# Monte Carlo integration

**Lode Pollet**

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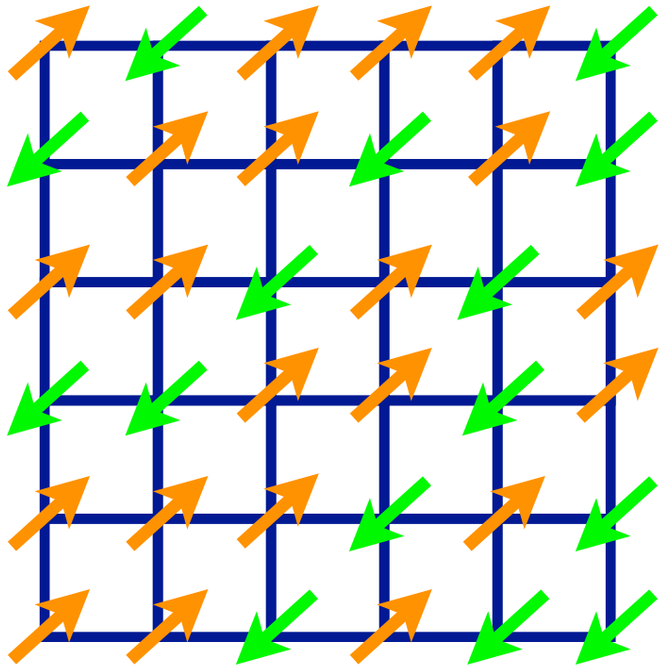
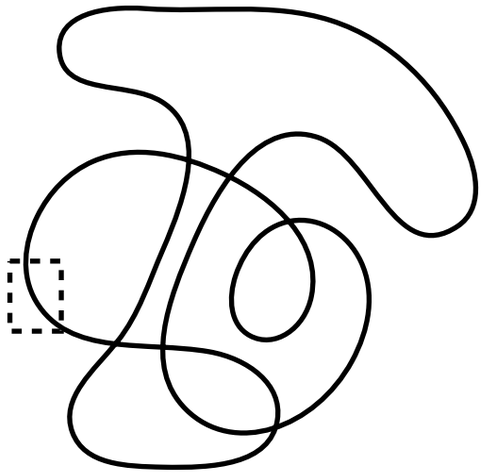
# Loops

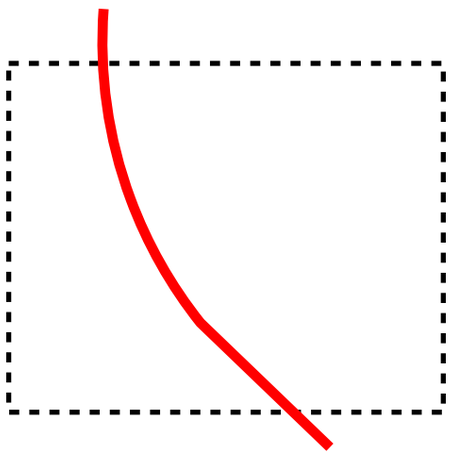
N. V. Prokof'ev

Consider the Ising model

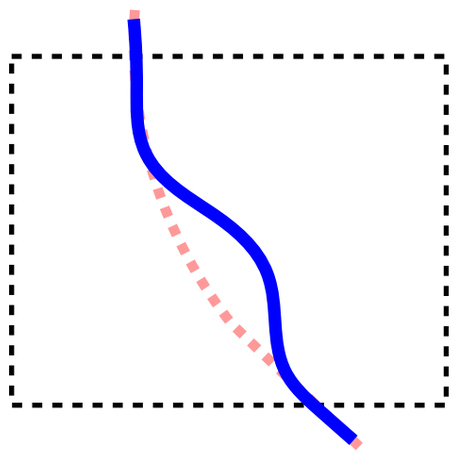




anything you can draw
without loose ends



local shape
change

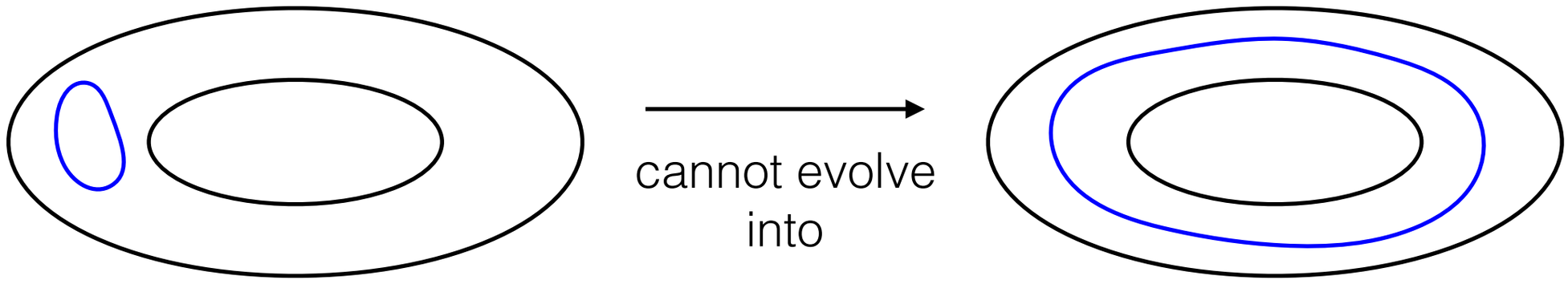


http://mcwa.csi.cuny.edu/umass/izing/Ising_text.pdf

# Loops

N. V. Prokof'ev

this is non-ergodic:




critical slowing down

$$\frac{N_{\mathrm{updates}}}{L^d} \sim L^z$$

z is the dynamical critical exponent
typically, z ~ 2

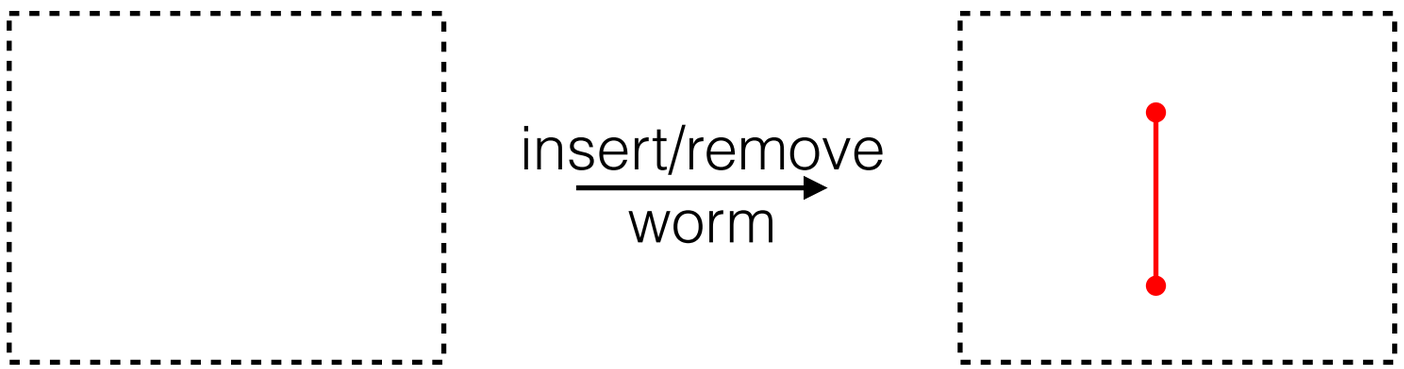
A global update to switch between the two would have exponentially low acceptance factors

