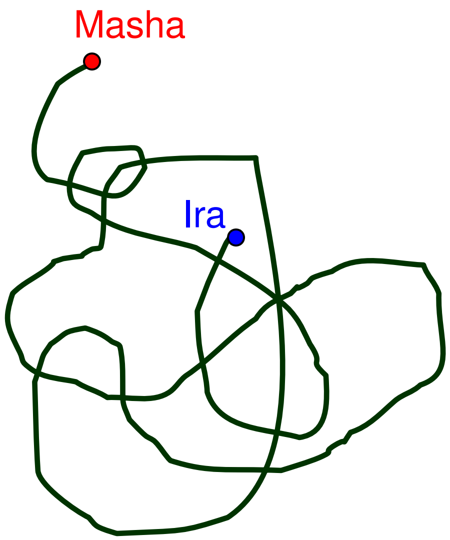
WORM ALGORITHM



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National Science Foundation
WHERE DISCOVERIES BEGIN

Los Angeles, January 23, 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!

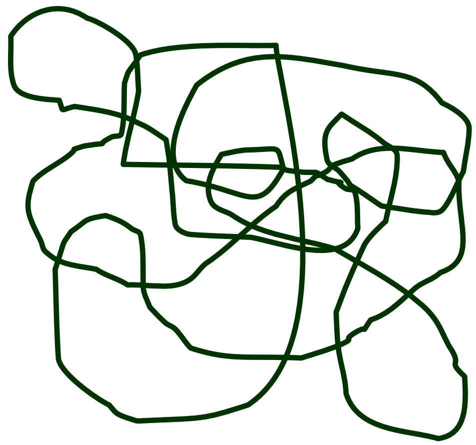
New quantities, more theoretical tools to address physics

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

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

Worm algorithm idea

Consider:

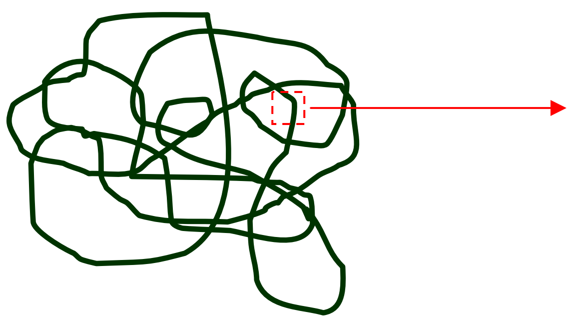


- **configuration space = arbitrary closed loops**

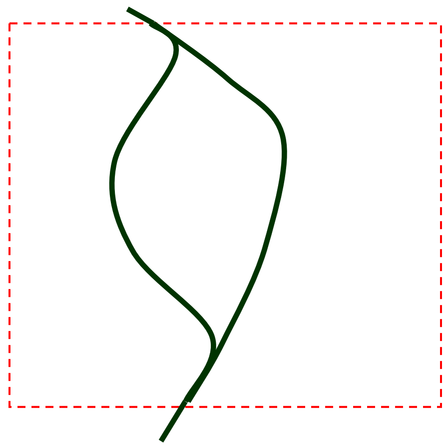
- **each cnf. has a weight factor** W_{cnf}

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

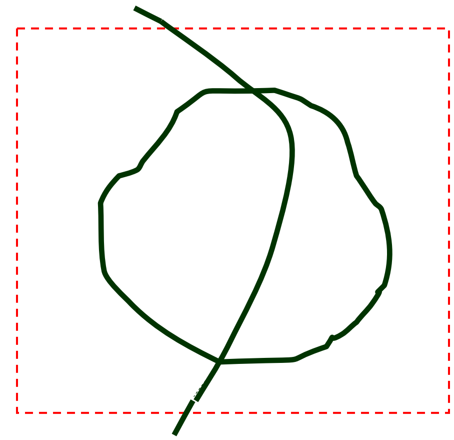
“conventional” sampling scheme:



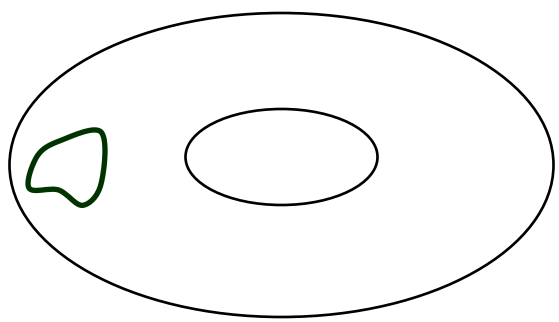
local shape change



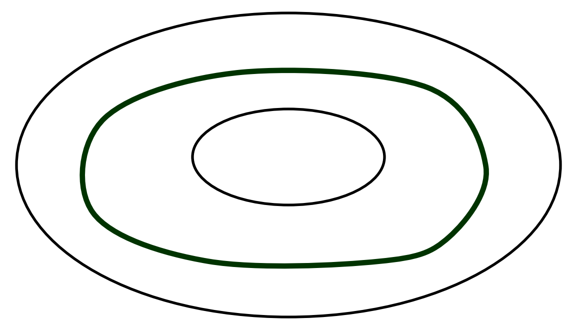
Add/delete small loops



No sampling of topological classes
(non-ergodic)



can not evolve to



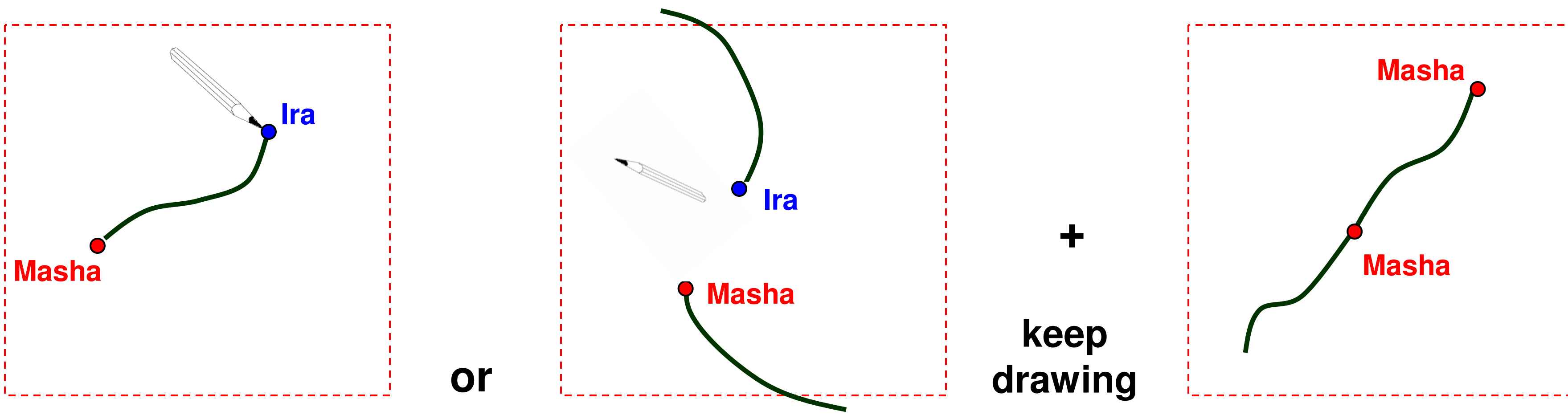
Critical slowing down
(large loops are related to critical modes)

