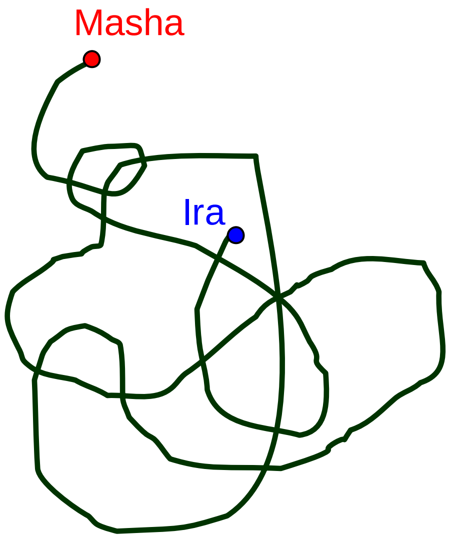
# WORM ALGORITHM

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WHERE DISCOVERIES BEGIN

ISSP, August 2006

# 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!**

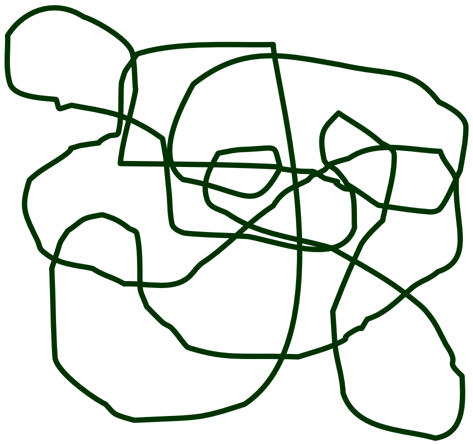
**New quantities, more theoretical tools to address physics**

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

**Examples from**: **superfluid-insulator transition, spin chains, helium solid & glass, deconfined criticality, resonant fermions, holes in the t-J model, …**

## Worm algorithm idea

**Consider:**

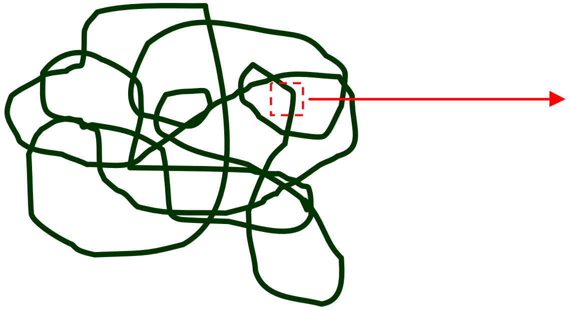


**- configuration space = arbitrary closed loops**

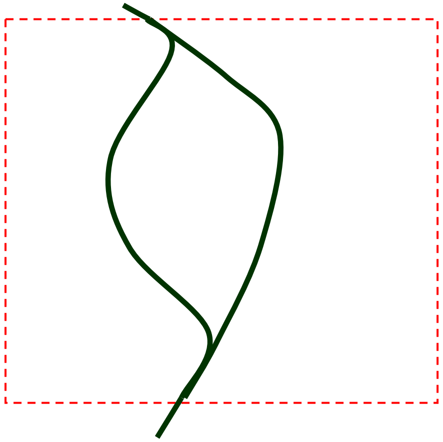
**- each cnf. has a weight factor** $W_{cnf}$

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

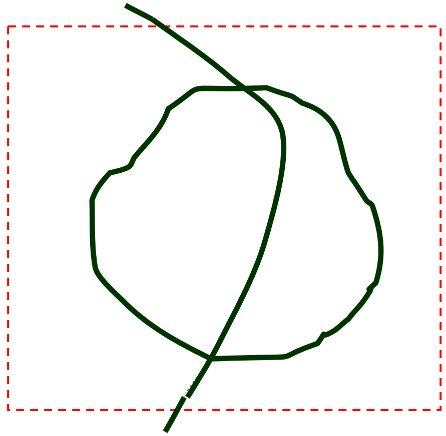
**“conventional” sampling scheme:**



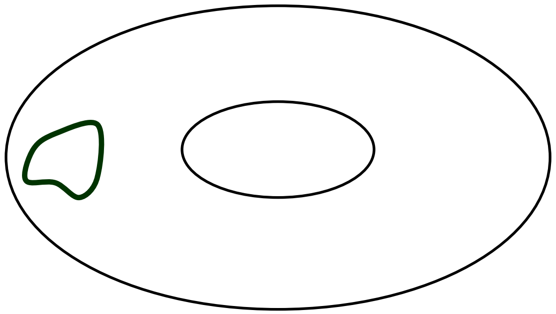
**local shape change**



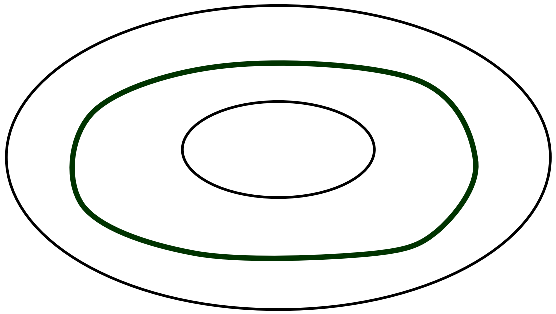
**Add/delete small loops**



**No sampling of topological classes**
**(non-ergodic)**



**can not evolve to**



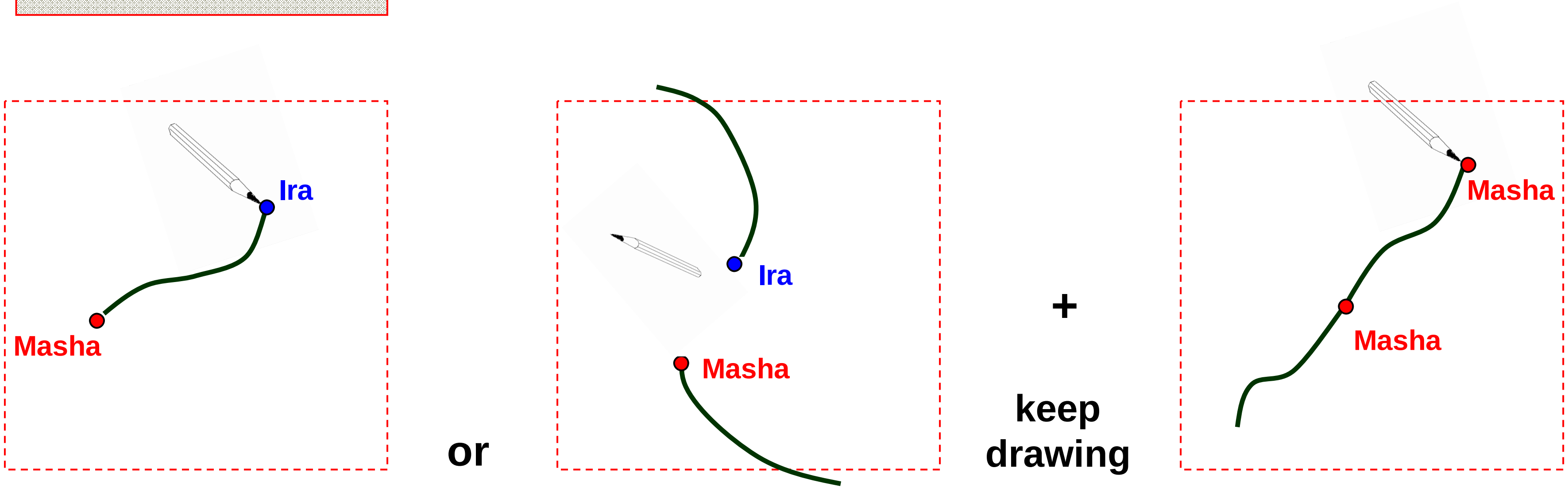
**Critical slowing down**
**(large loops are related to critical modes)**

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

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

# Worm algorithm idea

**draw and erase:**




- **Topological are sampled** (whatever you can draw!)