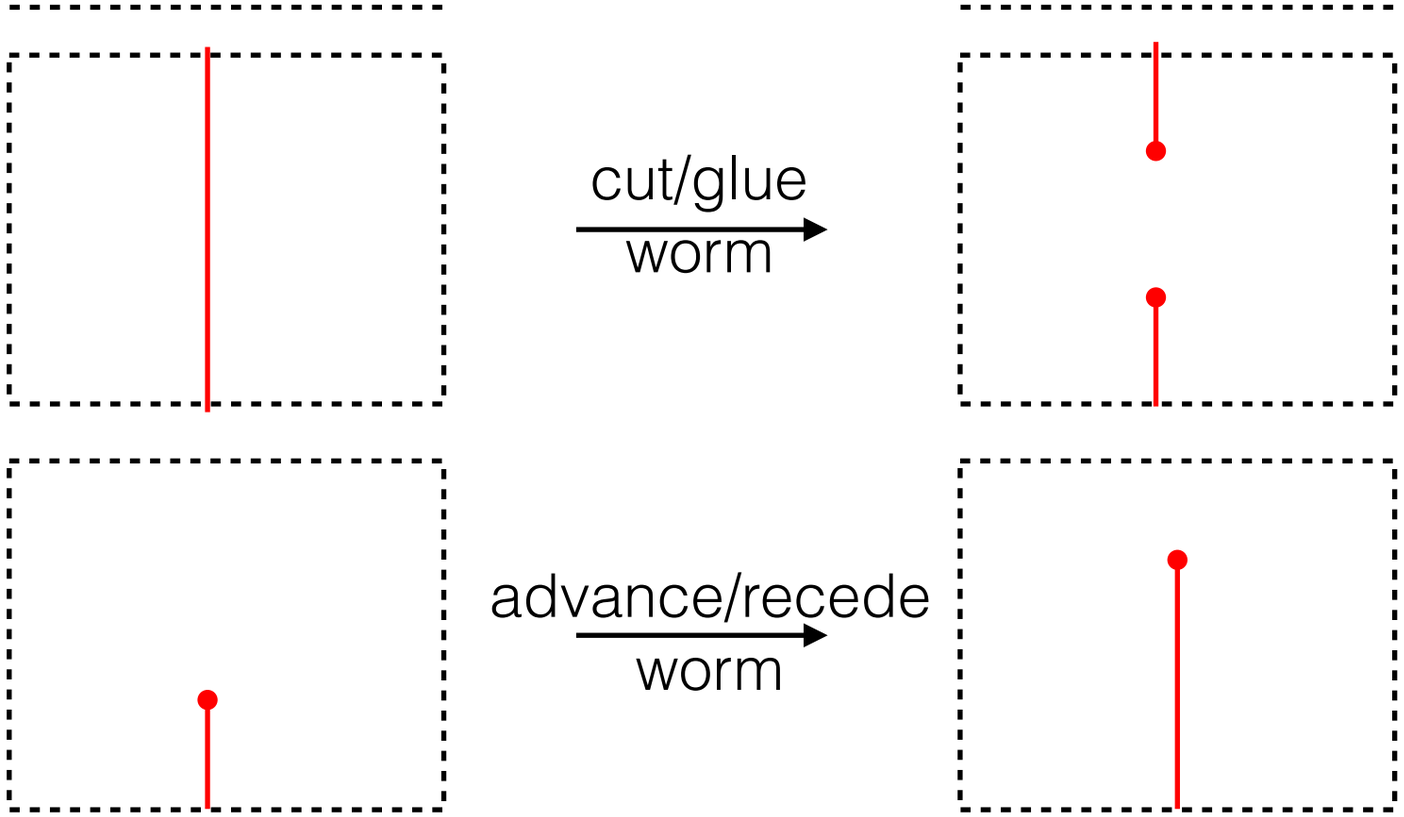
how to solve this problem?

# Worm algorithm

N. V. Prokof'ev

Idea: work in an extended space with open ends:



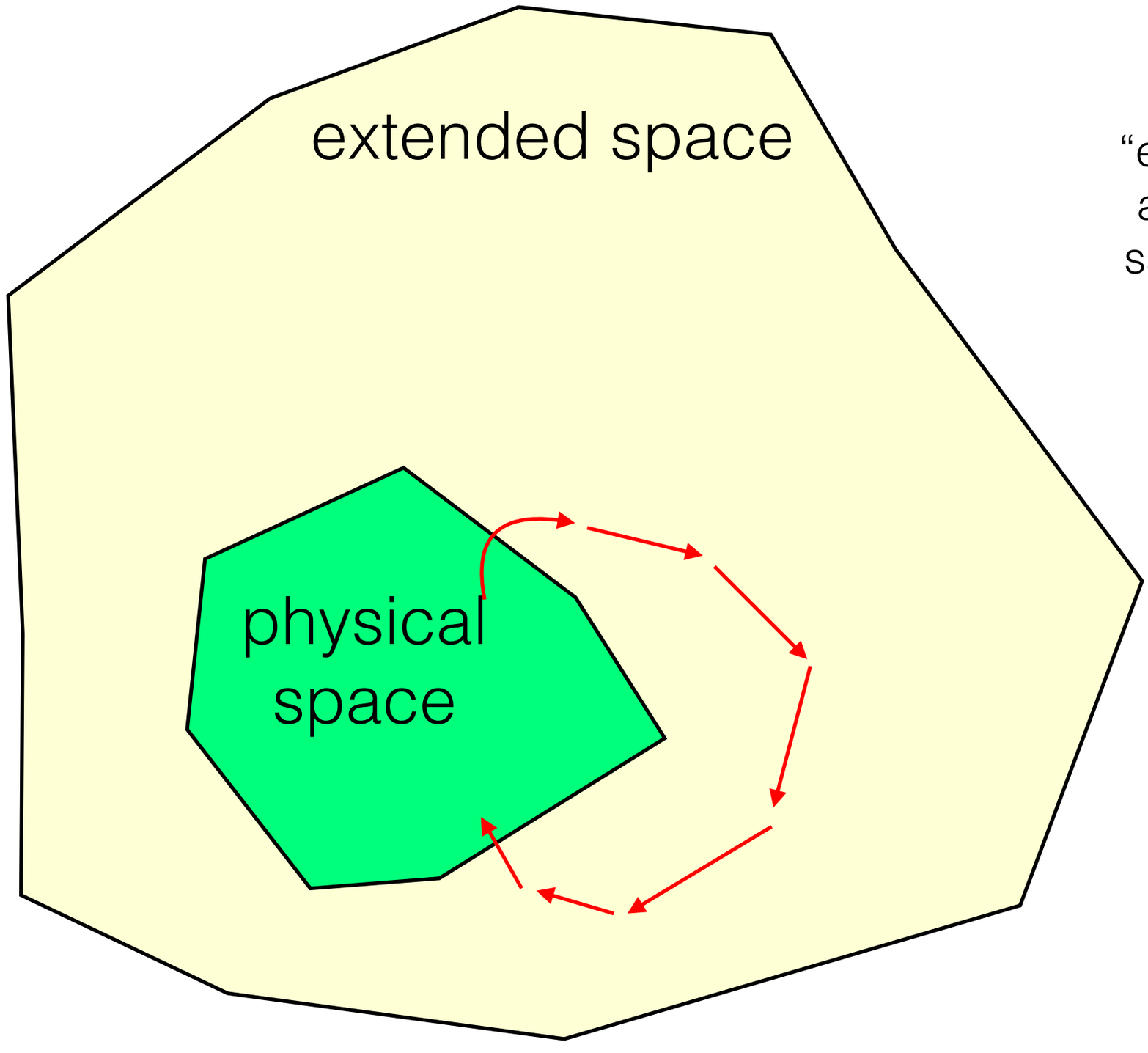




keep at most 1 worm pair
in the configuration

Because of the open ends, it is easy to
sample different topological sectors

# Worm algorithm

N. V. Prokof'ev




we will see that the "extended space" also has a precise meaning (it is a sampling of the correlation function)

# High temperature expansion of the Ising model

N. V. Prokof'ev

partition function:

$$Z = \sum_{\{\sigma_i\}} e^{\sum_{\langle i,j\rangle} K\sigma_i\sigma_j}$$

$$Z = \sum_{\{\sigma_i\}} \left( \prod_{b=\langle i,j\rangle} e^{K\sigma_i\sigma_j} \right)$$

Specific for the Ising model, we have the following trick following trick (instead of the more general Taylor expansion of the exponential):

$$e^{K\sigma_i\sigma_j} = \cosh(K)[1 + \tanh(K)\sigma_i\sigma_j]$$

plug in:

$$Z = 2^N \cosh^{dN}(K) \sum_{\{N_b=0,1\}}^{\text{loops}} \left( \prod_{b=\langle i,j\rangle} \tanh^{N_b}(K) \right)$$