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

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

Worm algorithm idea

draw and erase:



- **Topological classes are sampled** (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

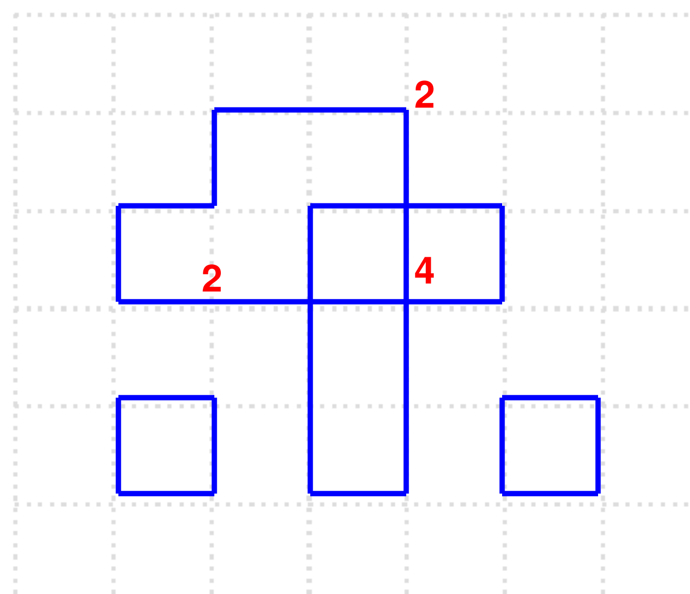
$$-\frac{H}{T} = K\sum_{<ij>} \sigma_i \sigma_j \quad (\sigma = \pm 1)$$

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

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

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

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



Graphically:

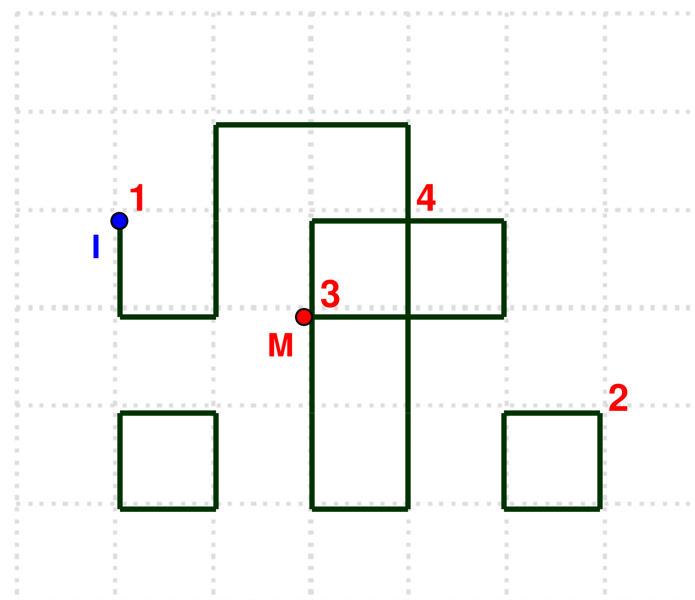
N_b = number of lines;

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 = $Z \cup G$



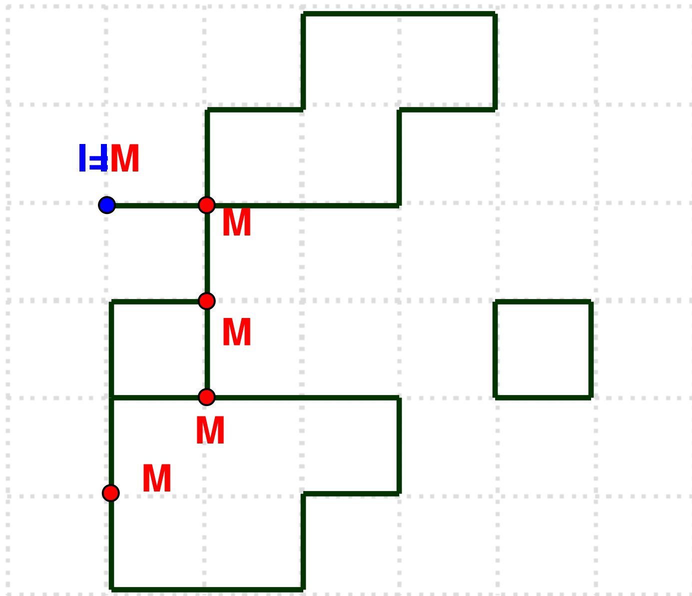
Complete algorithm:

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

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

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

Easier to implement then single spin-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 $\longrightarrow$ XY-model

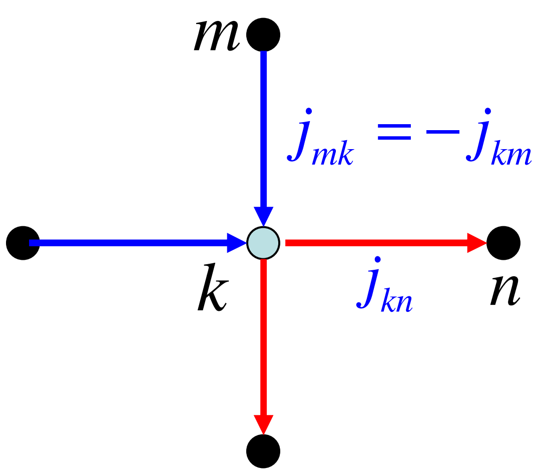
$$-\frac{H}{T} = K \sum_{\langle ij \rangle} \cos\left(\theta_i - \theta_j\right)$$

$$Z = \left(\prod_k \int_0^{2\pi} d\theta_k \right) e^{-H/T} \equiv \left(\int d\theta_k \right) \prod_{b=\langle kn \rangle} e^{K\cos(\theta_k - \theta_n)} \equiv \left(\int d\theta_k \right) \prod_{b=\langle kn \rangle} \sum_{j_b=-\infty}^{j_b=\infty} F(j_b)\, e^{-i(\theta_k - \theta_n) j_b}$$

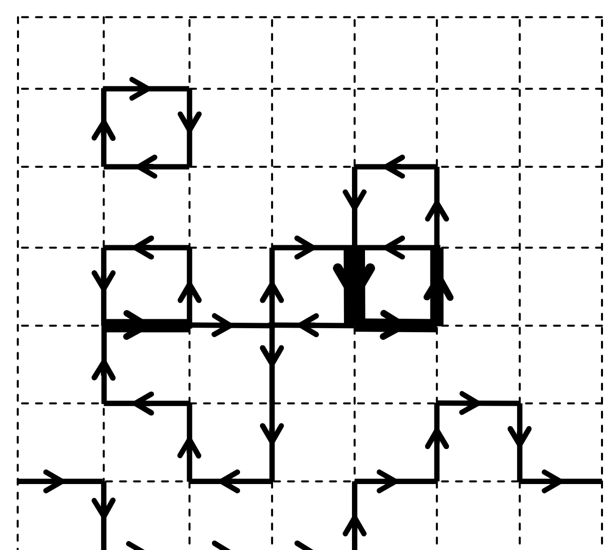
$$Z = \sum_{\{j_b=-\infty\}}^{\{j_b=\infty\}} \prod_b F(j_b) \left(\int_0^{2\pi} d\theta_k \, e^{-i\theta_k M_k} \right) = \sum_{\{j_b\}}^{\{loops\}} \prod_b F(j_b)$$

$$M_k = \sum_{\nu} j_{k,k+\nu} = 0$$

Flux in = Flux out ⇨ **closed oriented loops of integer j-currents; “zero-divergence” constraint**



