\beta H_1(\tau)\, H_1(\tau')\; d\tau\, d\tau' + \ldots \right\}$$

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

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

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

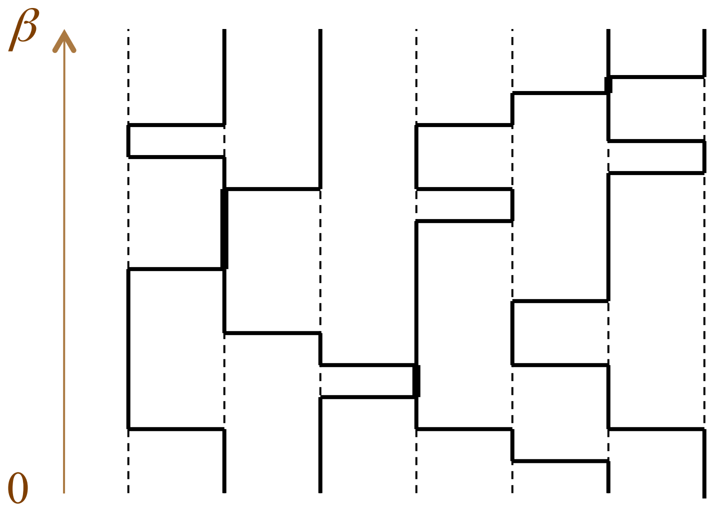
all possible trajectories for N particles with K hopping transitions

potential energy contribution

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

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

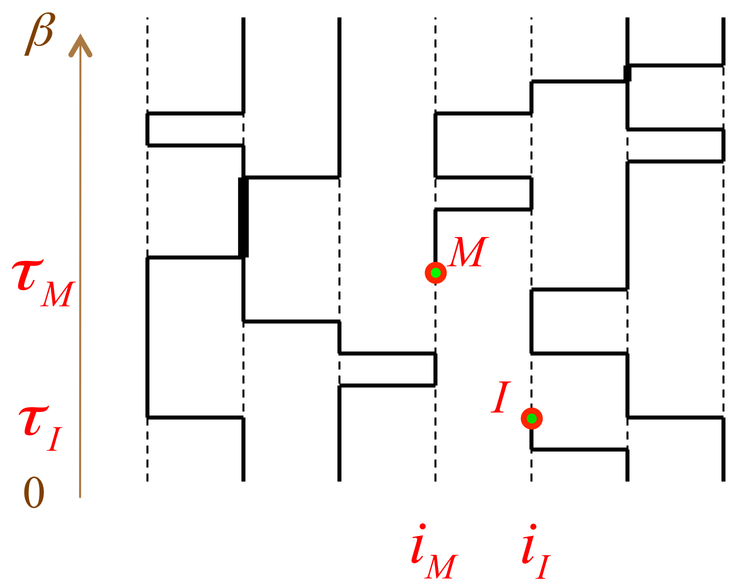
high-order term for $Z = \mathrm{Tr}\, e^{-\beta H}$



Similar expansion in hopping terms for

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

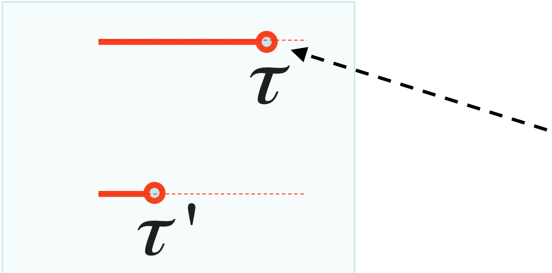
+ two special points for Ira and Masha



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

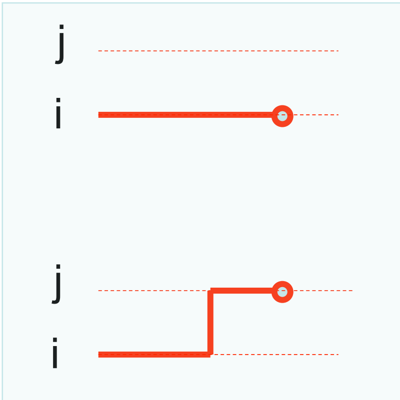
ergodic set of local updates

time shift:

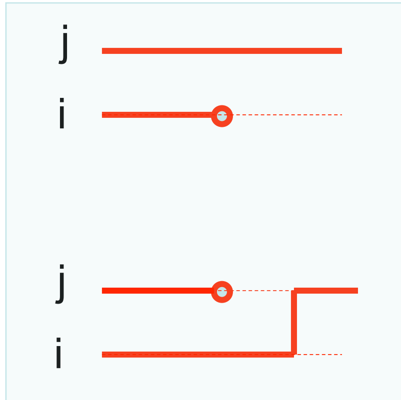


Ira or Masha

space shift ("particle" type):

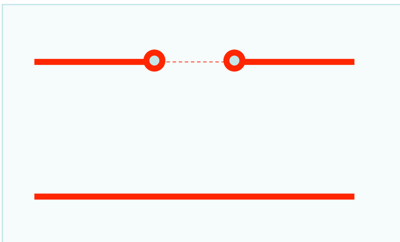


space shift ("hole" type):