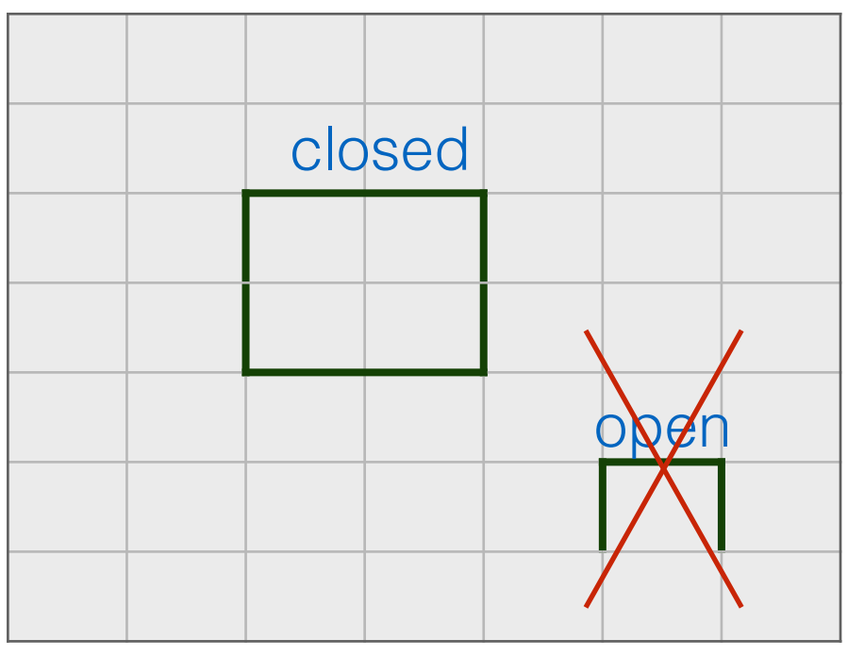
# High temperature expansion of the Ising model

How does the sum over closed loops come about?

consider $1 + \tanh(K)\sigma_i\sigma_j$

if 1 is taken, do nothing

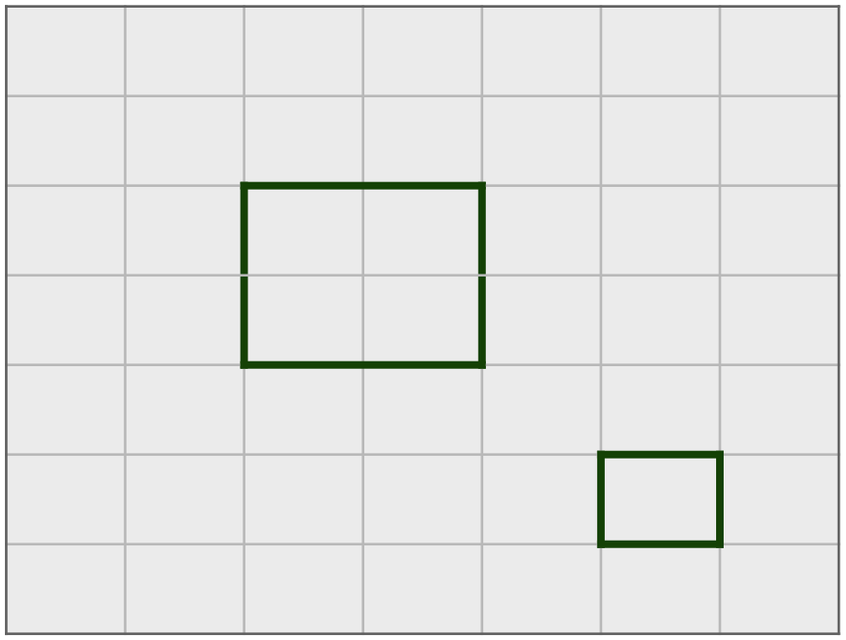
if $\tanh(K)\sigma_i\sigma_j$ is taken, put a bond on the graph (with weight tanh(K))




on site i: $\sum_{\sigma_i=\pm 1} \sigma_i{}^{\#\mathrm{bonds}(i)}$

The number of bonds incident on every site must hence be even

# partition function sector



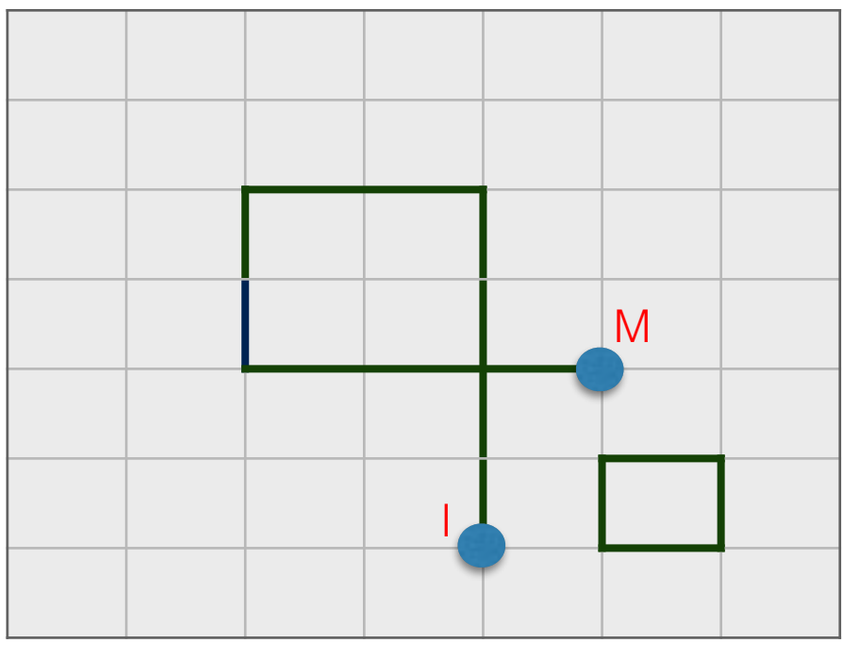
No overlaps!

# Spin correlation function

consider the correlation function

$$g_{IM} = \frac{G_{IM}}{Z} = \sum_{\{\sigma_i\}} e^{KH} \sigma_I \sigma_M$$

$$\equiv 2^N (\cosh K)^{dN} \sum_{\{N_b\}=0,1}^{\text{loops+IM-worm}} \left( \prod_b (\tanh K)^{N_b} \right)$$




the space for the worm algorithm is Z U G, the same as for the generalized partition function

$$Z_W = Z + \lambda G$$

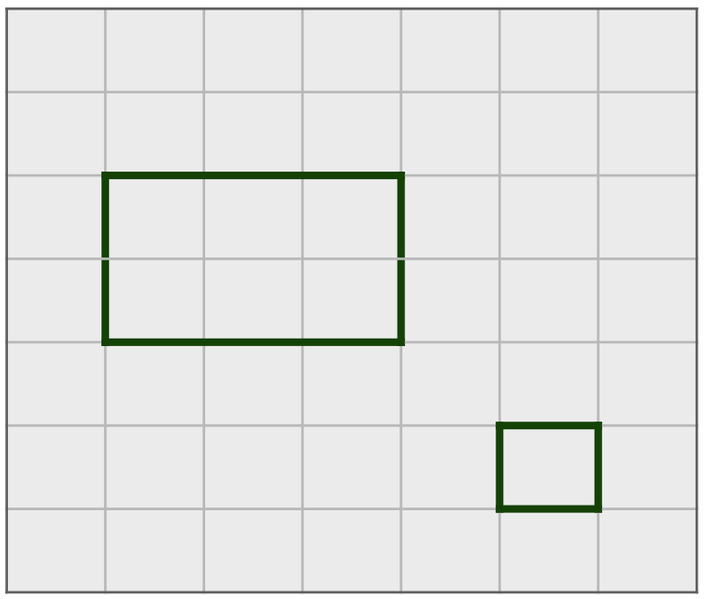
the constant λ can be seen as an optimization constant governing the relative frequency one is in the Z or G space

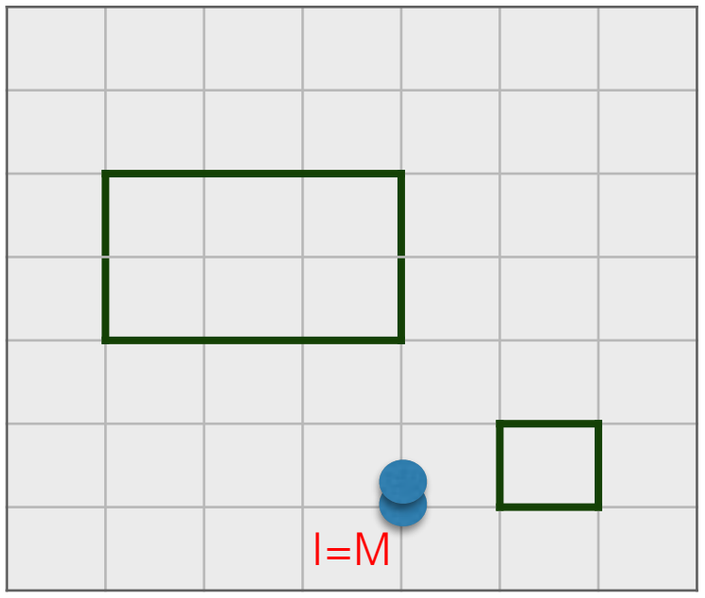
question: how would you incorporate a magnetic field in this loop representation?