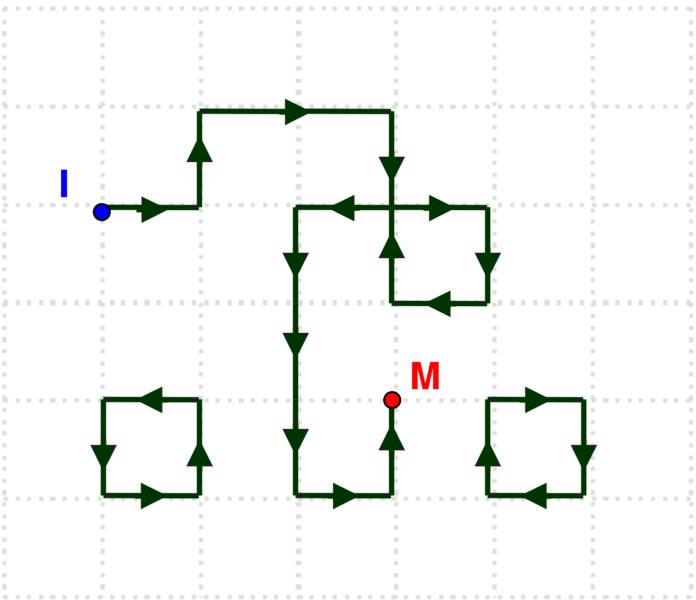
$$e^{-i(\theta_m - \theta_k) j_{mk}} \equiv e^{-i(\theta_k - \theta_m) j_{km}}$$



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

$$g(I-M) = \langle e^{i\theta_I} e^{-i\theta_M} \rangle = \frac{G(I-M)}{Z}$$

(one open loop)



Same algorithm:

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

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

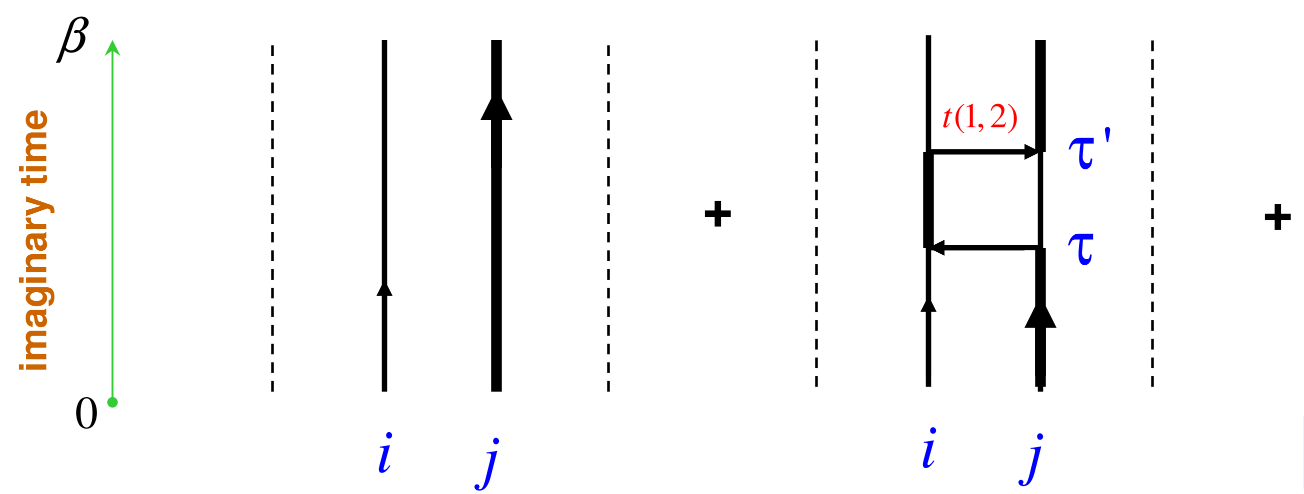
- $j_b^{new} = \begin{cases} j_b - 1 \\ j_b + 1 \end{cases}$ for positive/negative directions; accept with prob. $R = \min\left[1, \frac{F(j_b^{new})}{F(j_b)}\right]$

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

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

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

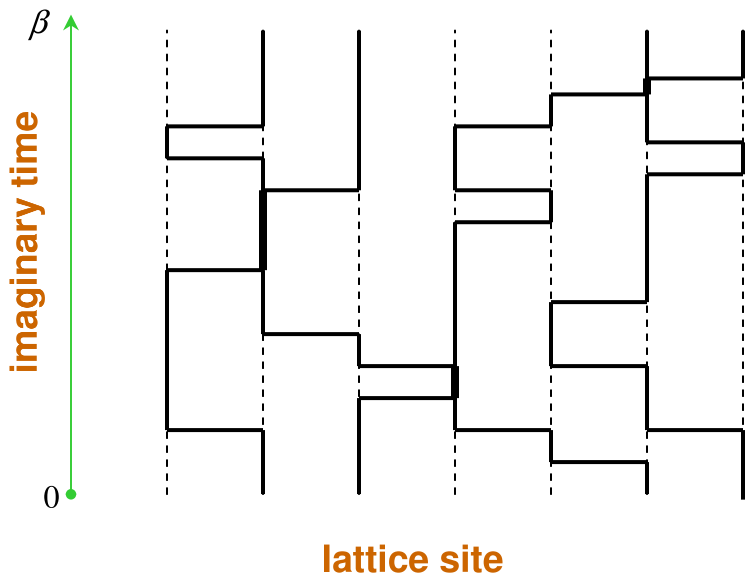
$$= \mathrm{Tr}\, e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau)\, d\tau + \int_0^\beta \int_\tau^\beta H_1(\tau)\, H_1(\tau)\;\; d\tau\, d\tau' + \ldots \right\}$$