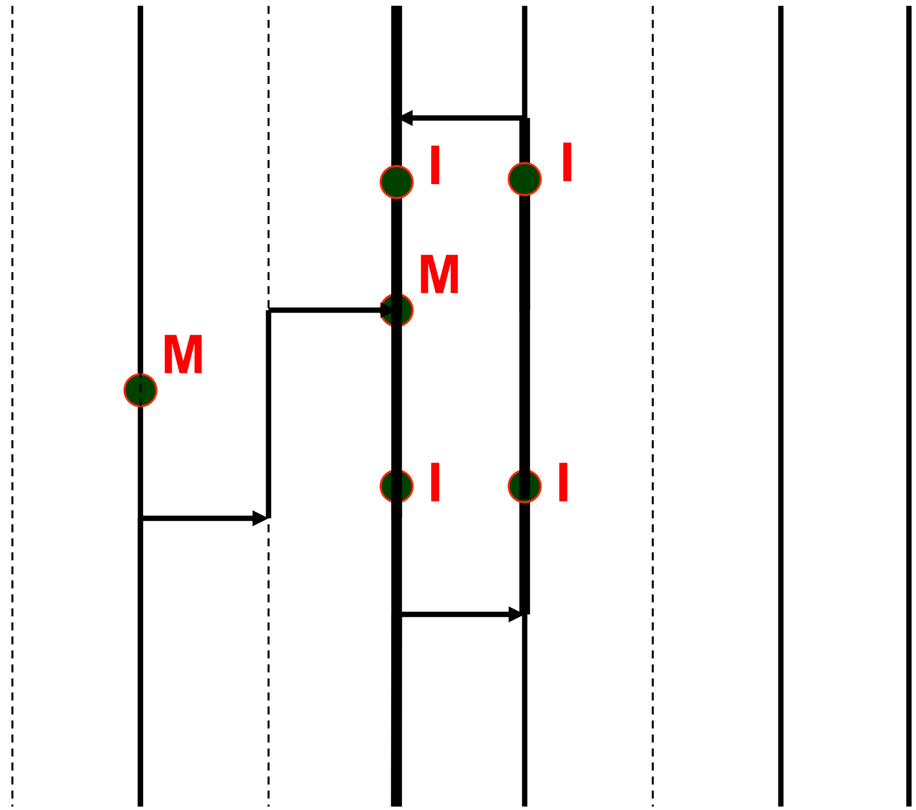


Insert/delete Ira and Masha:

$Z \leftrightarrow G$



connects Z and G configuration spaces


M
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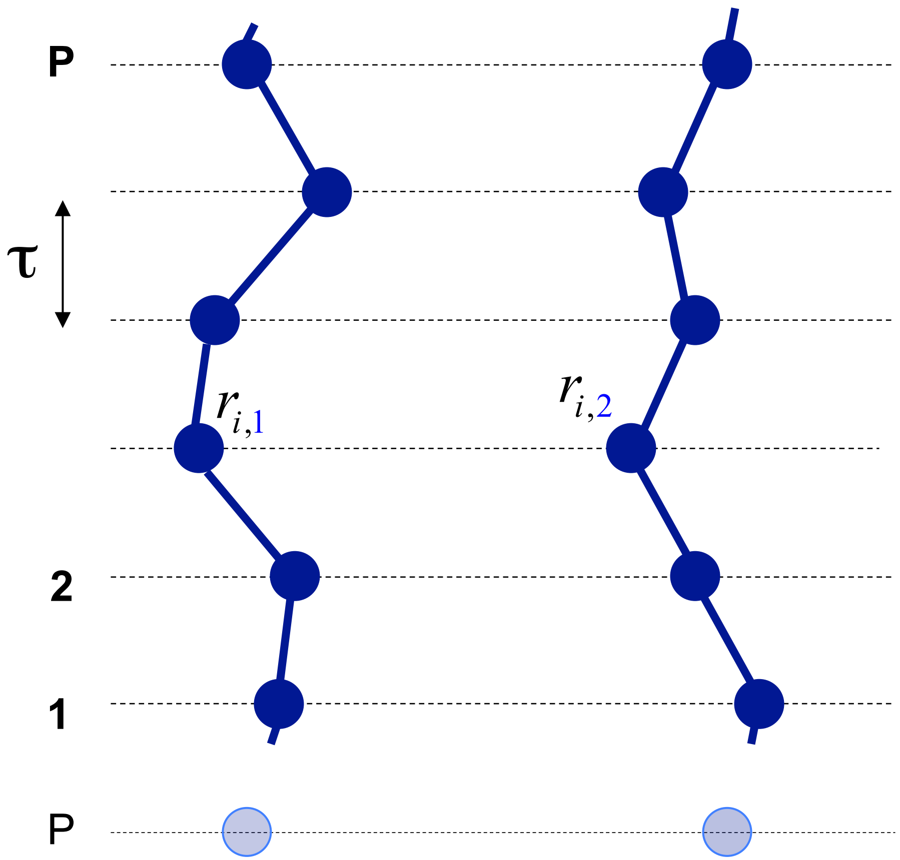
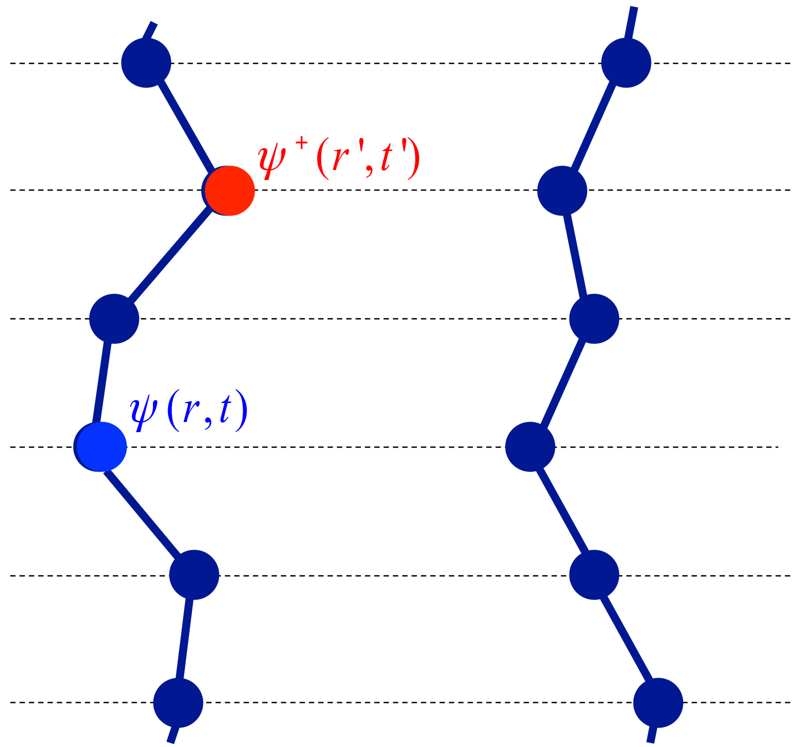
Path-integrals in continuous space