# Algorithm

1. if I == M choose a new site at random and go to step 2
2. move M around until M reaches I again as follows:

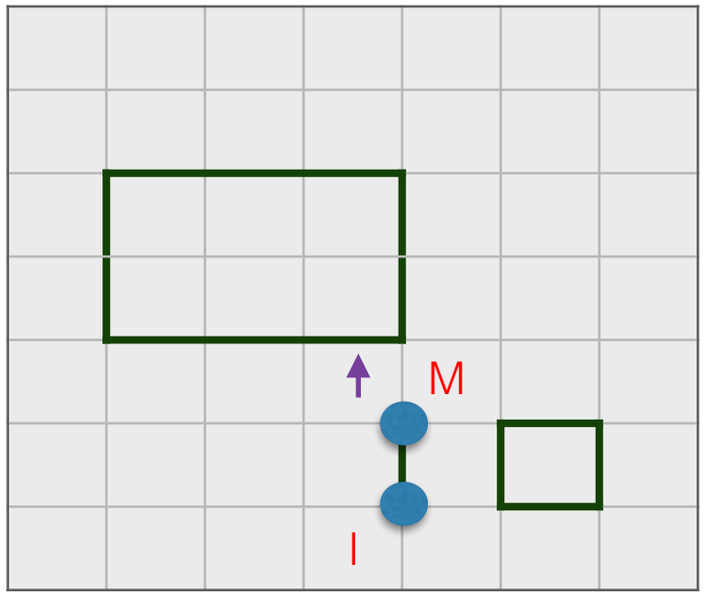
    1. choose direction, let it be bond b
    2. if Nb == 0 then change Nb to Nb =1 with probability R = tanh(K); if Nb == 1 then change Nb to Nb=0 with probability 1