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

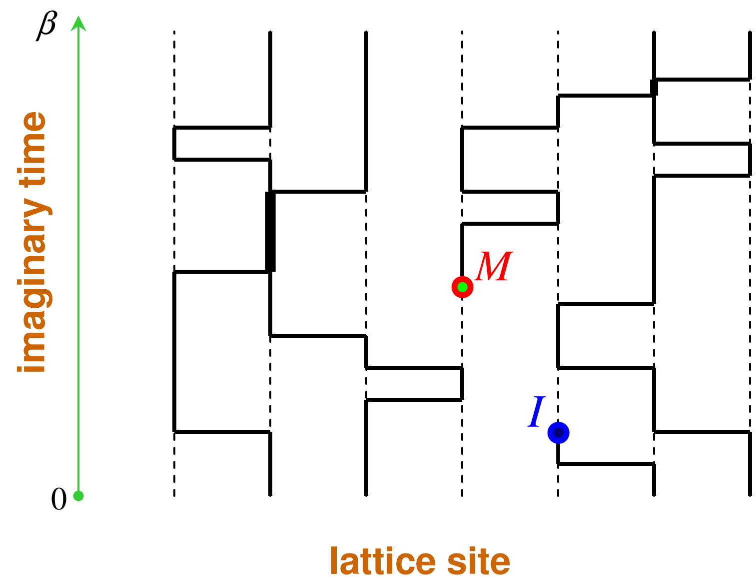
Diagrams for

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



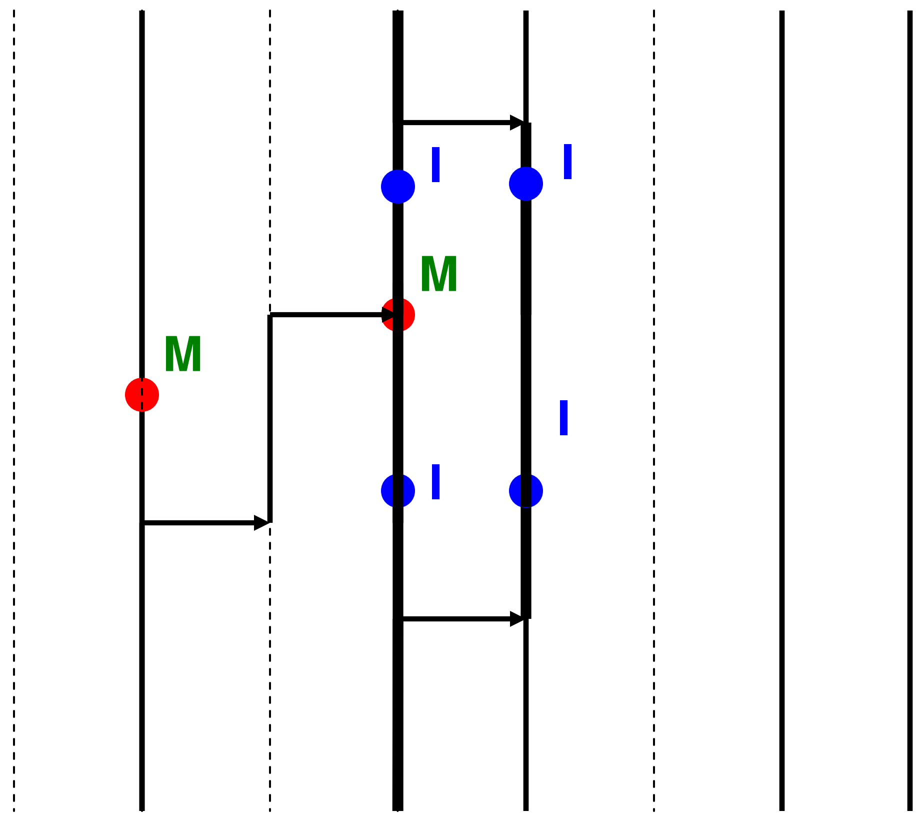
Diagrams for

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



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)


M
M
I
I
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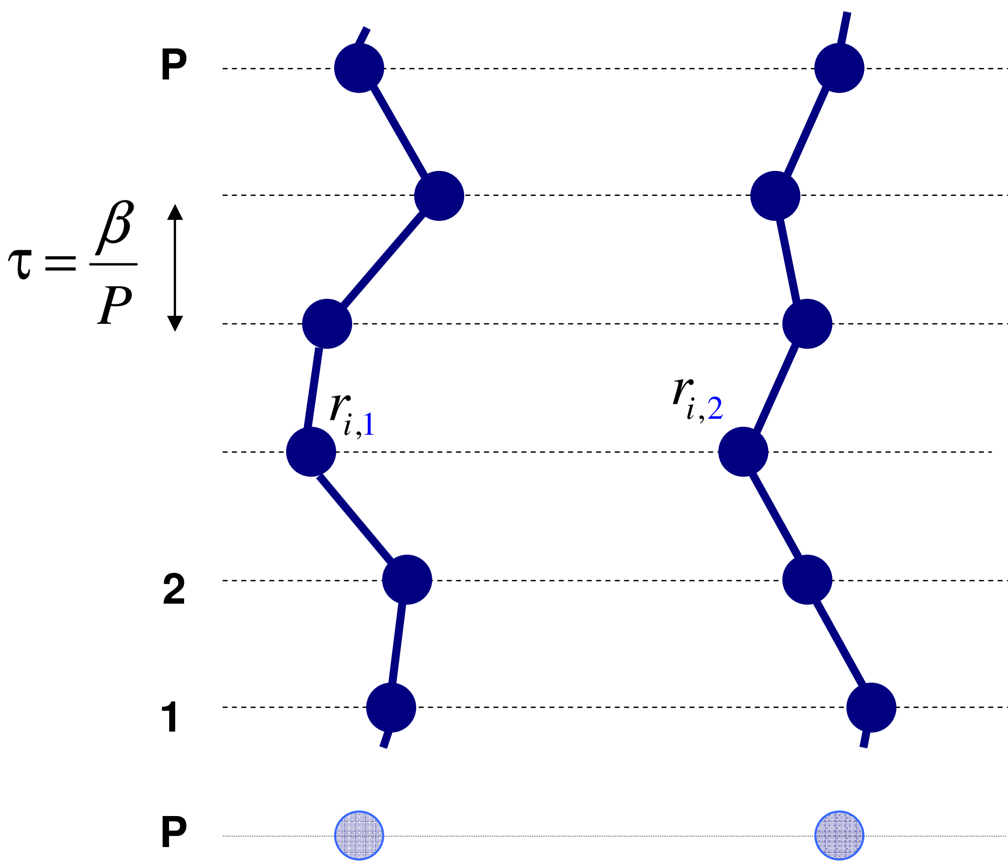
I