- **No critical slowing down in most cases**

**Disconnected loops are related to correlation functions and are not merely an algorithm trick!**

# High-T expansion for the Ising model

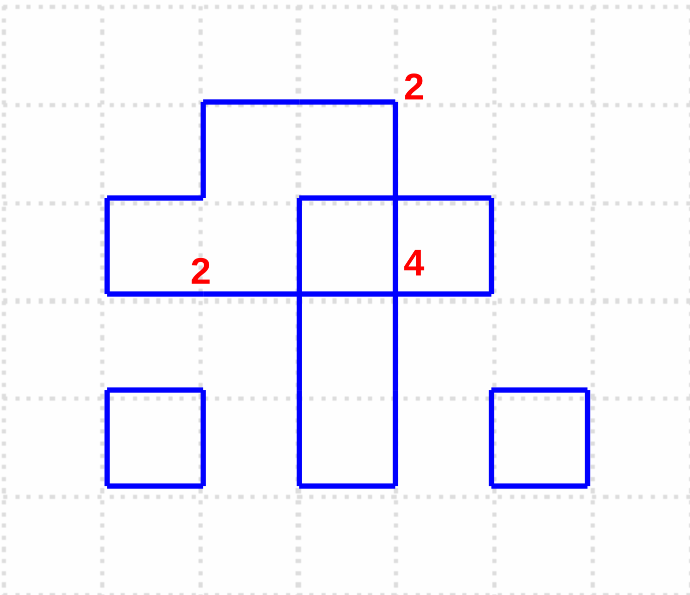
$$-\frac{H}{T} = K \sum_{<ij>} \sigma_i \sigma_j \quad (\sigma = \pm 1)$$

$$Z = \sum_{\{\sigma_i\}} e^{-H/T} \equiv \sum_{\{\sigma_i\}} \prod_{b=<ij>} e^{K\sigma_i\sigma_j} \equiv \sum_{\{\sigma_i\}} \prod_{b=<ij>} \cosh K \; (1 + \tanh K \; \sigma_i \sigma_j)$$

$$\sim \sum_{\{\sigma_i\}} \prod_{b=<ij>} \sum_{N_b=0,1} \left(\tanh K \; \sigma_i \sigma_j\right)^{N_b} = \sum_{\{N_b=0,1\}} \left( \prod_{b=<ij>} \tanh^{N_b} K \right) \prod_i \left( \sum_{\sigma_i = \pm 1} \sigma_i^{M_i} \right)$$

$$\sim \sum_{\{N_b\}=loops} \left( \prod_{b=<ij>} \tanh^{N_b} K \right)$$

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




**Graphically:**

$N_b$ = **number of lines;**

**continuity (enter/exit)** $\rightarrow M_i = even$

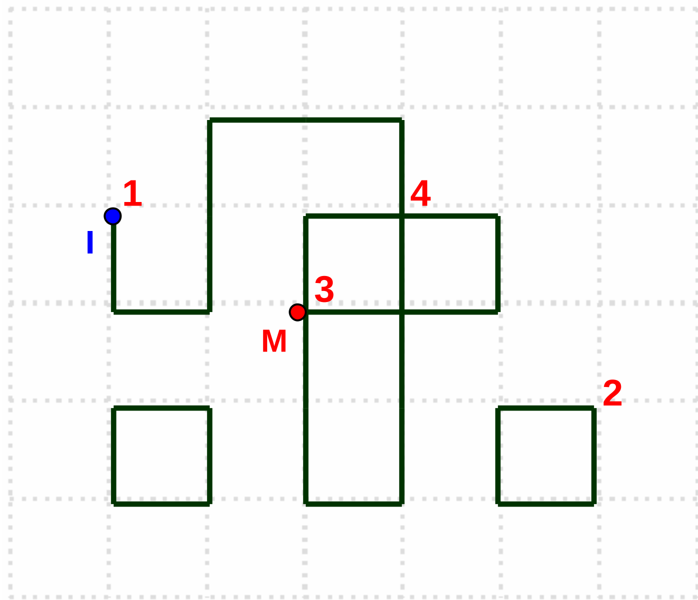
Spin-spin correlation function: $g_{IM} = \frac{G_{IM}}{Z}$ , $G_{IM} = \sum_{\{\sigma_i\}} e^{-H/T} \sigma_I \sigma_M$

$$G \equiv \sum_{\{N_b\}} \left( \prod_{b=<ij>} \tanh^{N_b} K \right) \prod_i \left( \sum_{\sigma_i = \pm 1} \sigma_i^{M_i + \delta_{iI} + \delta_{iM}} \right) \sim \sum_{\substack{\{N_b\}=loops \\ +IM\ worm}} \left( \prod_{b=<ij>} \tanh^{N_b} K \right)$$

**Worm algorithm cnf. space =** $Z$ $G$

**Same as for generalized partition**

$$Z_W = Z + \kappa G$$



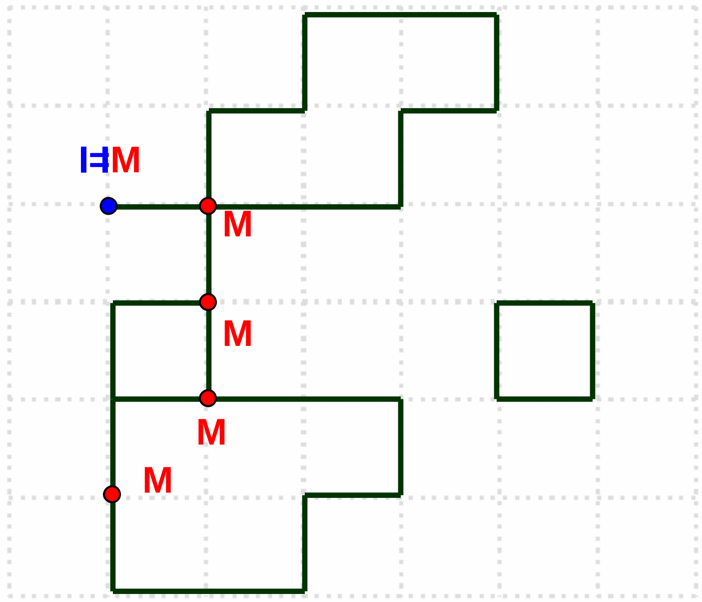
## Complete algorithm:

- If $I = M$, select a new site for $I, M$ 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. $R = \begin{cases} \min(1, \tanh(K)) \\ \min(1, \tanh^{-1}(K)) \end{cases}$

Easier to implement then single-flip!