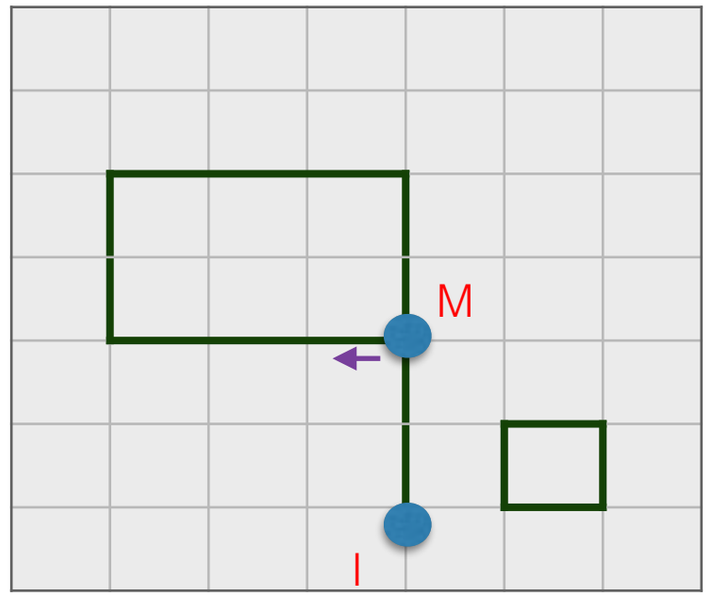


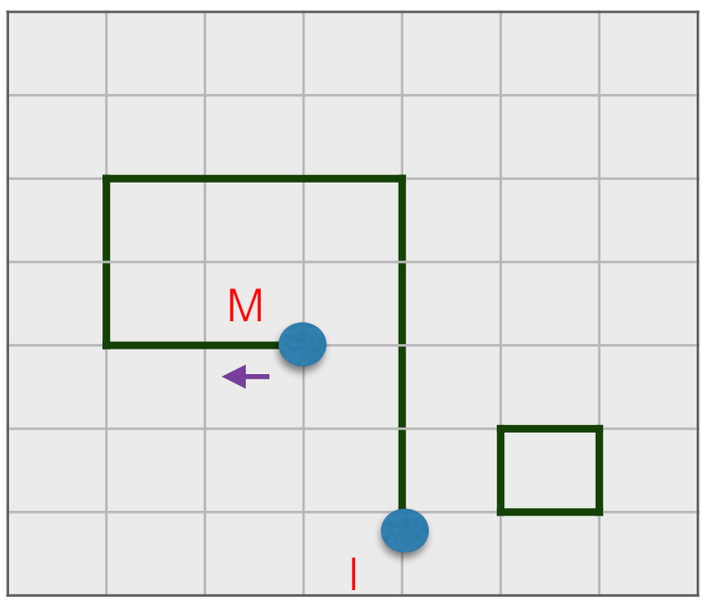


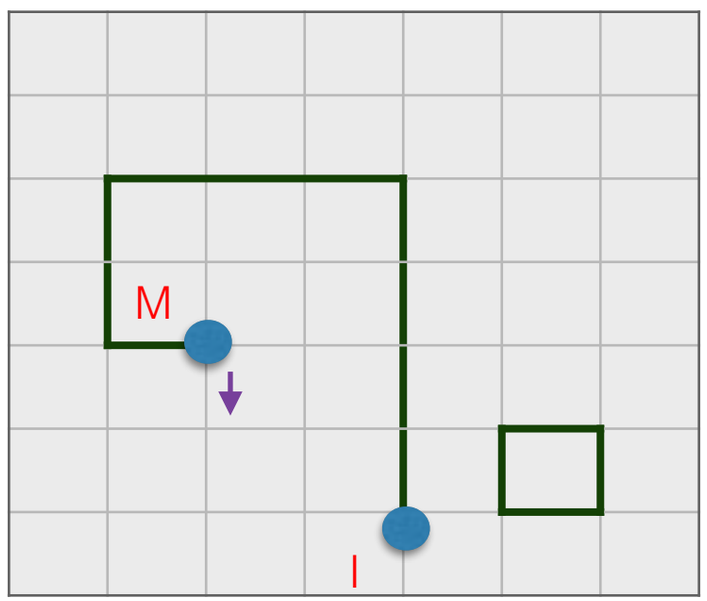
# Algorithm

N. V. Prokof'ev



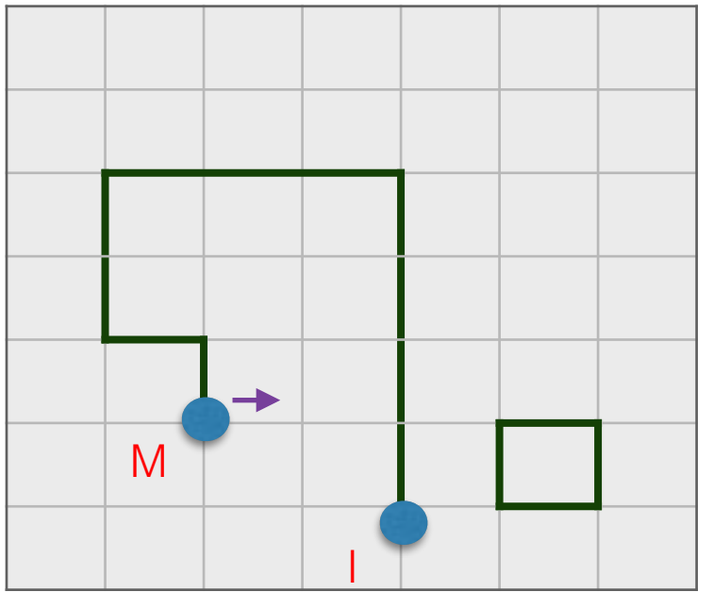



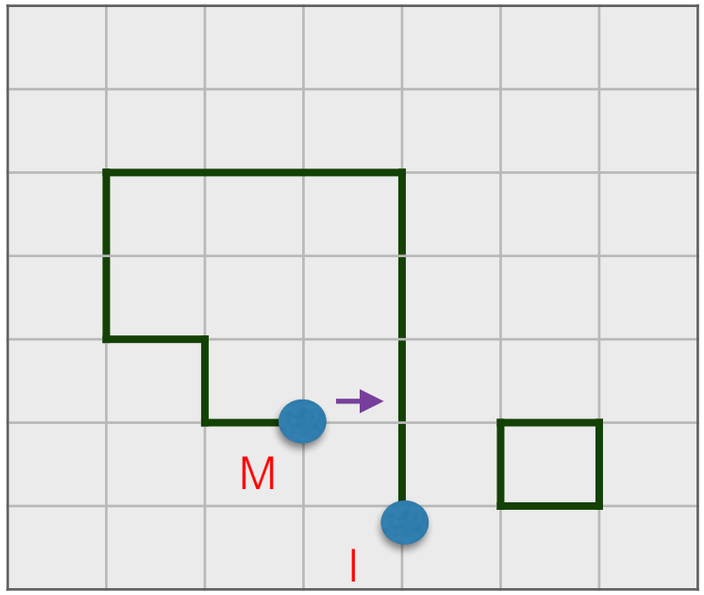



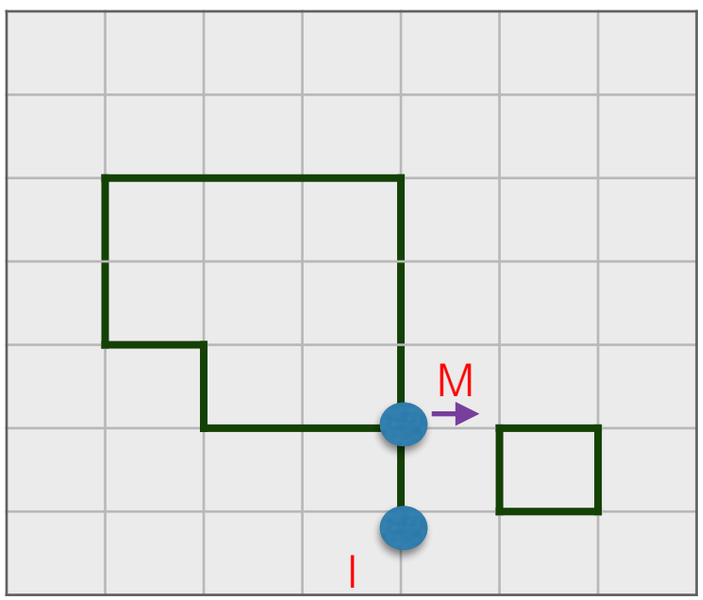



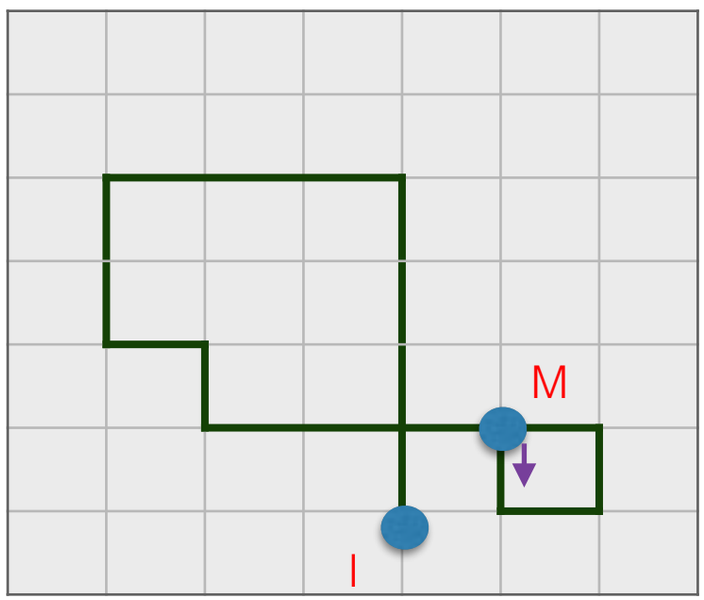
# Algorithm

N. V. Prokof'ev



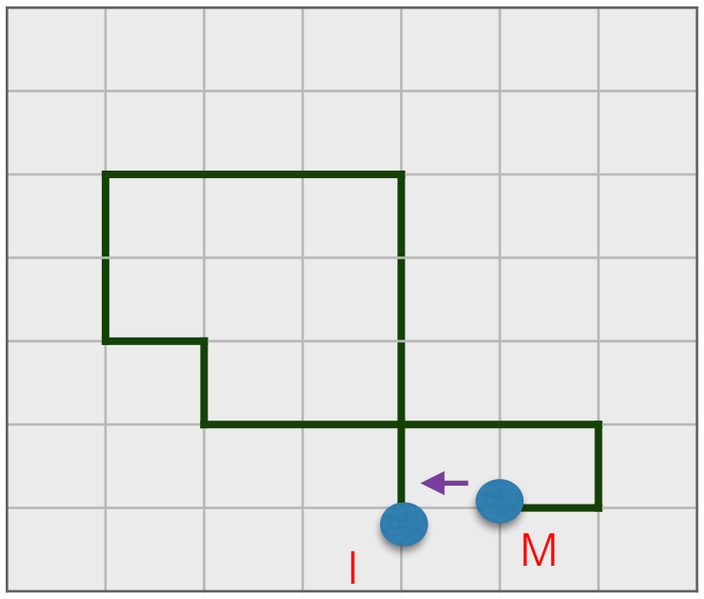



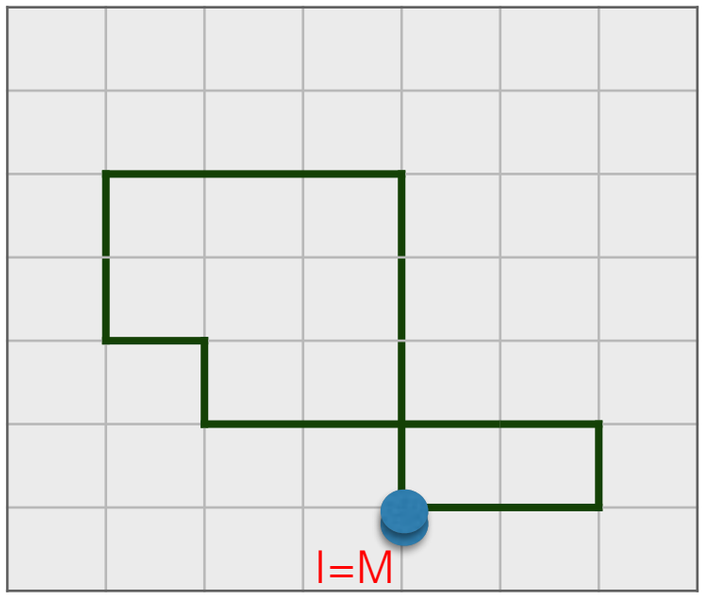



# Algorithm

N. V. Prokof'ev




Estimators:

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

$$Z = Z + \delta_{IM}$$

$$N_{\text{links}} = N_{\text{links}} \pm 1$$

$$M2 = M2 + 1$$

$$g(i-j) = \langle \sigma_i \sigma_j \rangle = G(i-j)/Z$$

$$\langle M^2 \rangle = \left\langle \left( \sum_i \sigma_i \right)^2 \right\rangle = \sum_{ij} \langle \sigma_i \sigma_j \rangle = N \times M2/Z$$

$$E = -JNd \langle \sigma_1 \sigma_2 \rangle = -Jndg(1)$$

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

# Scope and extensions

- Phase transitions (second order)
- finite size scaling
- Potts model, higher dimensions, XY model, …
- superfluidity and winding number

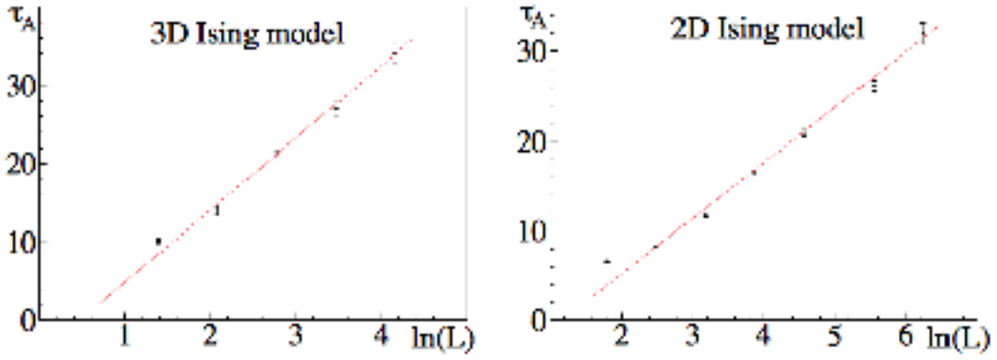



FIG. 2. Autocorrelation times for various universality classes. The 3D Ising model is fitted to $\tau = -4.3 + 9.2\ln(L)$, and $z(L = 64) = 0.18$ (see text). The 2D Ising model is fitted to $\tau = -7.2 + 6.2\ln(L)$, and $z(L = 512) = 0.25$. The 3D $XY$-model is fitted to $\tau = 1.7 + 3.85\ln(L)$, and $z(L = 128) = 0.2$. The 2D $XY$-model is fitted to $\tau = 1.85 + 2.05\ln(L)$, and $z(L = 640) = 0.16$. The 3D Gaussian model is fitted to $\tau = 18.9 + 5.8\ln(L)$, and $z(L = 64) = 0.17$. The $q = 3$ Potts model in 2D is fitted to the power law $\tau = 4.3L^{0.55}$.