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

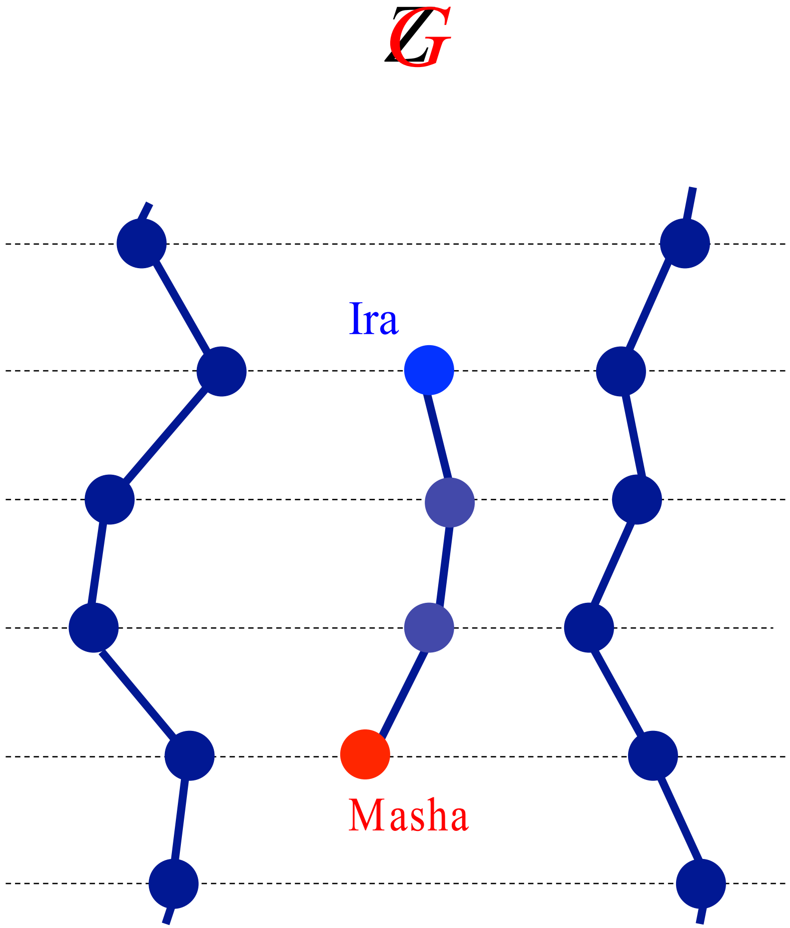


$$R_i = (r_{i,1}, r_{i,2}, \ldots, r_{i,N})$$