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

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

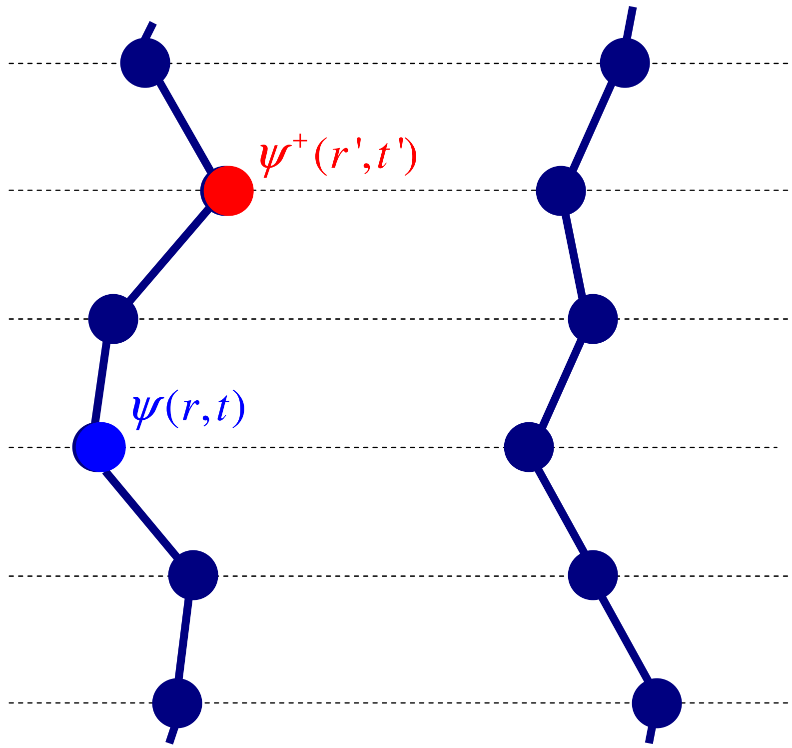
$$Z = \iiint dR_1 \ldots dR_P \exp\left\{ -\sum_{i=1}^{P=\beta/\tau} \left(\frac{m(R_{i+1} - R_i)^2}{2\tau} + U(R)\tau \right) \right\}$$