**MC estimators**

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

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

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

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

**Magnetization fluctuations:** $$\left\langle M^2\right\rangle=\left\langle\left(\sum\sigma_i\right)^2\right\rangle=N\sum g(i)$$

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

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

**Ising** $\longrightarrow$ **lattice field theory**

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

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

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

$$Z=\sum_{\{N_{i\nu}\}}\left(\prod_{i,\nu}\frac{t^{N_{i\nu}}}{N_{i\nu}!}\right)\prod_i\left(\int d\psi_i\;\underbrace{\psi_i^{M_{1i}}\left(\psi^{*}_i\right)^{M_{2i}}}_{e^{i\varphi(M_1-M_2)}\to M_1=M_2=M}\;e^{\mu|\psi_i|^2-U|\psi_i|^4}\right)$$

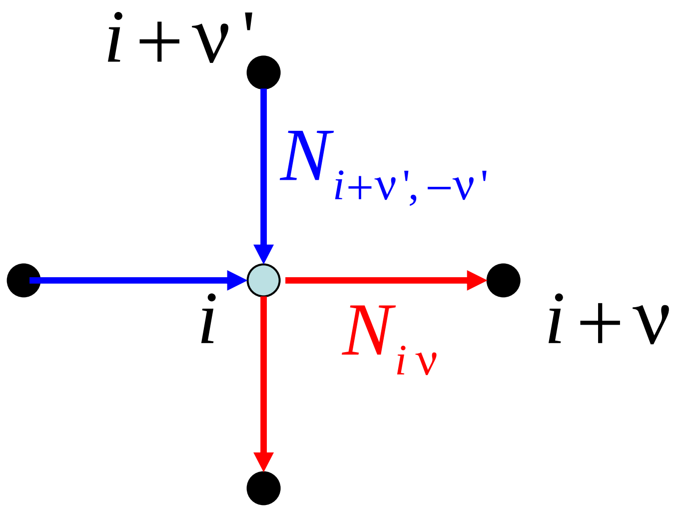
$$\prod_i Q(M_i)$$

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

$\longrightarrow$ **closed oriented loops**

$=$ **tabulated numbers**

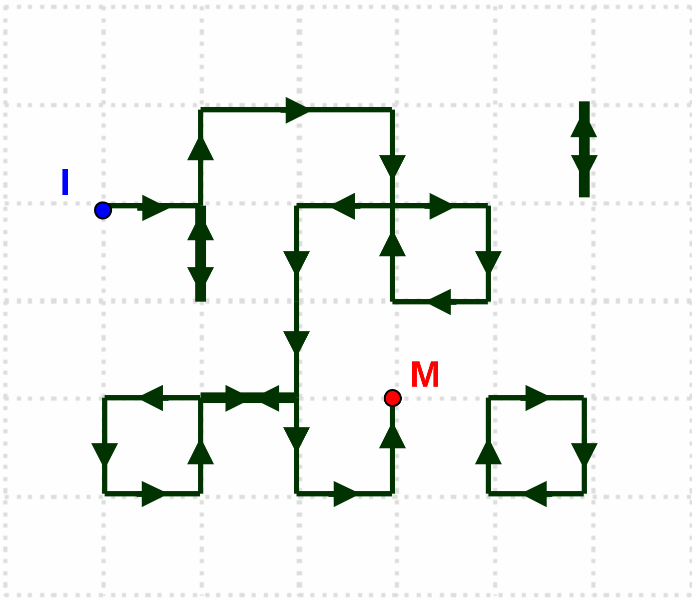
$$\psi_i^{\sum_\nu N_{i\nu}} (\psi^*_i)^{\sum_\nu N_{i+\nu,-\nu}}$$




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

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

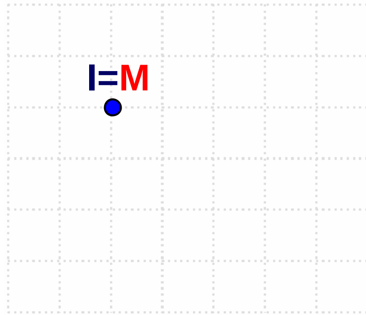
**(one open loop)**



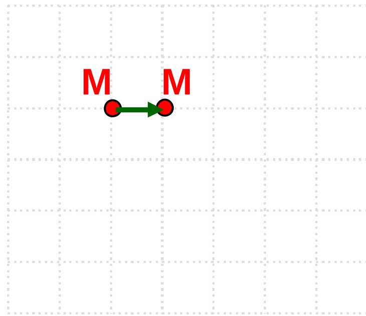

**Worm algorithm cnf. space =** $Z \quad G$

## Same algorithm:

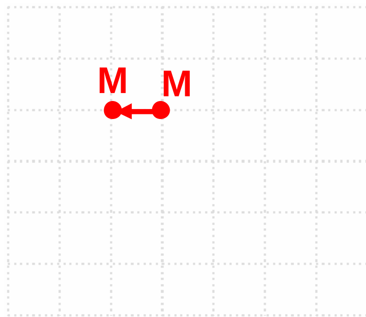
- $Z \leftrightarrow G$ **sectors, prob. to accept** $R_{Z\to G} = \min\left[1, \frac{Q(M_I+1)}{Q(M_I)}\right]$




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



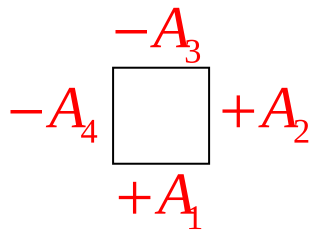

- $N_{M+\nu,-\nu} \to N_{M+\nu,-\nu}-1$ **erase** $R = \min\left[1, \frac{(N_{M+\nu,-\nu})\,Q(M_M-1)}{t\,Q(M_M)}\right]$




**Keep drawing/erasing …**

**Multi-component gauge field-theory**
**(deconfined criticality, XY-VBS and Neel-VBS quantum phase transitions…**

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




$U_{11} = U_{22} \neq U_{12}$ XY-VBS transition
no DCP, always first-order

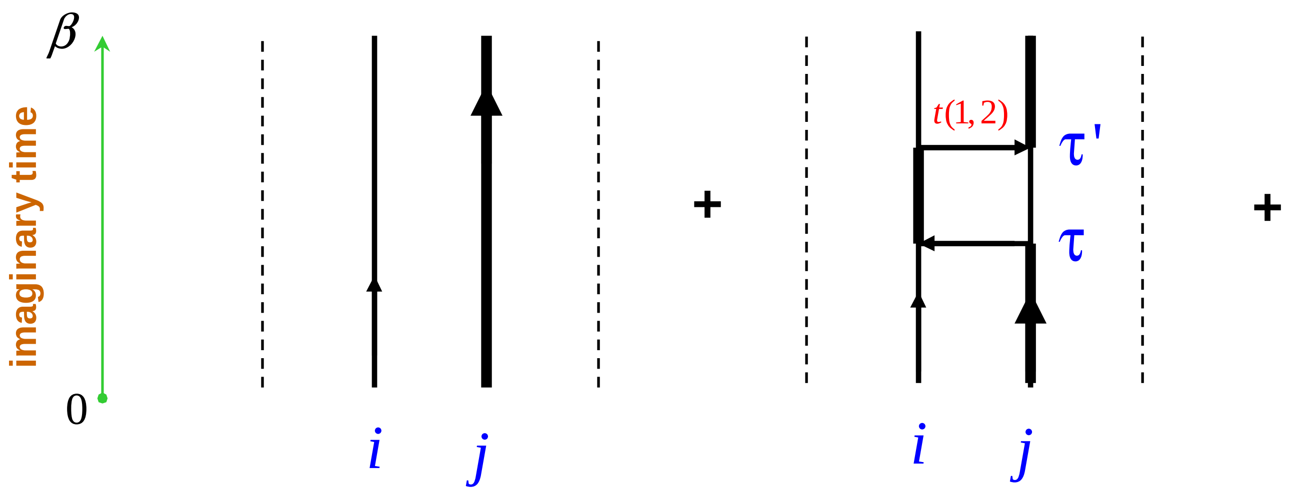
$U_{11} = U_{22} = U_{12}$ Neel-VBS transition, unknown !