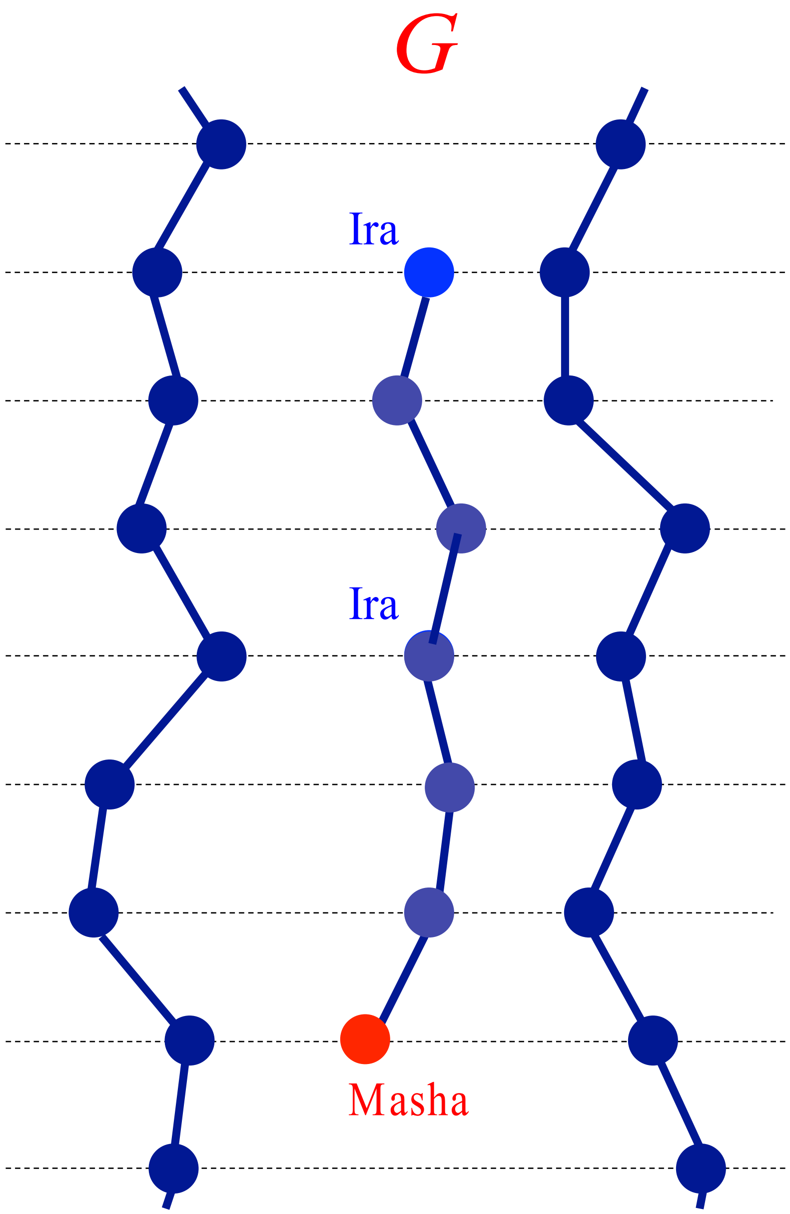
Z G



(open/close update)

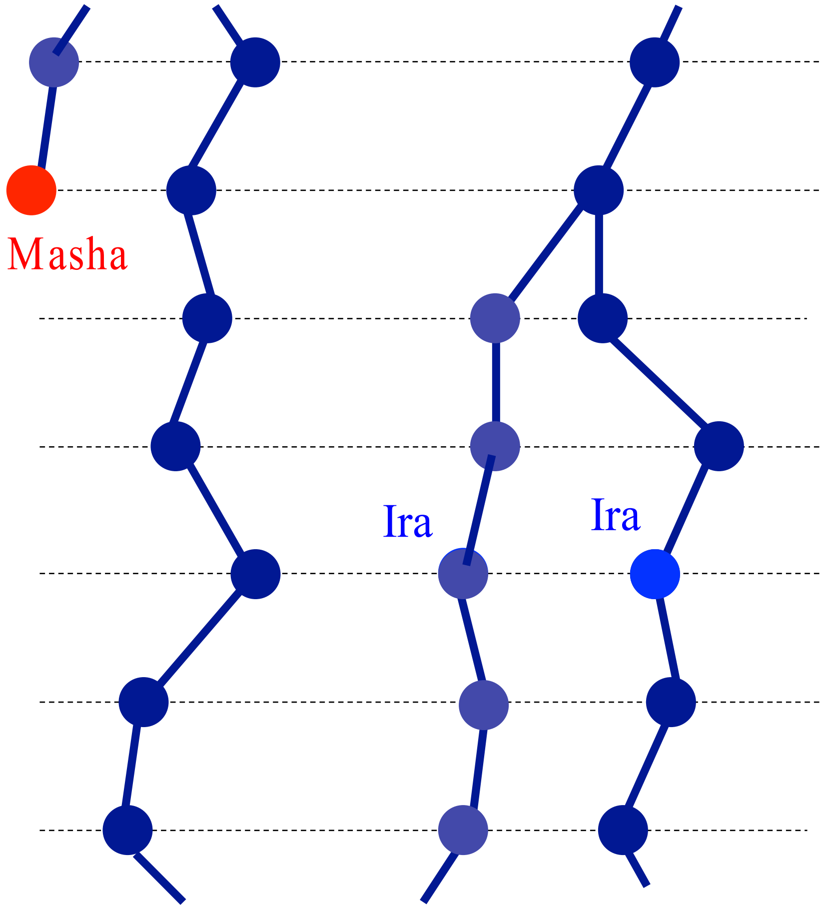


(insert/remove update)



(advance/recede update)