Feynman path-integral

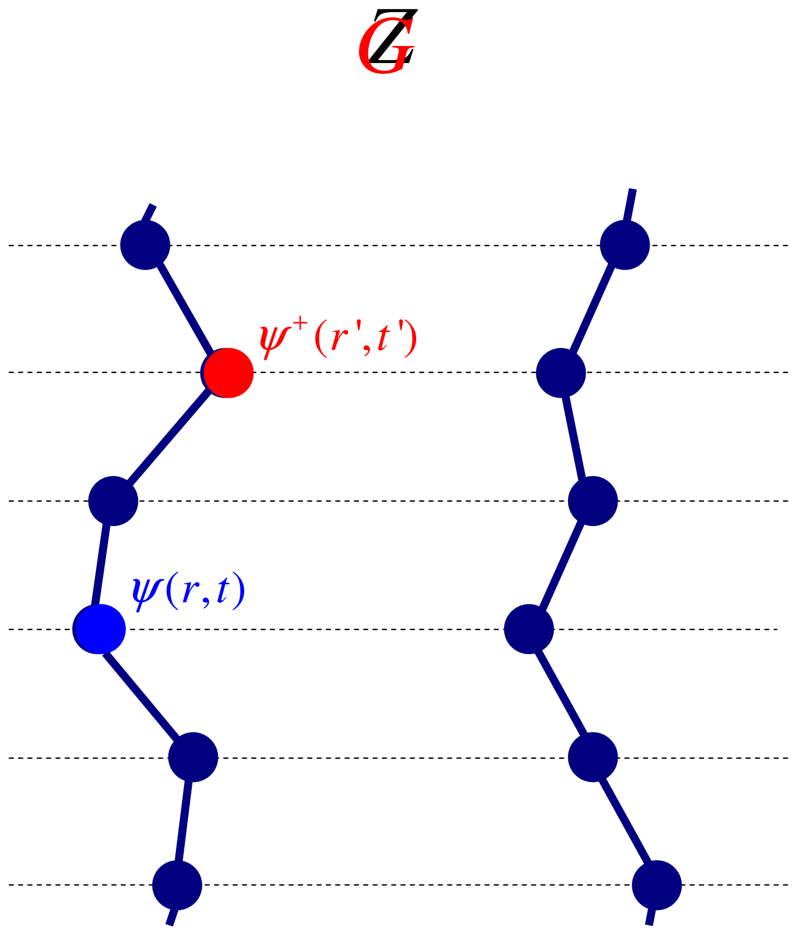


$$R_i = (r_{i,1}, r_{i,2}, \ldots, r_{i,N})$$

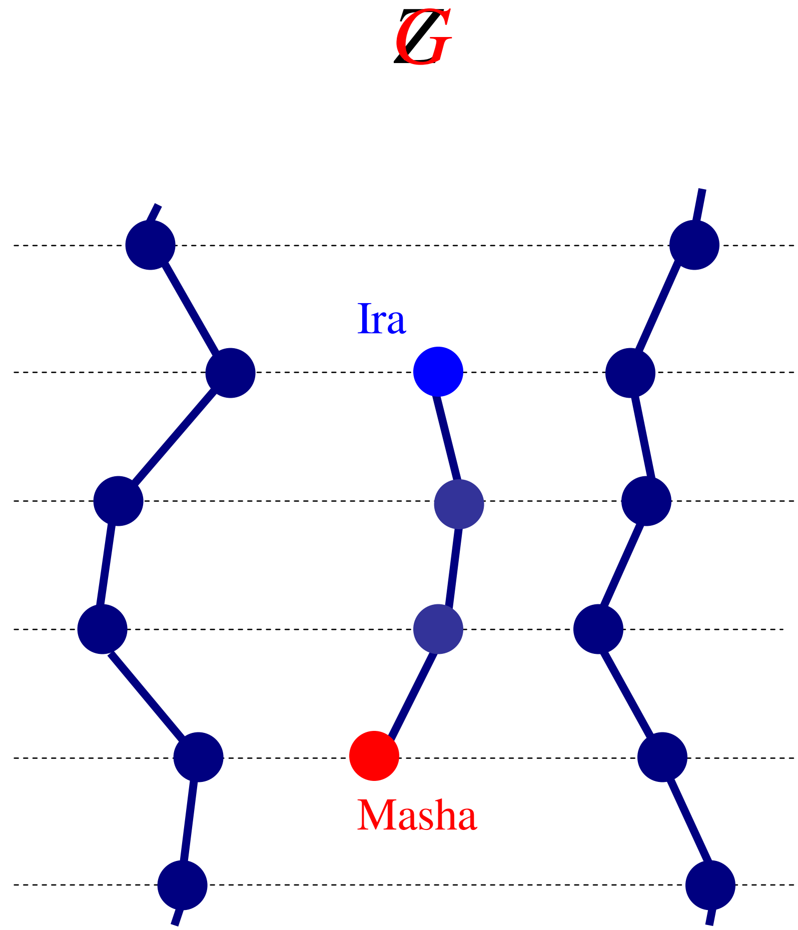
Z G



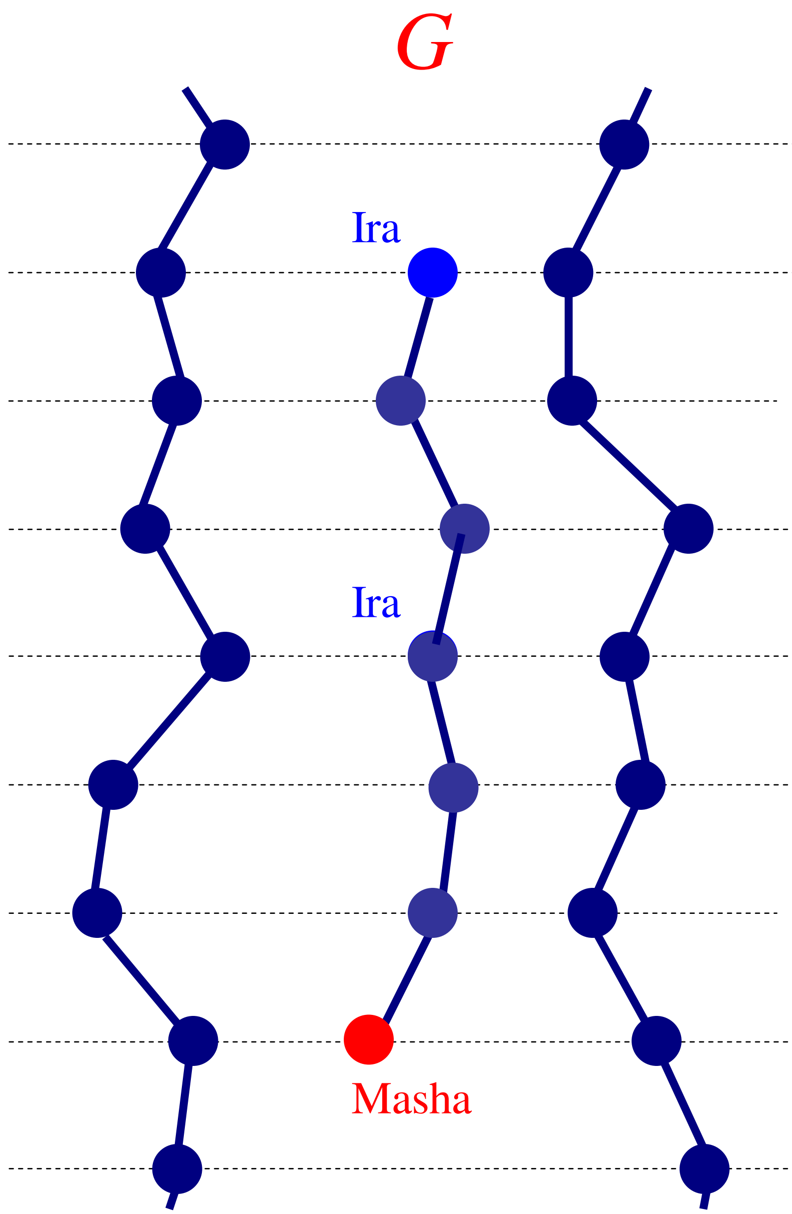
Perform simulations in the extended configuration space $Z \cup G$



(open/close update)

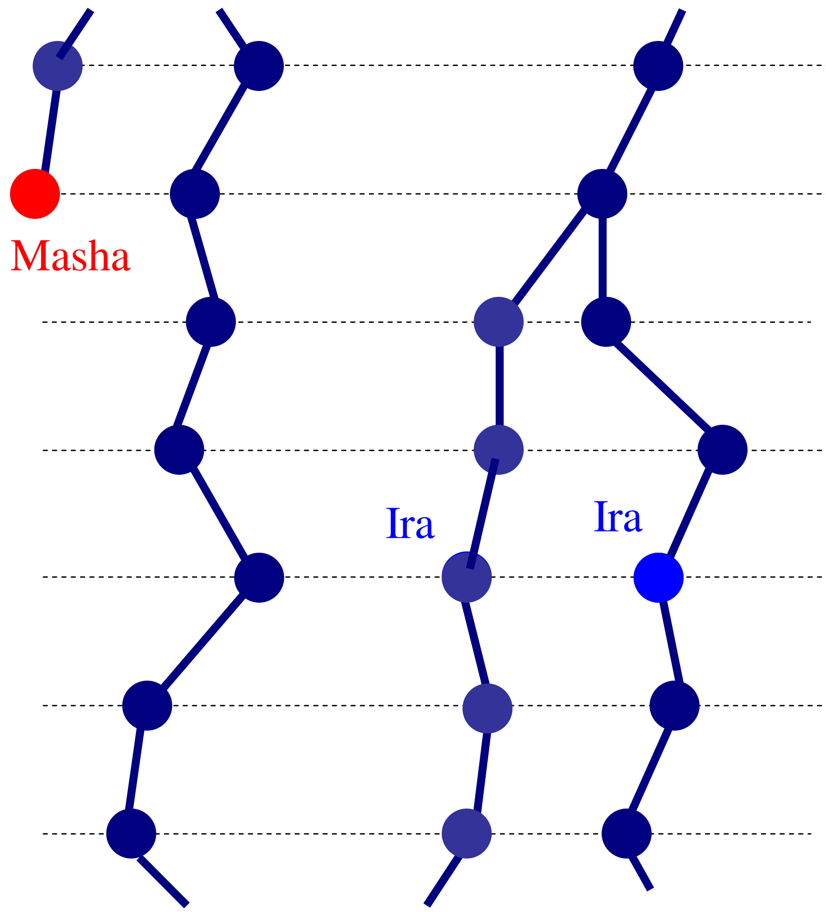


(insert/remove update)



(advance/recede update)

G

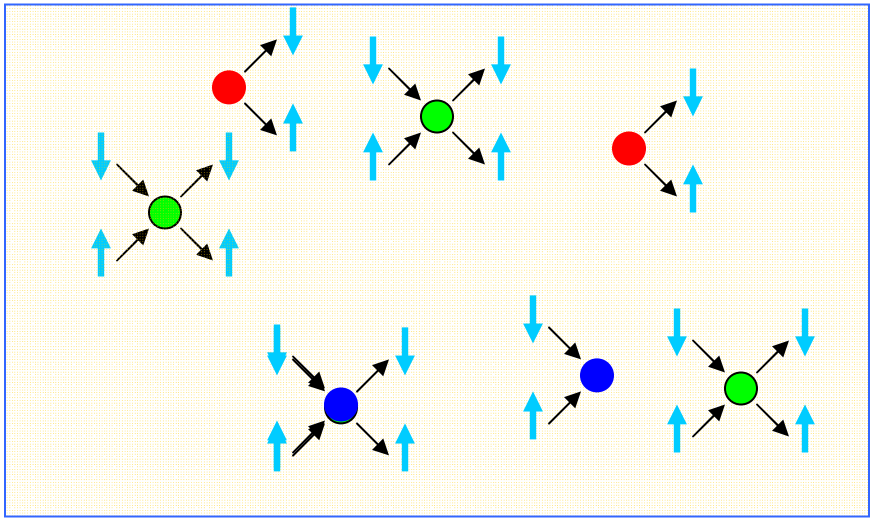


(swap update)

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) ● $= -U$



Pair correlation function

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

General ideas: 1. Enlarge the configuration space

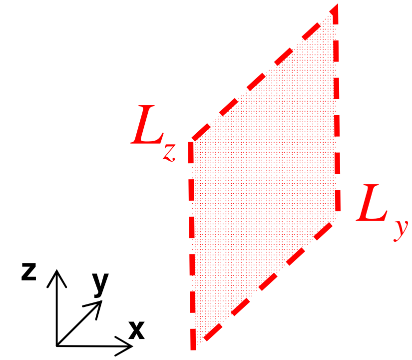
(using correlation functions, source operators, even unphysical structures!)