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

**Lattice path-integrals for bosons and spins are "diagrams" of closed loops!**

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

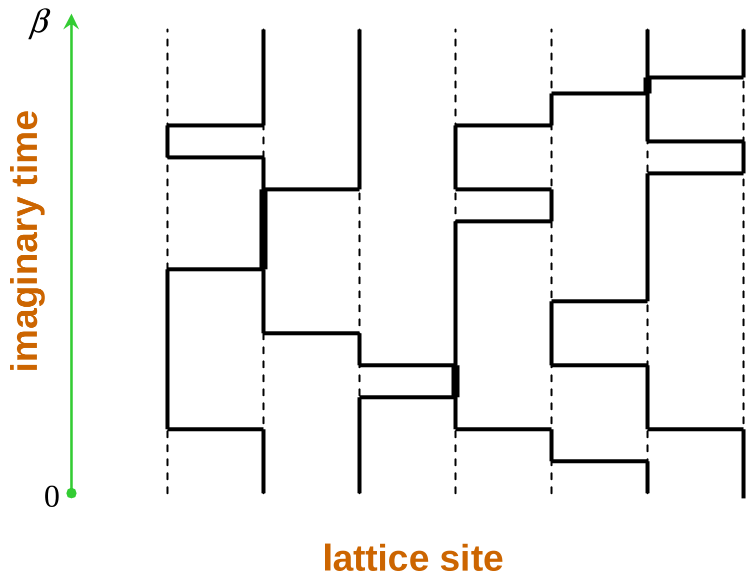
$$= \mathrm{Tr}\, e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau)\, d\tau + \int_0^\beta \int_\tau^\beta H_1(\tau)\, H_1(\tau)\; d\tau\, d\tau' + \ldots \right\}$$




$$|n_i = 0, 1, 2, 0\rangle$$

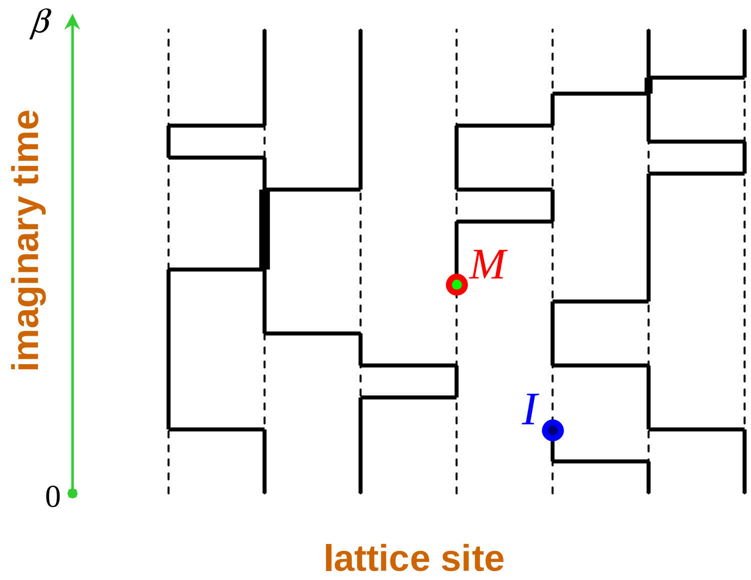
Diagrams for

$$Z = \mathrm{Tr}\, e^{-\beta H}$$




Diagrams for

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




## The rest is conventional worm algorithm in continuous time

**(there is no problem to work with arbitrary number of continuous variables as long as an expansion is well defined)**

## Diagrammatic Monte Carlo (not in this lecture)

$$A(\vec{y}) = \sum_{n=0}^{\infty} \sum_{\xi} \iiint d\vec{x}_1 d\vec{x}_2 \dots d\vec{x}_n D_n(\xi; \vec{x}_1, \vec{x}_2, \dots \vec{x}_n, \vec{y})$$

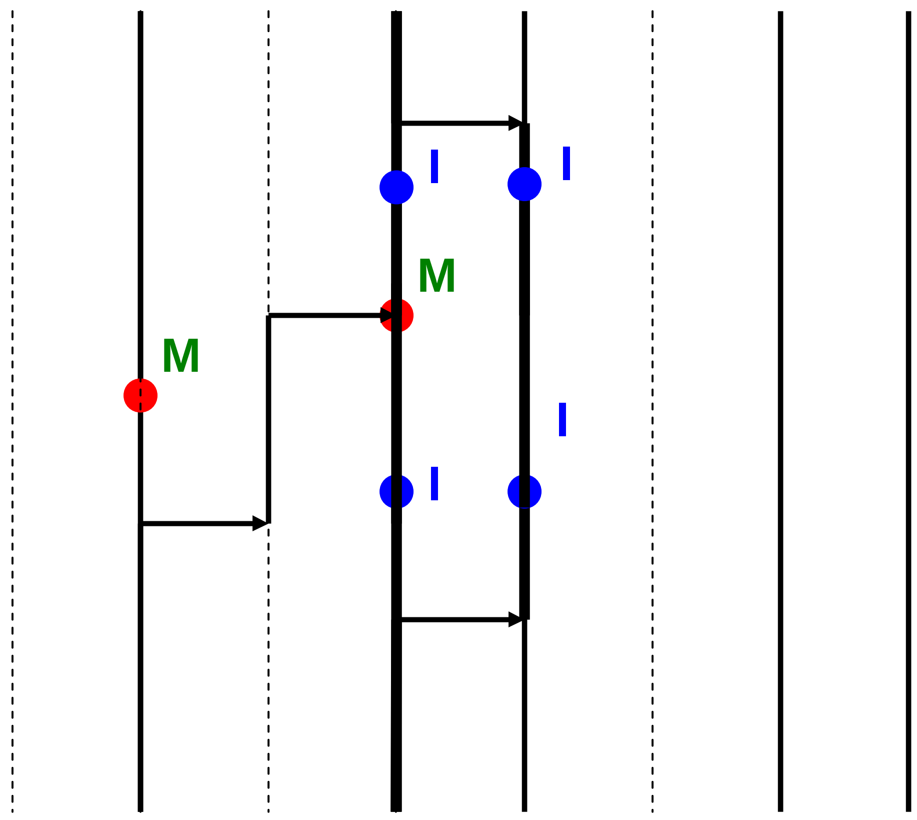
Diagram order

Same-order diagrams

Integration variables

Contribution to the answer
or the diagram weight
(positive definite, please)