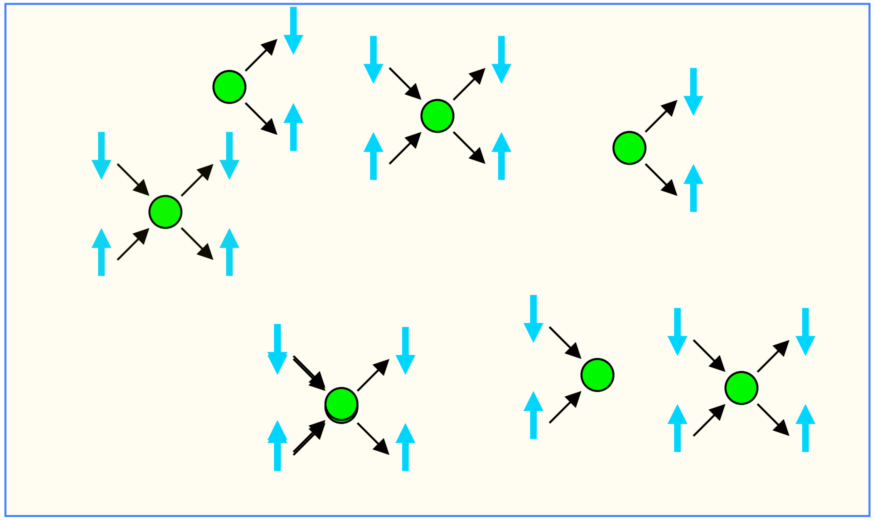
G



(swap update)

Not necessarily for closed loops!

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



Pair correlation function

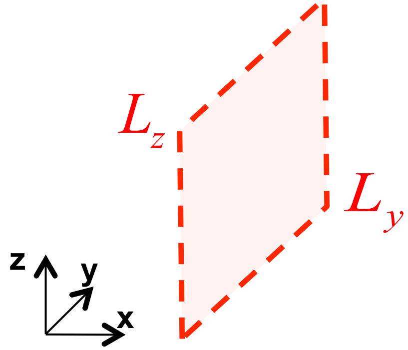
$$\langle a_{\uparrow}^{+}(r_1,\tau_1)a_{\downarrow}^{+}(r_1,\tau_1)\;\; a_{\downarrow}(r_2,\tau_2)a_{\uparrow}(r_2,\tau_2)\rangle$$

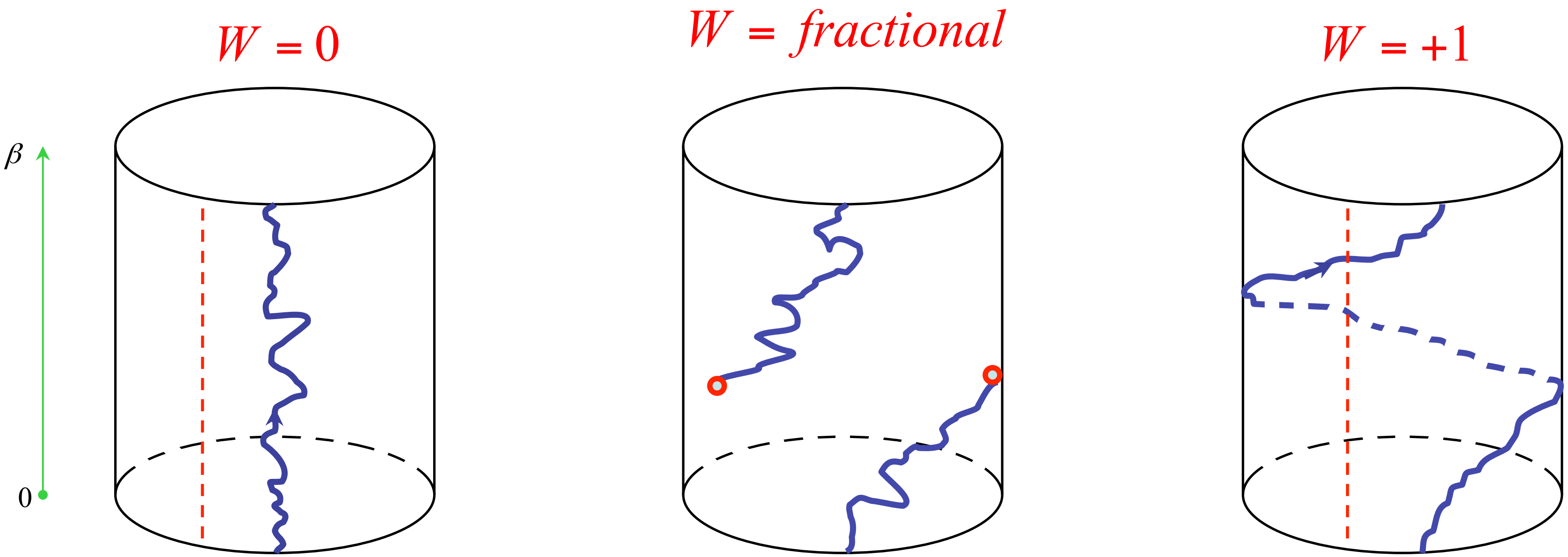
The rest is worm algorithm in this $Z \cup G_{IM}$ configuration space:
draw and erase interaction vertexes using exclusively Ira and Masha