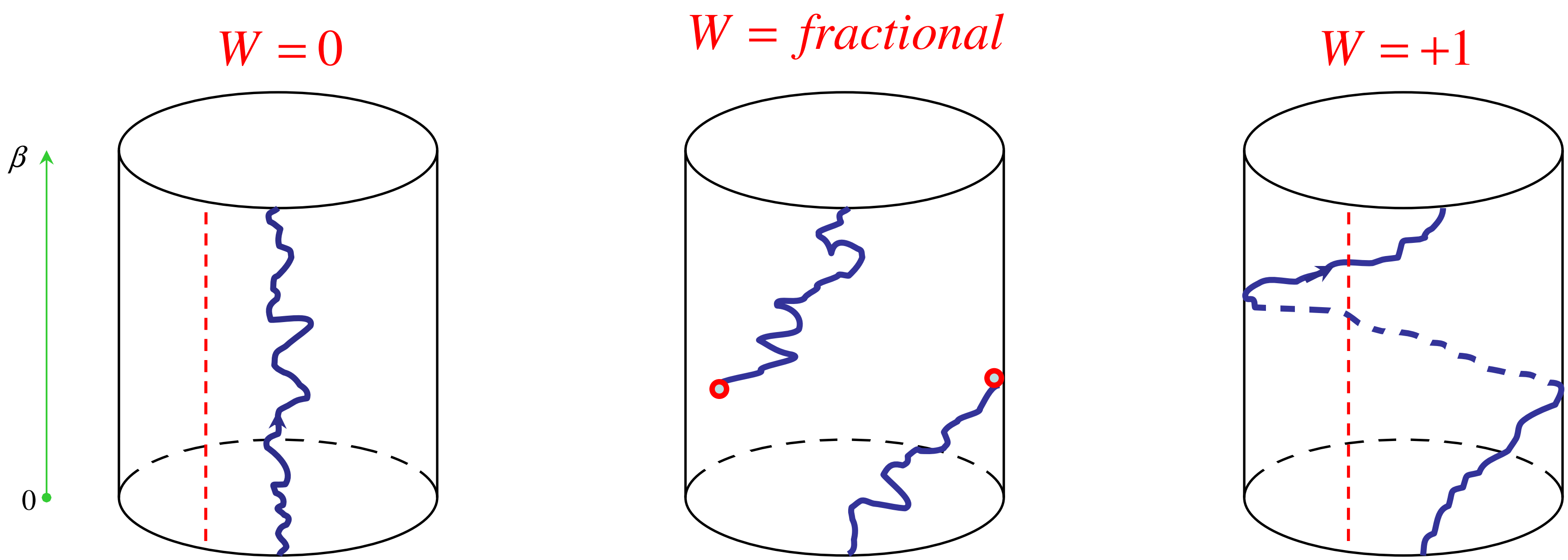
2. Perform local updates through the special points

More: winding numbers and superfluid density

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

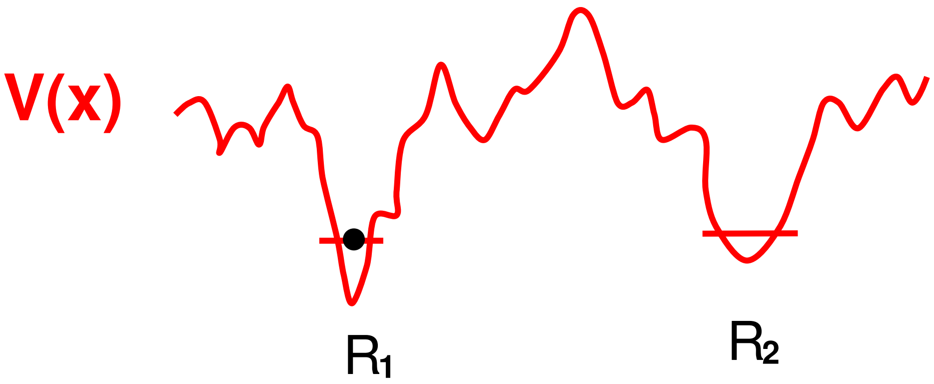
(cross-section independent in Z-sector)