http://arxiv.org/pdf/cond-mat/0103146.pdf

## continuous-time expansion (strong coupling)

basis = Fock states, $H_1$ = kinetic term

$$Z = \sum_{\{n_i\}} \langle n_i | e^{-\beta H_0} \mathcal{T} e^{-\int_0^\beta H_1(\tau) d\tau} | n_i \rangle$$

$$Z = \sum_{\{n_i\}} \langle n_i | e^{-\beta H_0} \left( 1 - \int_0^\beta H_1(\tau) d\tau + \int_0^\beta d\tau \int_0^\tau d\tau' H_1(\tau) H_1(\tau') + \dots \right) | n_i \rangle$$


by virtue of the time-ordered product and the Heisenberg operators

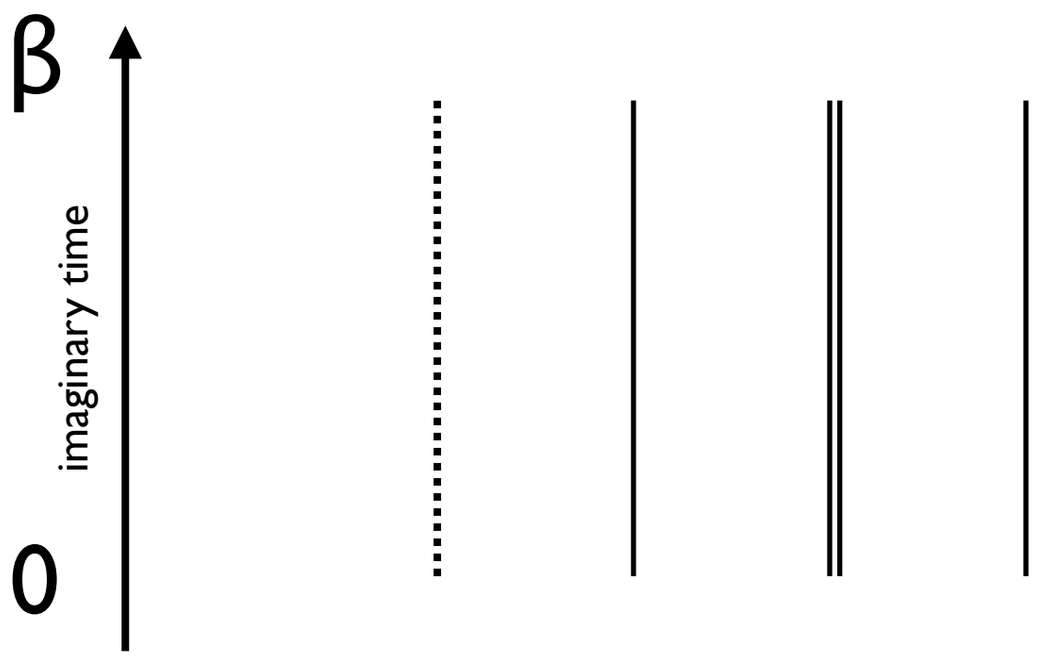
$$H_1(\tau) = e^{\tau H_0} H_1 e^{-\tau H_0}$$

each term describes the evolution of the occupation numbers (insert complete set of states before and after $H_I$)

zeroth order:

$$Z = \sum_{\{n_i\}} \langle n_i | e^{-\beta H_0} | n_i \rangle = \sum_{\{n_i\}} e^{-\beta H_0(n_i)}$$

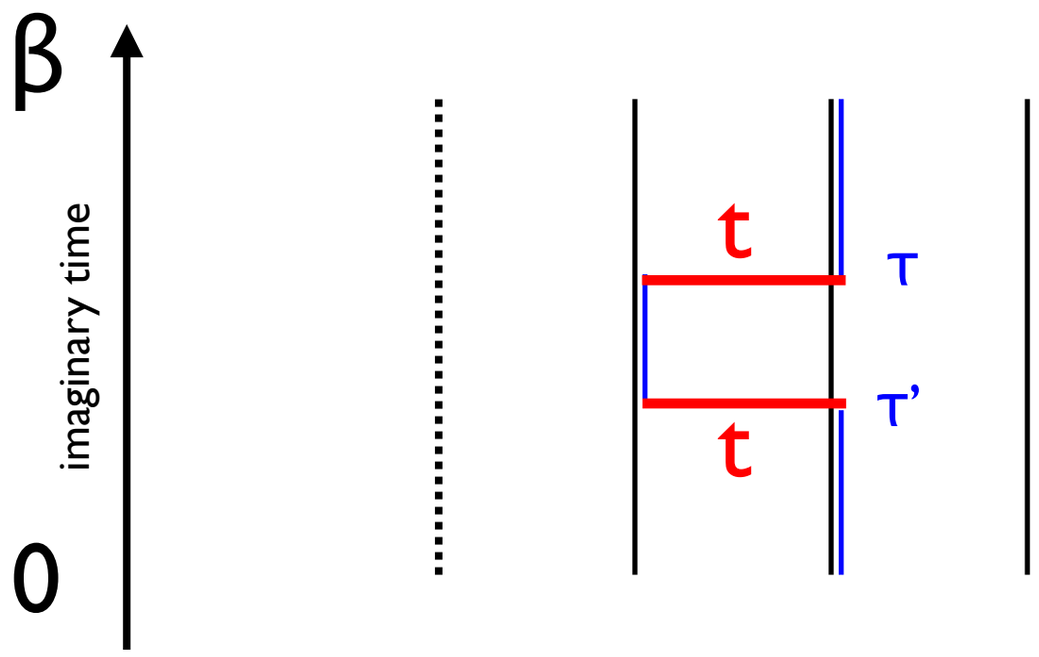
This is the atomic limit. Graphical representation:




4-site problem;
occupation numbers
are 0-1-2-1

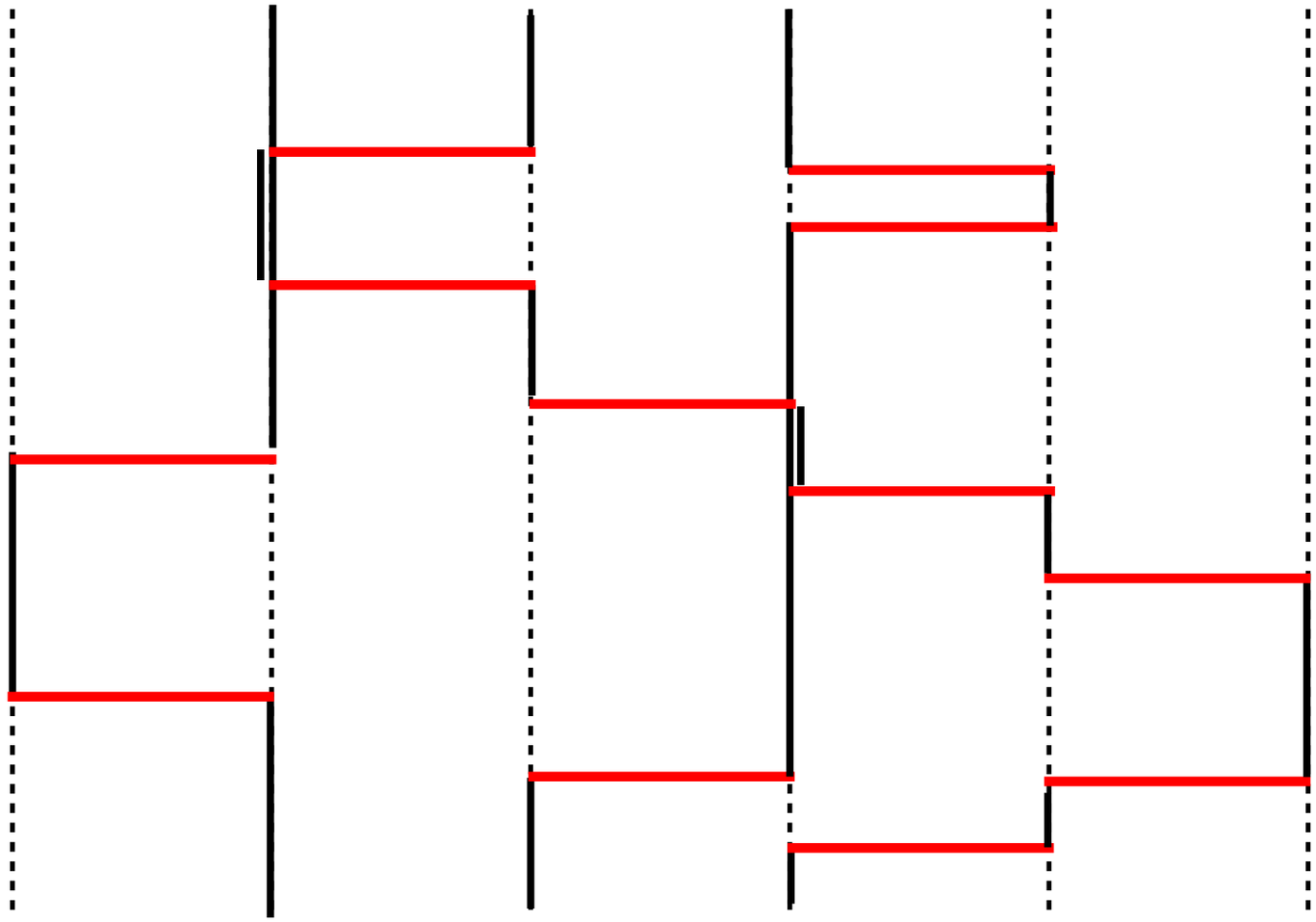
## second order

$$\sum_{\{n_1\},\{n_2\}} \int_0^\beta d\tau \int_0^\tau d\tau' (-1)^2 e^{-(\beta-\tau)H_0(n_1)} \langle n_1|H_1|n_2\rangle e^{-(\tau-\tau')H_0(n_2)} \langle n_2|H_1|n_1\rangle e^{-\tau' H_0(n_1)}$$




brute force evaluation of this expansion : high temperature series expansion (also done for log Z) — see the book by Oitmaa and coworkers. Stochastic evaluation —> PIMC

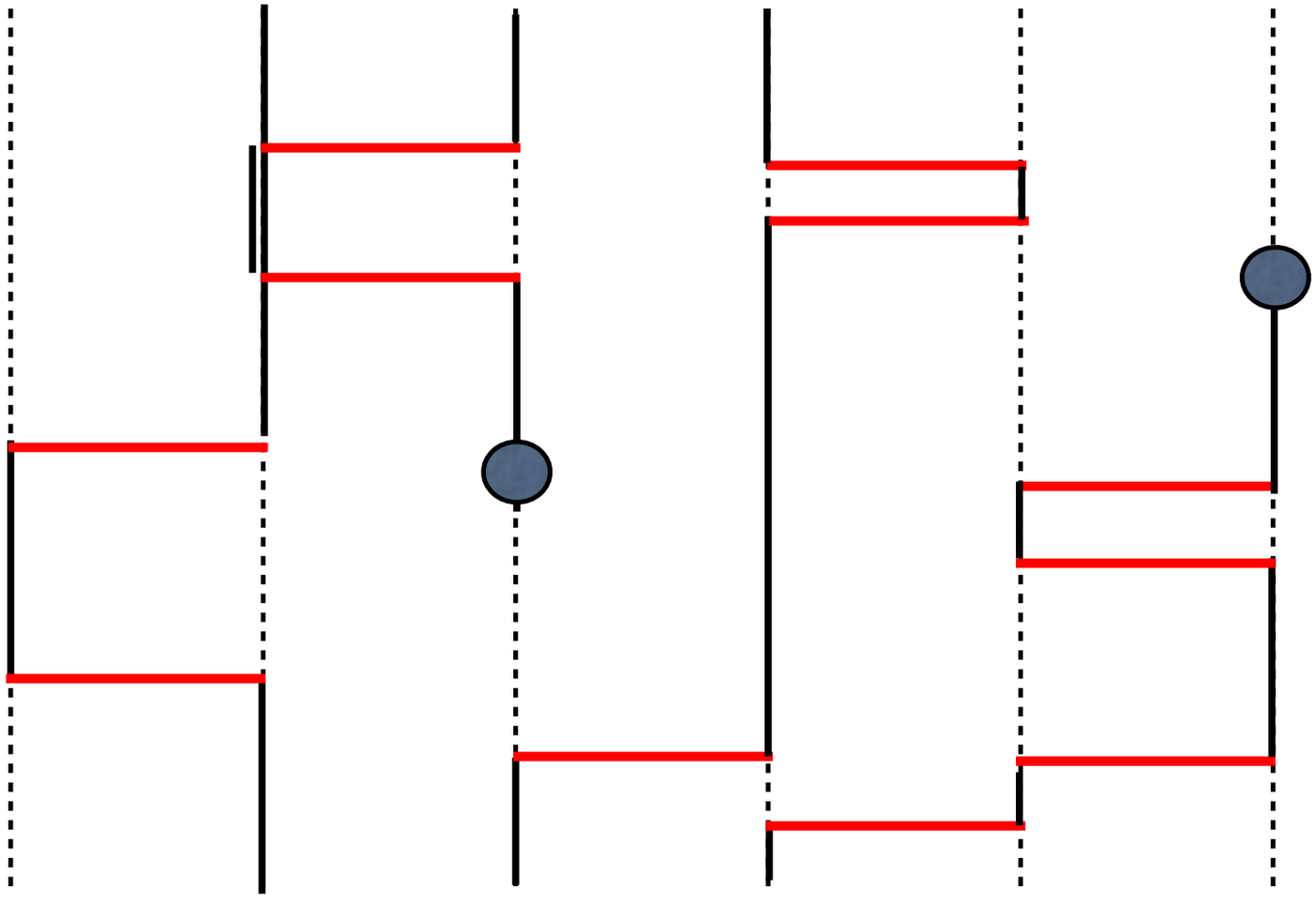
higher order graphical representation:



# PIMC

Green function:

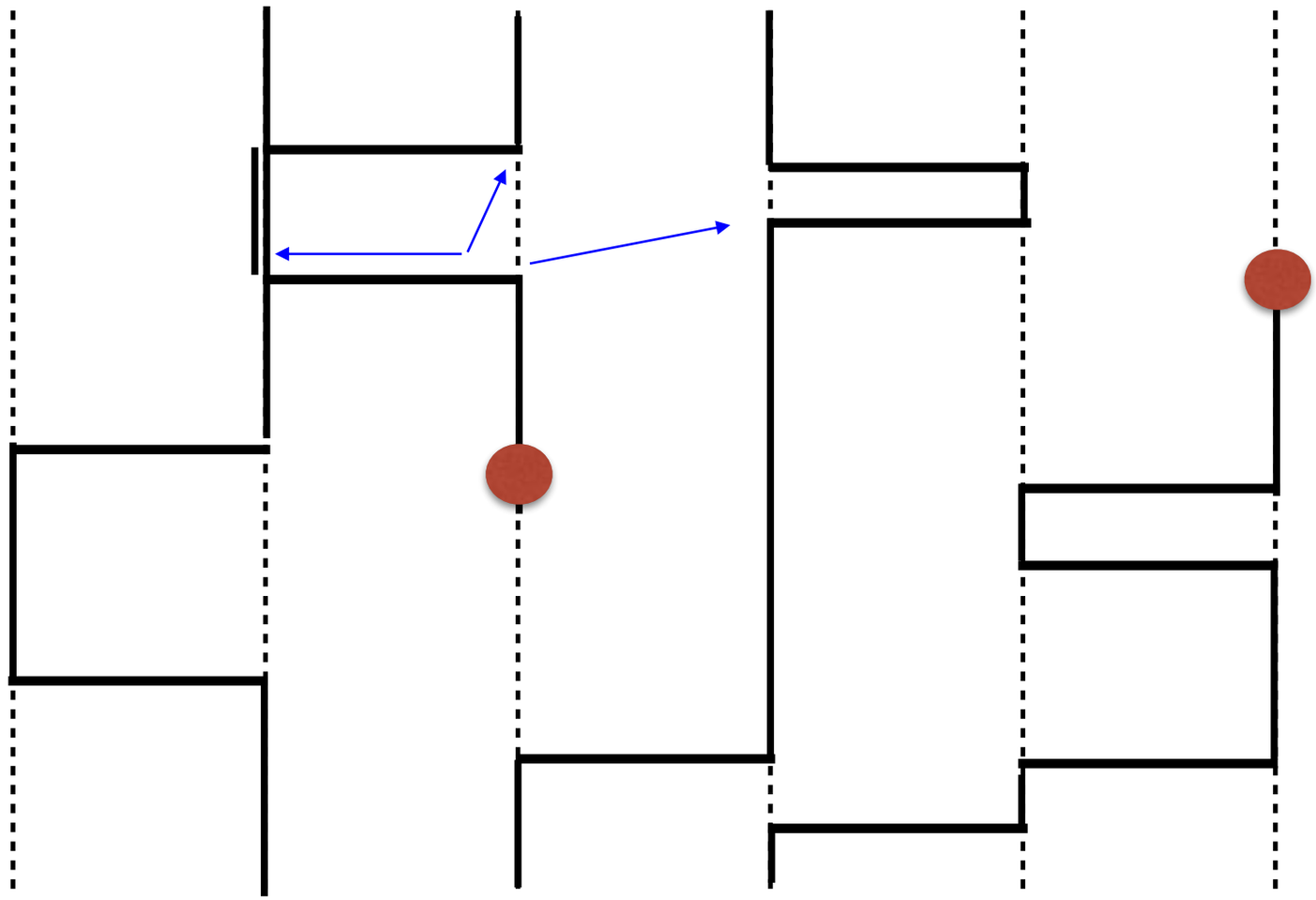
$$G(i-j,\tau_i-\tau_j)=\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta H}\mathcal{T}b(i,\tau_i)b^{\dagger}(j,\tau_j)\right]$$