More: winding numbers and superfluid density

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

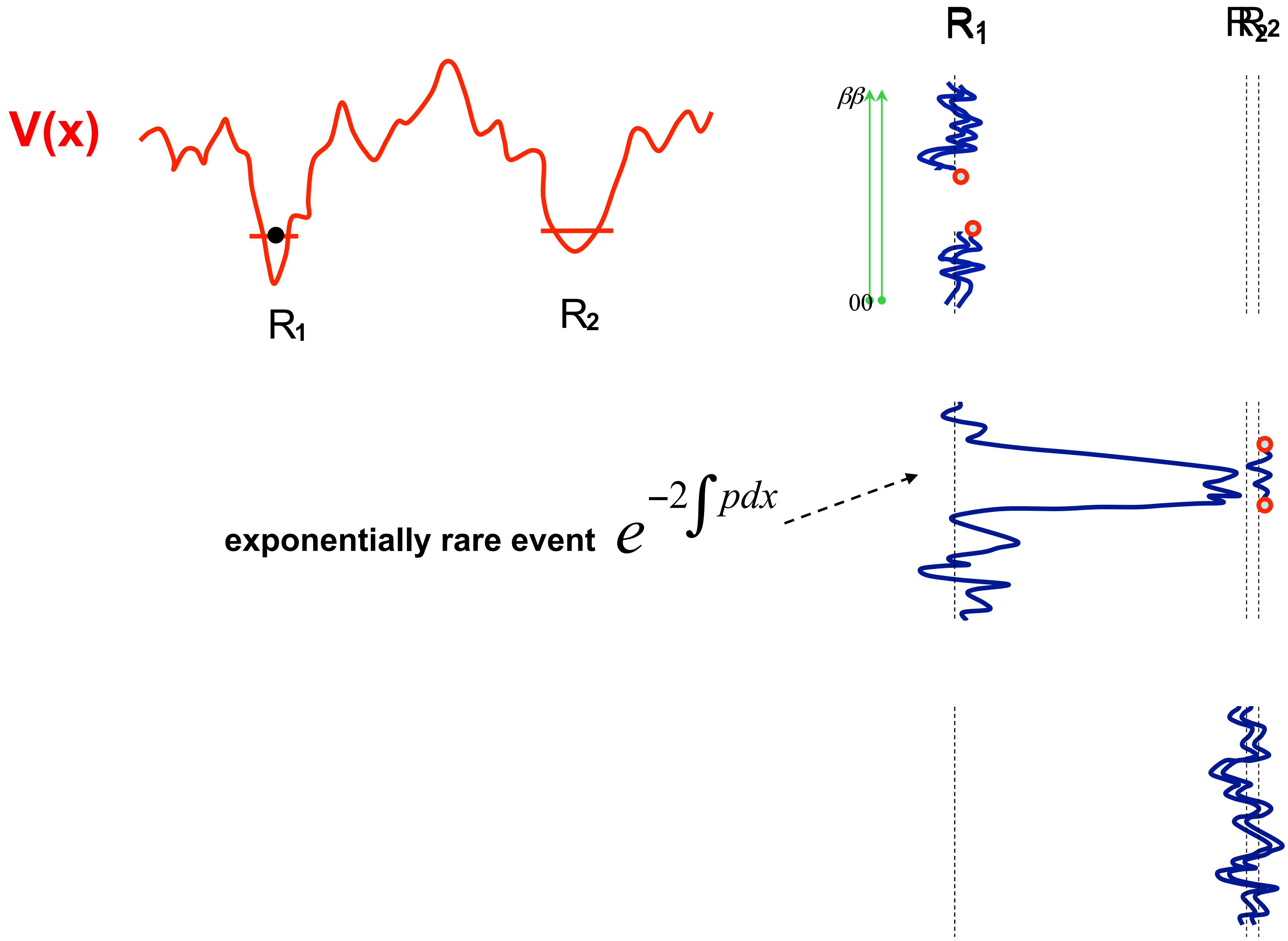
(cross-section independent in Z-sector)





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

Grand canonical ensemble (a "must" for disorder problems!)



More tools:

1. Density matrix $n(r',r) = \langle \psi^\dagger(r',\tau)\psi(r,\tau) \rangle$ (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:

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

mobility thresholds, participation ratio, etc.

Why bother with algorithms?

Efficiency

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

Reliably!

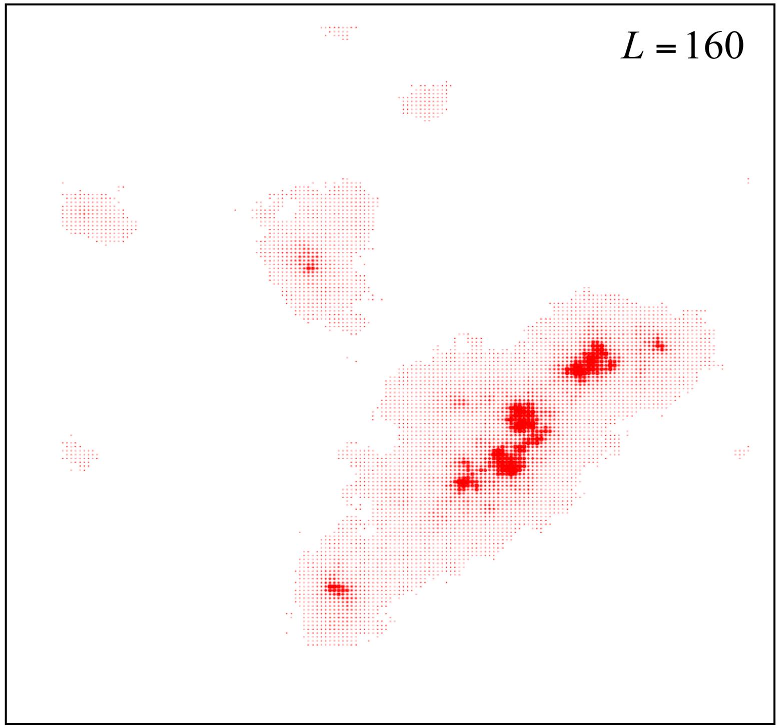
New quantities, more theoretical tools to address physics