ENTER



I
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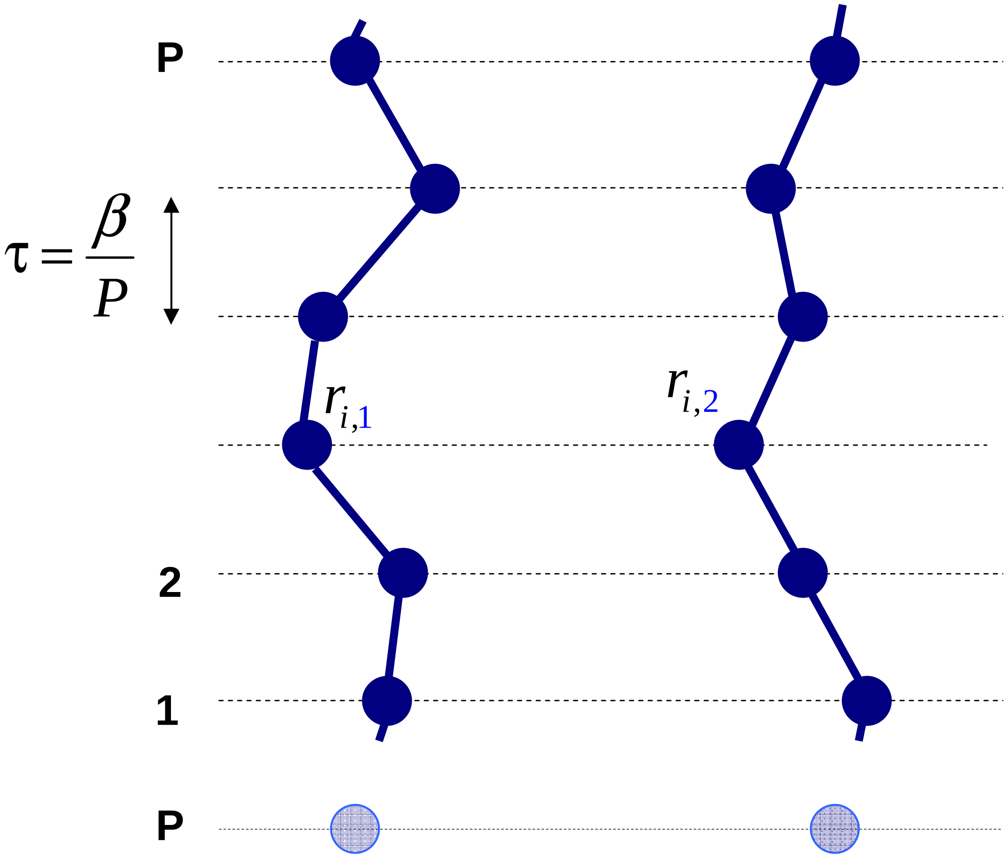
**Path-integrals in continuous space are consist of closed loops too!**

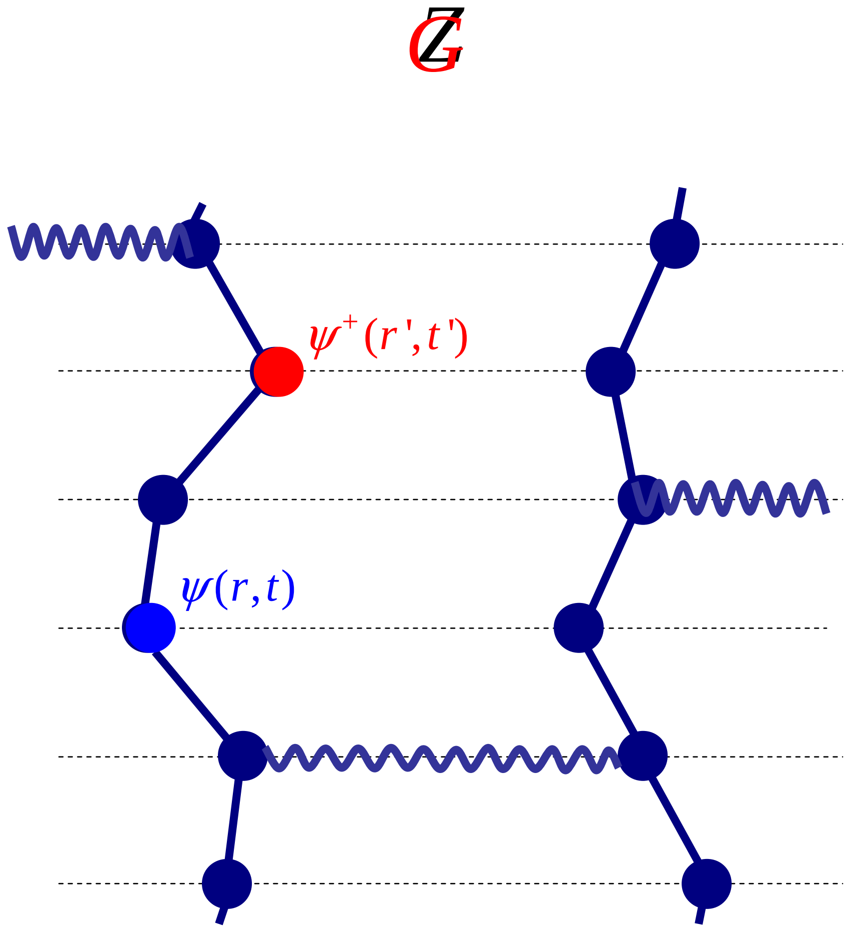
$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} V(r_i - r_j)$$

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

Feynman path-integral




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

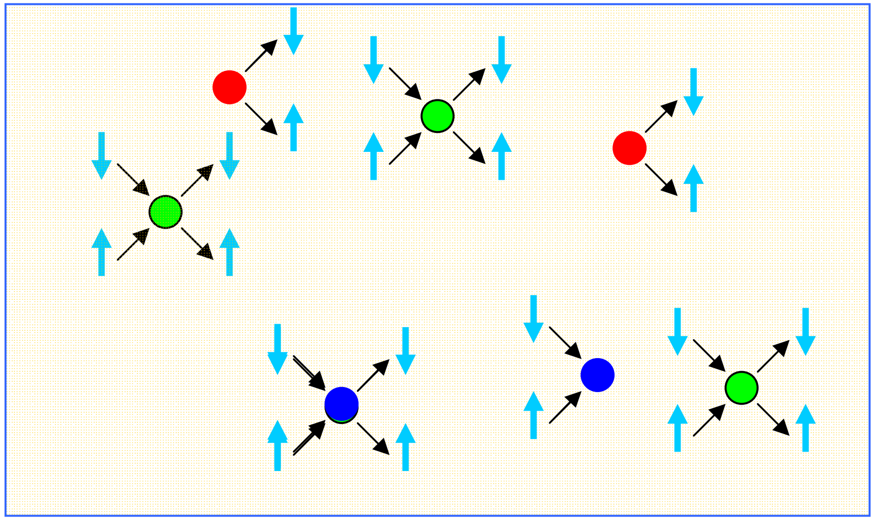



**diagrammatic expansion**
**for** $V(r) < 0$

**Not necessarily for closed loops!**

$$H = \sum_{i,\sigma=\uparrow\downarrow} \varepsilon(k_{i\sigma}) + \sum_{i<j} V(r_{i\uparrow} - r_{j\downarrow})$$