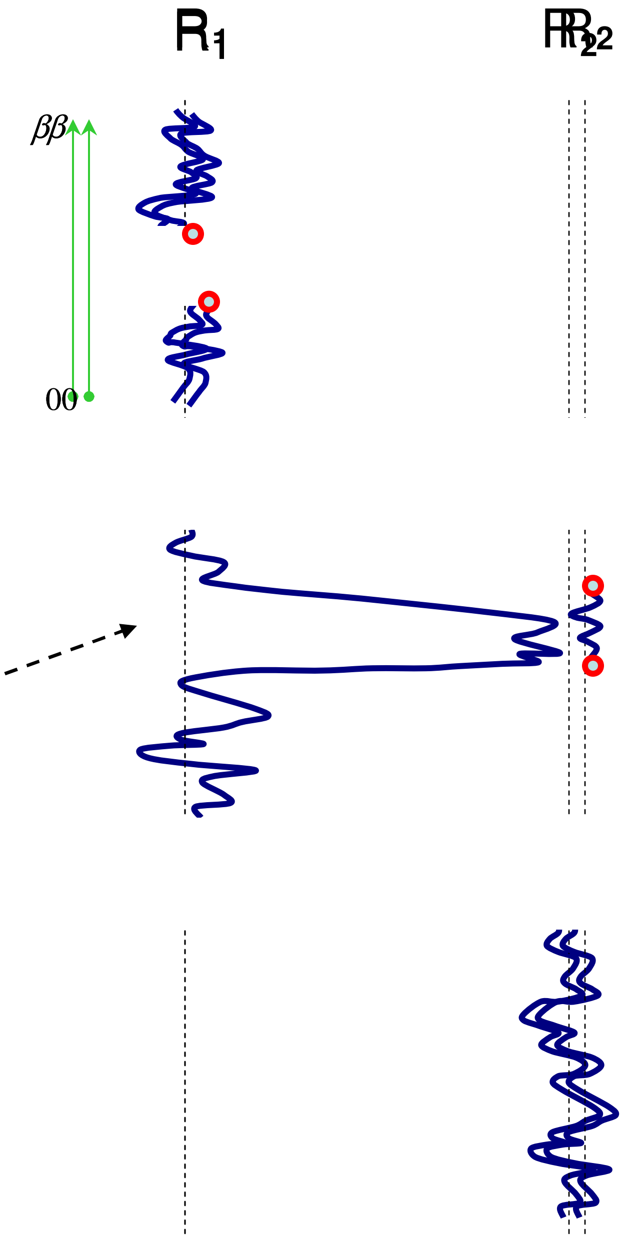




$$\rho_S = (m / \beta d L^{d-2}) \langle W^2 \rangle$$

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

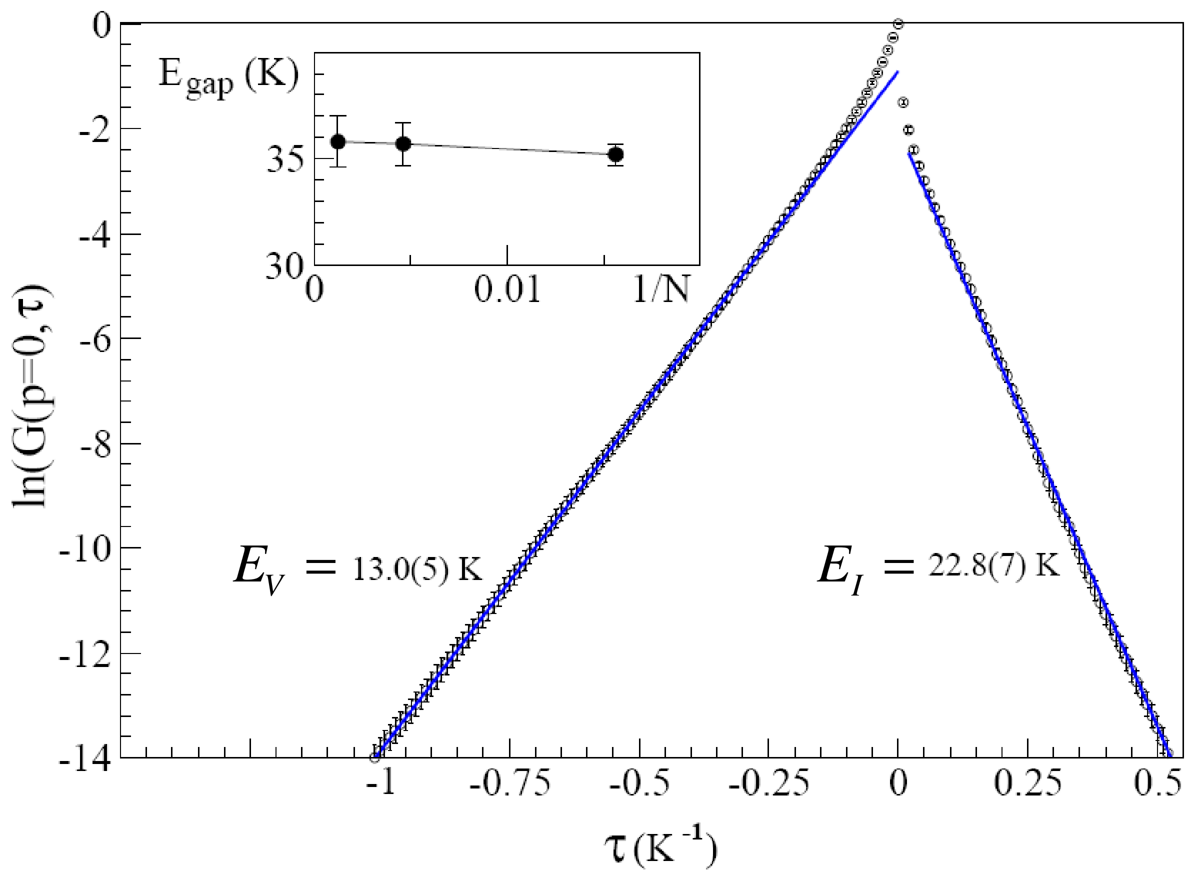




exponentially rare event $e^{-2\int p dx}$

Ideal equilibrium crystals of He-4

Vacancy & interstitial gaps from exponential decay of $G(p,\tau \to \infty) \to Z e^{-E_{i,v}|\tau|}$



$T = 0.25\ K,\ \ n = 0.0287\ A^{-3},\ \ N = 800$ (melting density)

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

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

Continuous variables (any number of them) is not a problem.

Let …

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

Diagram order

Same-order diagrams

Integration variables

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

ENTER

Balance Equation:

If the desired probability density distribution of diagrams in the stochastic sum is P_ν then the MC process of updating diagrams should be stationary with respect to P_ν (equilibrium condition) (in most cases it is the same as the diagram weight D_ν)

$$\underbrace{D_\nu \sum_{updates\ \nu\to\nu'} W_\nu(\nu')\, R_{accept}^{\nu\to\nu'}}_{\text{Flux out of } \nu} = \underbrace{\sum_{updates\ \nu'\to\nu} D_{\nu'}\, W_{\nu'}(\nu)\, R_{accept}^{\nu'\to\nu}}_{\text{Flux to } \nu}$$

Flux out of ν **Flux to ν**

$W_\nu(\nu')$ **Is the probability density of "making" new variables, if any**

Detailed Balance: solve it for each pair of updates separately.

$$D_\nu\, W_\nu(\nu')\, R_{accept}^{\nu\to\nu'} = D_{\nu'}\, W_{\nu'}(\nu)\, R_{accept}^{\nu'\to\nu}$$

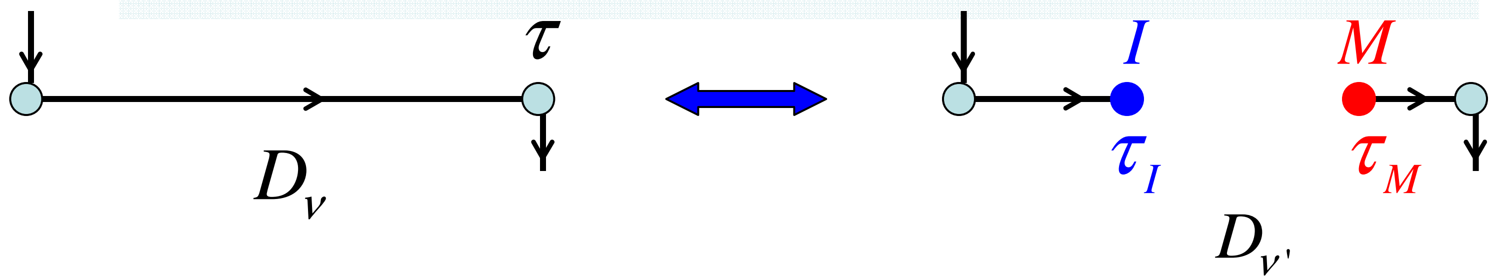
Equation:

$$D_n(\vec{x}_1,\ldots,\vec{x}_n)(d\vec{x})^n \, W(\vec{x}_{n+1},\ldots,\vec{x}_{n+m})(d\vec{x})^m \, p_{\to n+m} \, R_{accept}^{n\to n+m} = D_{n+m}(\vec{x}_1,\ldots,\vec{x}_{n+m})(d\vec{x})^{n+m} \, p_{n\leftarrow} \, R_{accept}^{n+m\to n}$$

Solution:

$$R = \frac{R_{accept}^{n\to n+m}}{R_{accept}^{n+m\to n}} = \frac{D_{n+m}(x_1,\ldots,x_{n+m})}{D_n(x_1,\ldots,x_n)} \frac{1}{W(x_{n+1},\ldots,x_{n+m})} \frac{p_{n\leftarrow}}{p_{\to n+m}}$$

Example: Create/Delete I & M



$$W = \frac{2}{\tau^2} \qquad p_{\to} = 1/K_{\text{intervals}} \qquad p_{\leftarrow} = 1$$ **This is it!**

$$\frac{D_\nu}{D_{\nu'}} = C_{G/Z} \; e^{[-U(n-1)+U(n)-\mu][\tau_I-\tau_M]} \; K_{\text{intervals}}$$