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

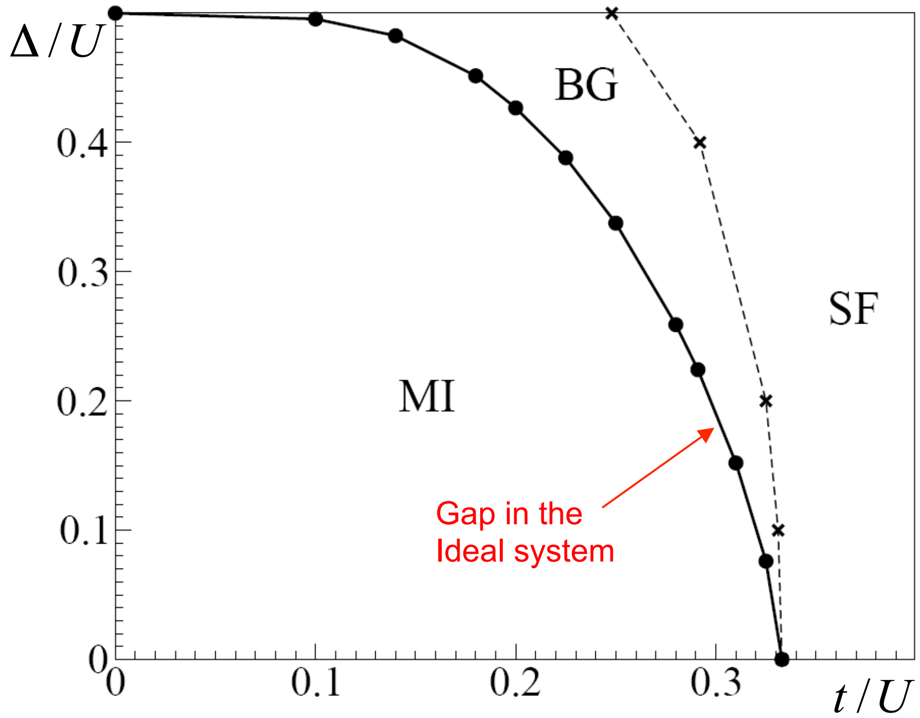
↔ **New physics**

“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

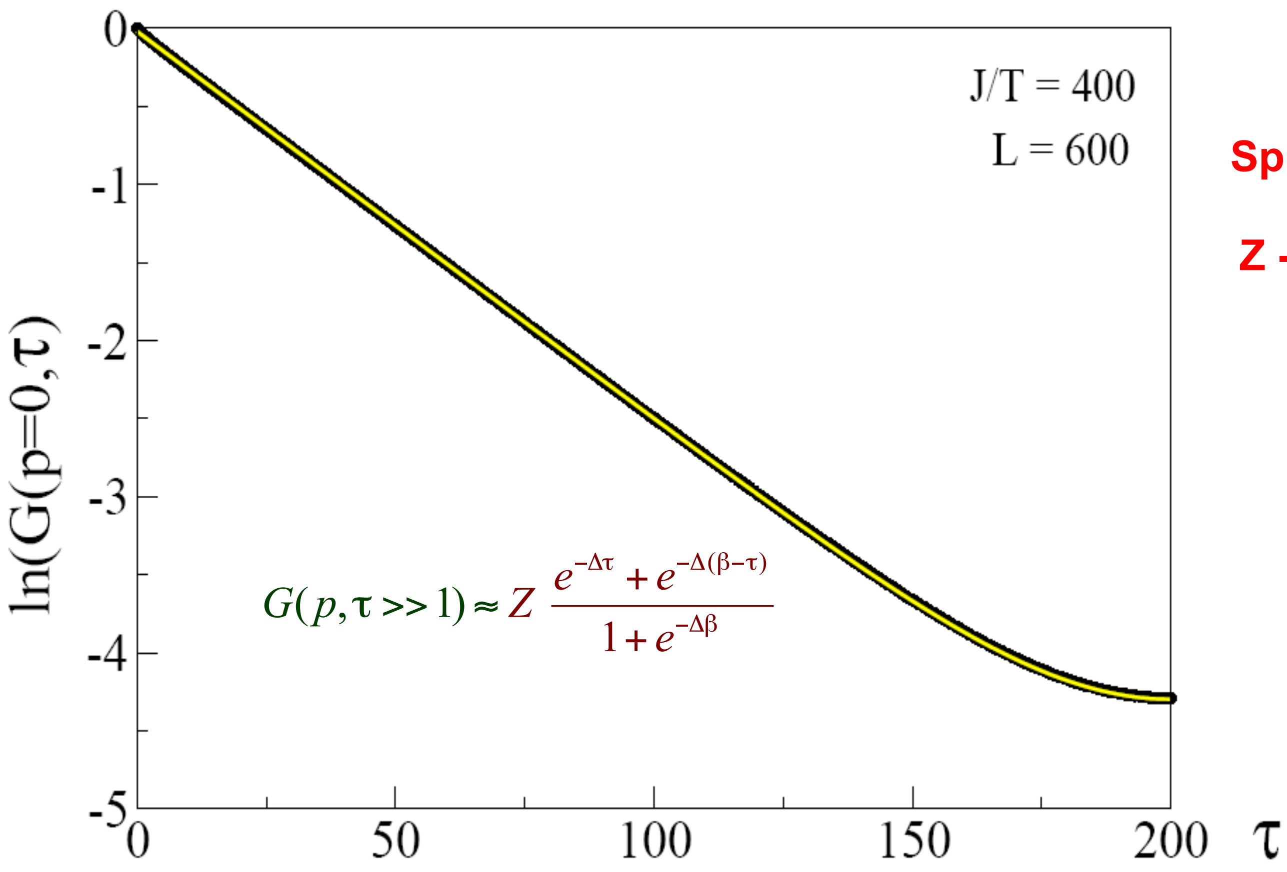


It is a theorem that for $\Delta > E_{GAP}$
the compressibility is finite