**Feynman (space-time) diagrams for fermions with contact interaction (attractive)** $\bullet = -U$



**Pair correlation function**

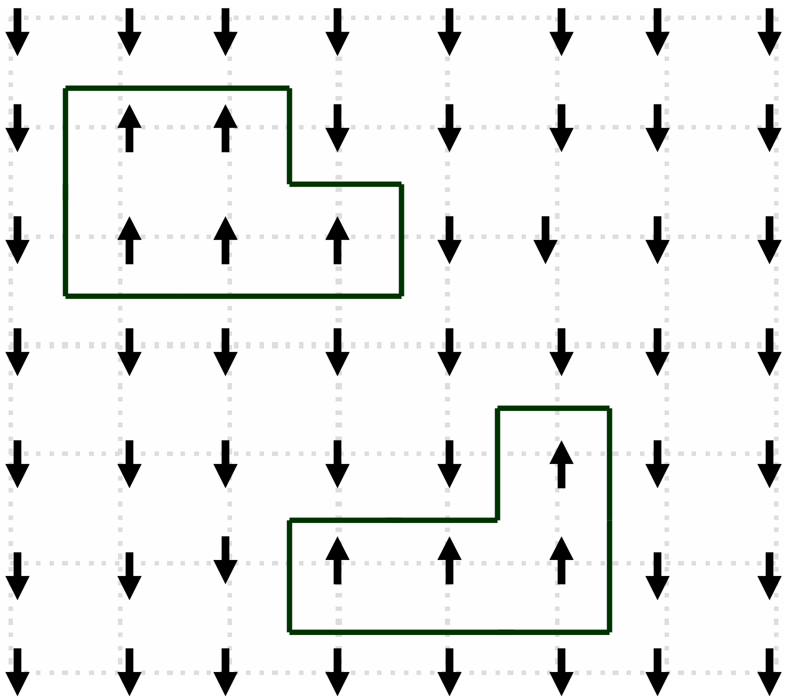
$$\left\langle a_\uparrow^+(r_1,\tau_1) a_\downarrow^+(r_1,\tau_1)\ a_\downarrow(r_2,\tau_2) a_\uparrow(r_2,\tau_2) \right\rangle$$

**connect vortexes with** $G_\downarrow$ **and** $G_\uparrow$ $\longrightarrow$ $D_n = (-U)^n G_\uparrow \ldots G_\uparrow G_\downarrow \ldots G_\downarrow (d\vec{r}d\tau)^n (-1)^{\text{perm}}$

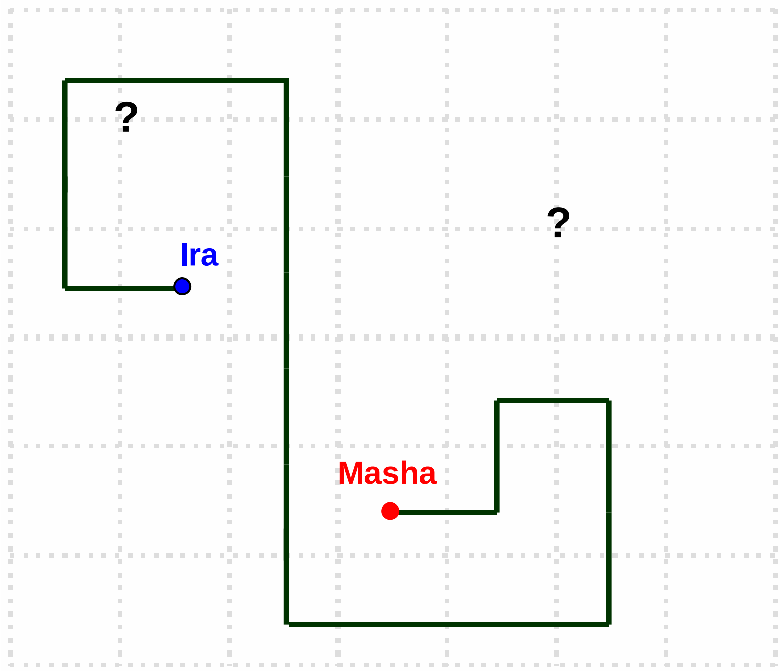
**sum over all possible** $(n!)^2$ **connections** $\sum_\xi D_n(\xi) = (-U)^n \det^2 G_\uparrow(\vec{x}_i, \vec{x}_j)(d\vec{r}d\tau)^n \geq 0$

## G space is NOT necessarily physical

**Domain walls in 2D Ising model are loops!**



**Disconnected loop is unphysical!**

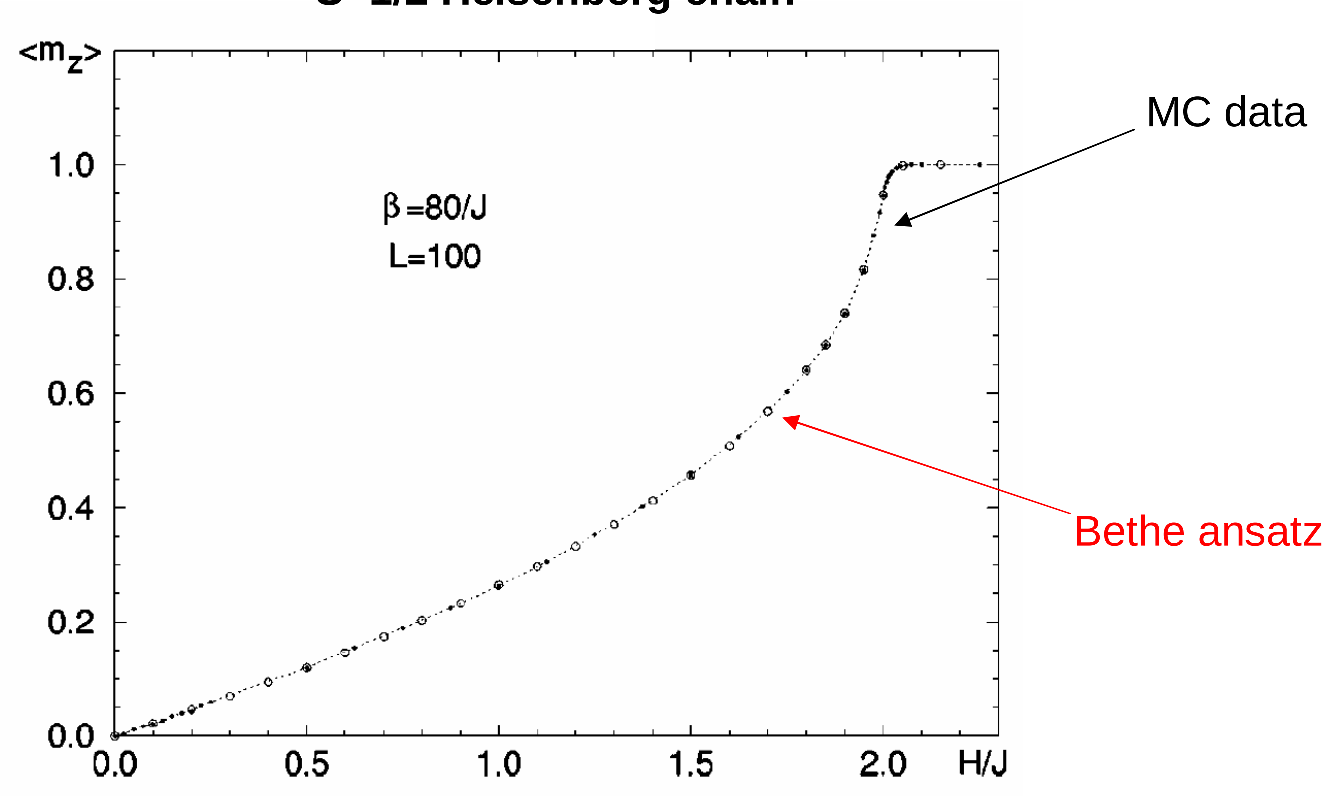


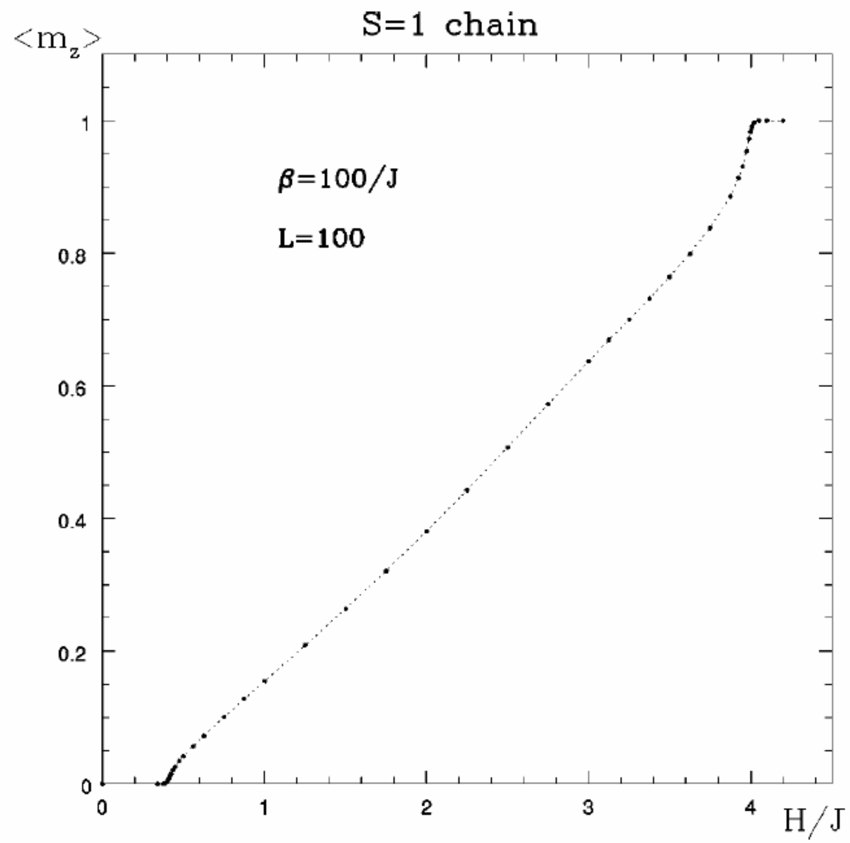

**Worm cnf. space =** $Z \cdot (G =$ **disconnected loop** $)$

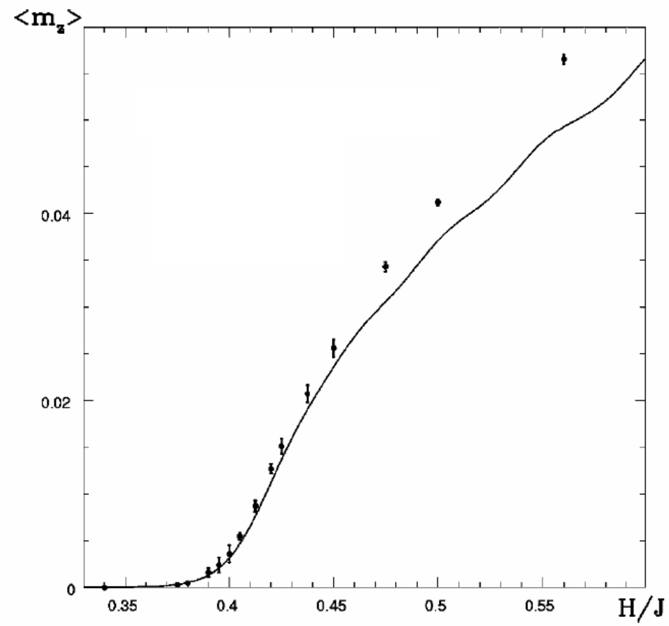
**Quantum spin chains magnetization curves, gaps, spin wave spectra**

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

**S=1/2 Heisenberg chain**






**Line is for the effective fermion theory with spectrum**

$$\varepsilon(p = 2\pi n / L) = \sqrt{\Delta^2 + cp^2}$$

$$\Delta = 0.4105(1)$$

$$c = 2.48(1)$$

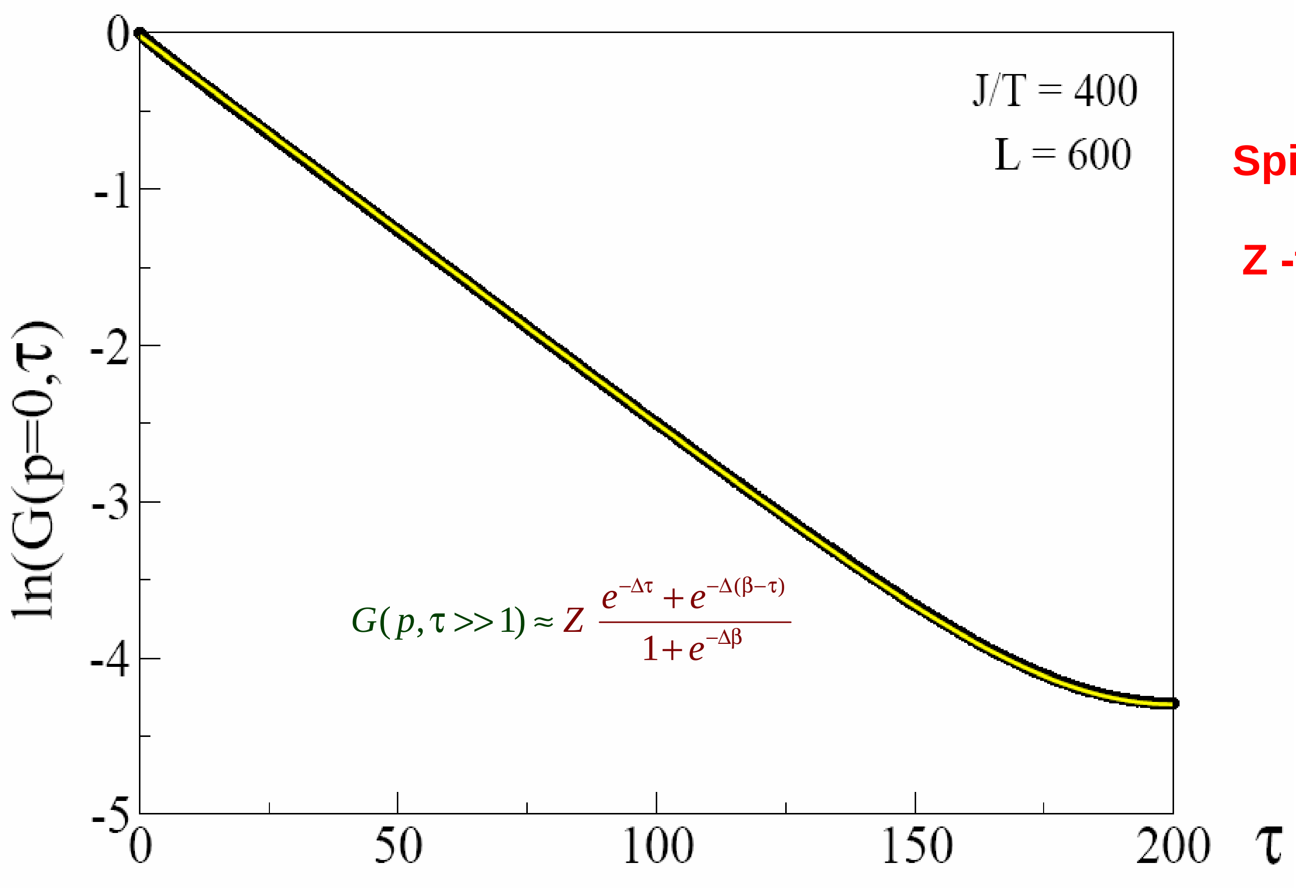
**deviations are due to magnon-magnon interactions**