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

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

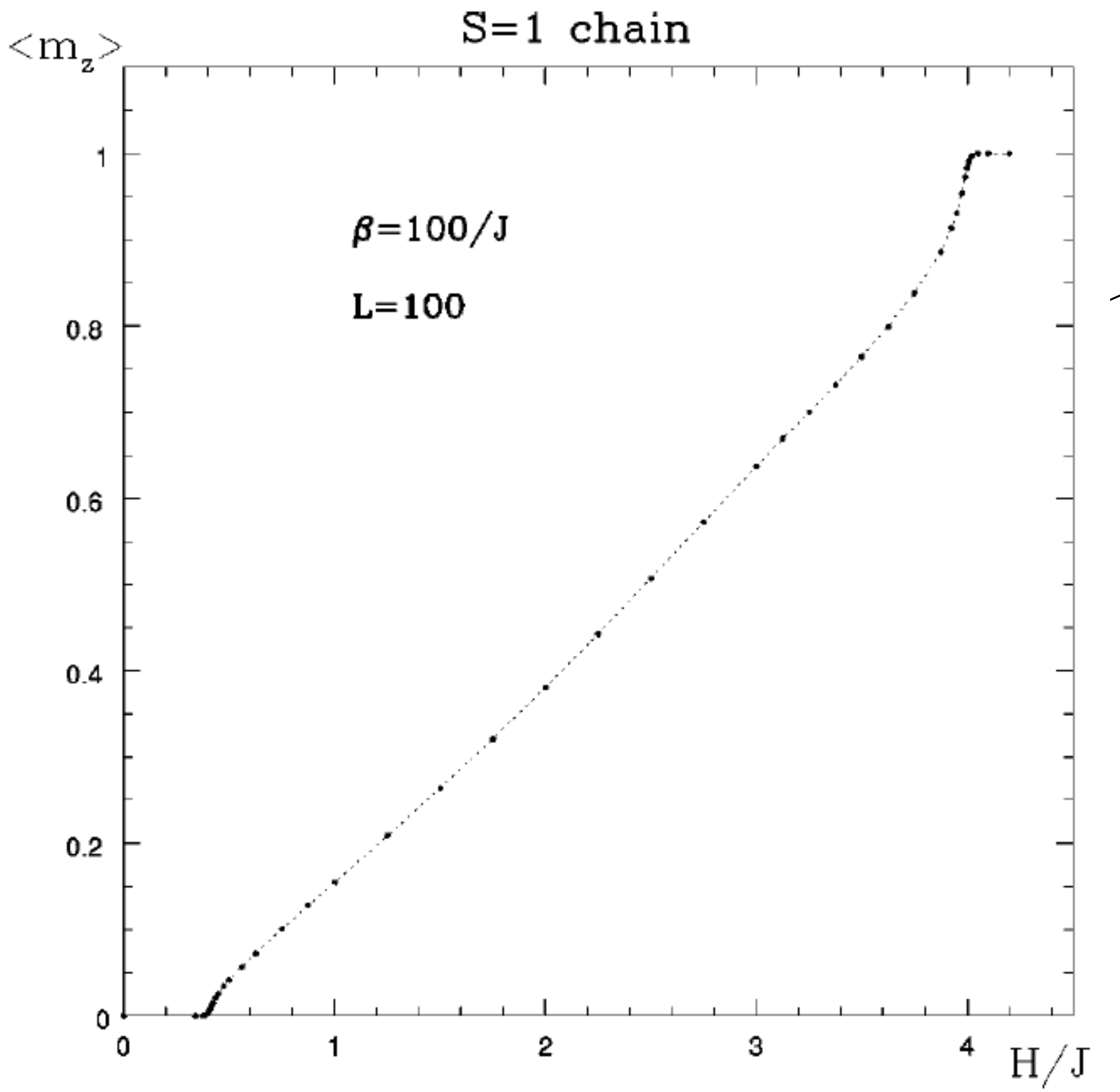
Energy gap: One dimensional S=1 chain with $J_z / J_x = 0.43$



Spin gap $\Delta = 0.02486(5)$

Z -factor $Z = 0.980(5)$

magnetization curves



MC data

Bethe ansatz