Lou, Qin, Ng, Su, Affleck '99

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

$$G(p,\tau) = \int e^{ipx}\, dx \left\langle T_\tau S^\dagger(x,\tau) S_I^-(0) \right\rangle$$

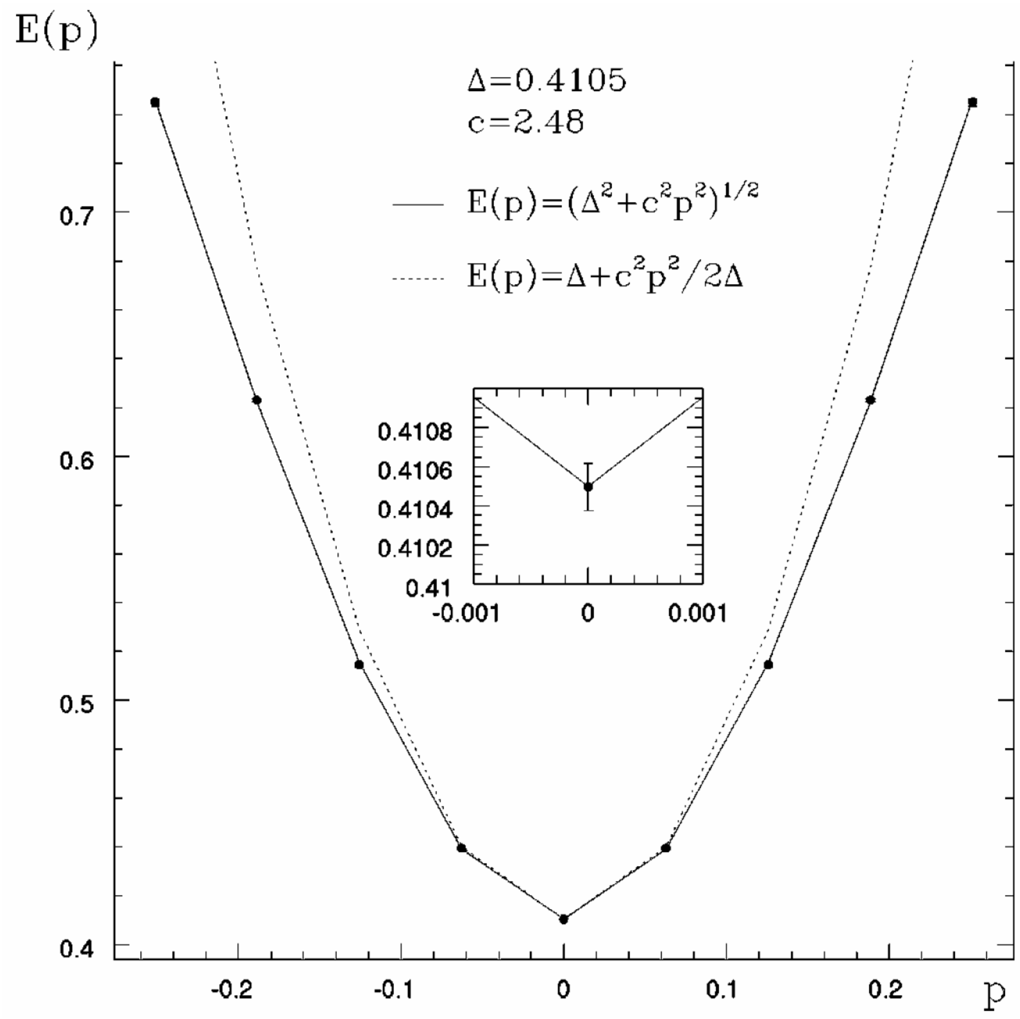
$$= \sum_{\alpha'} \left| \left(S_p^\dagger\right)_{G\alpha'} \right|^2 e^{(E_G - E_{\alpha'})\tau} \xrightarrow[\tau J >> 1]{} Z\, e^{-\Delta\tau}$$



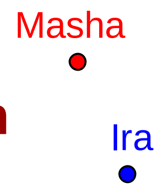

**Spin gap** $\Delta = 0.02486(5)$

**Z -factor** $Z = 0.980(5)$

**Spin waves spectrum:** **One dimensional S=1 Heisenberg chain**



# Conclusions:

**Worm algorithm = cnf. space of $Z$ $G$ + updates based on** 


**Can be formulated for:**

**- classical and quantum models (Bose/Fermi/Spin)**

**- different representations (path-integrals, Feynam diagrams,SSE)**

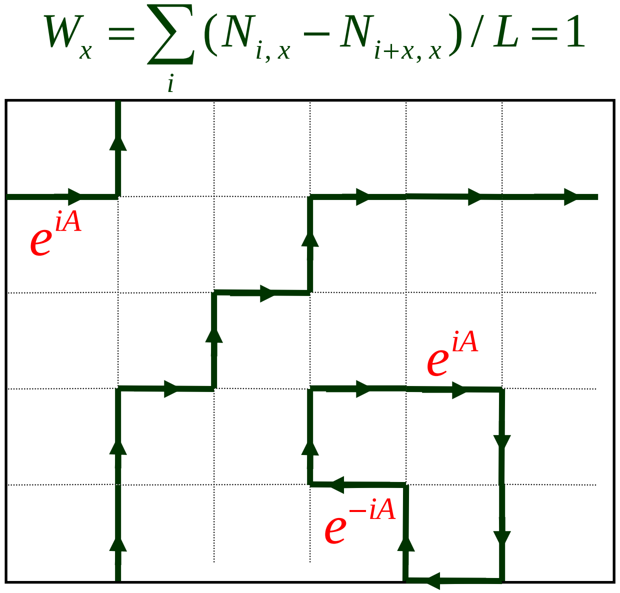
**- non-local solutions of balance Eqn. (clusters, directed loops, geom. worm)**

# Winding numbers

**Homogeneous gauge in x-direction:** $t \longrightarrow t e^{iA}, \quad A_x(r) = \varphi / L\,, \quad \oint A_x(r)\, dx = \varphi$

$$Z = \sum_{W_x} e^{i\varphi W_x} Z_{W_x}$$

$$F = -T \ln Z = F(0) + L^d \Lambda_S \frac{(\varphi / L)^2}{2}$$




$$\Lambda_S = L^{d-2} \frac{\partial^2 F}{\partial \varphi^2} = \frac{T \left\langle W_x^{\ 2} \right\rangle}{L^{d-2}}$$

**Ceperley**
**Pollock '86**