so there is a similar expansion but with two additional „end“ points

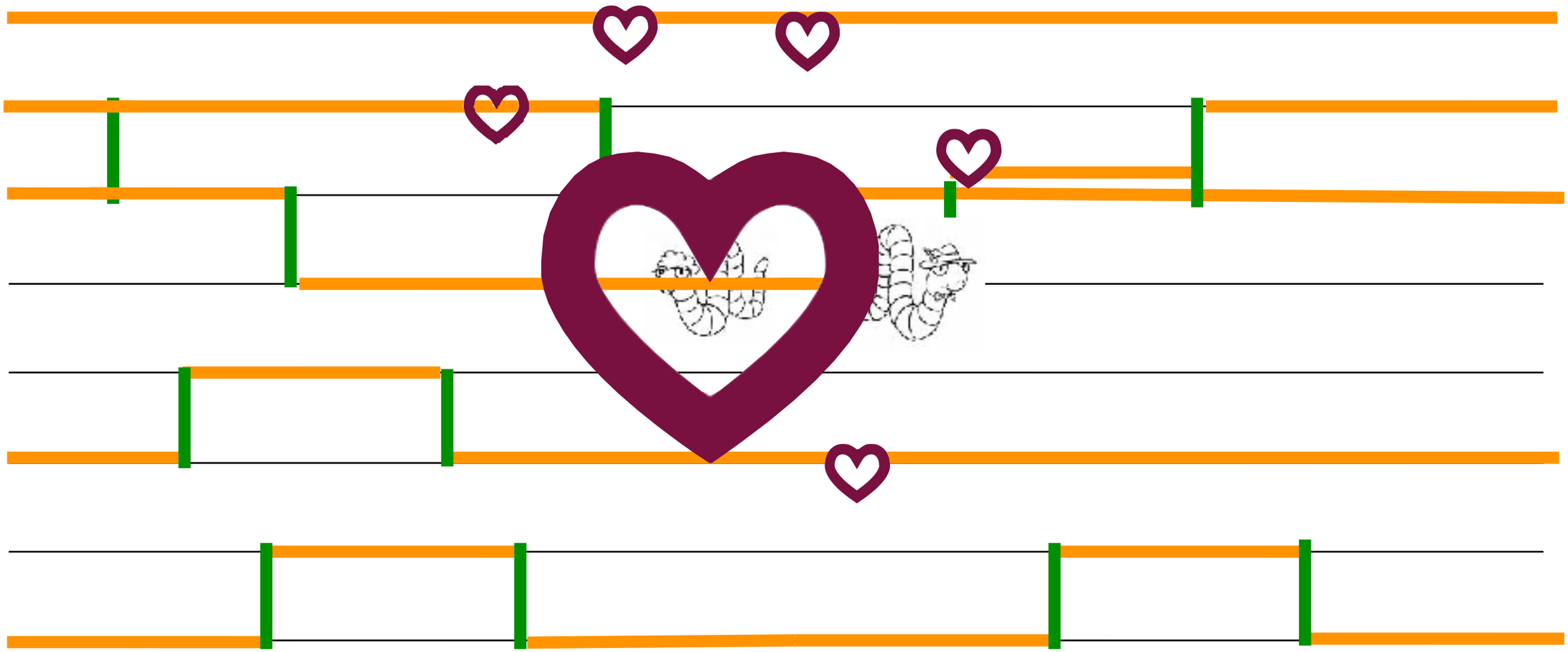
# PIMC

Data structure: get to know your neighbors.
My implementation: list of „kinks“ (alternatively, work with intervals)



(most tricky point of the code)

# Worm updates



grand-canonical

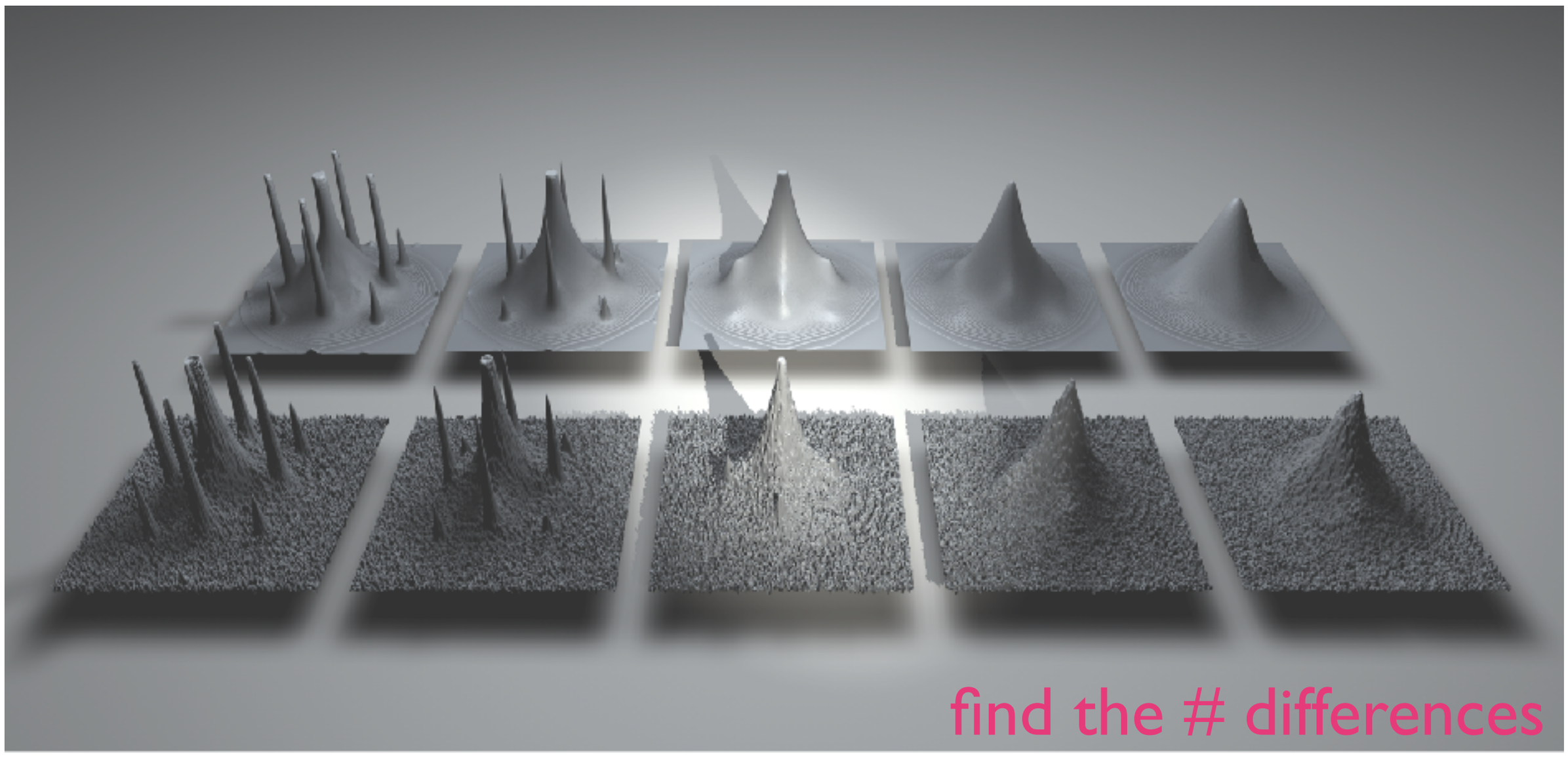
bosonic exchange

N.V. Prokof'ev, B.V. Svistunov and I. Tupitsyn, Sov. Phys. JETP **87**, 310 (1998).

# Ultracold atom quantum simulators pass first key test

\+ : control, clean, tunable

\- : temperature, detection, light-matter effects



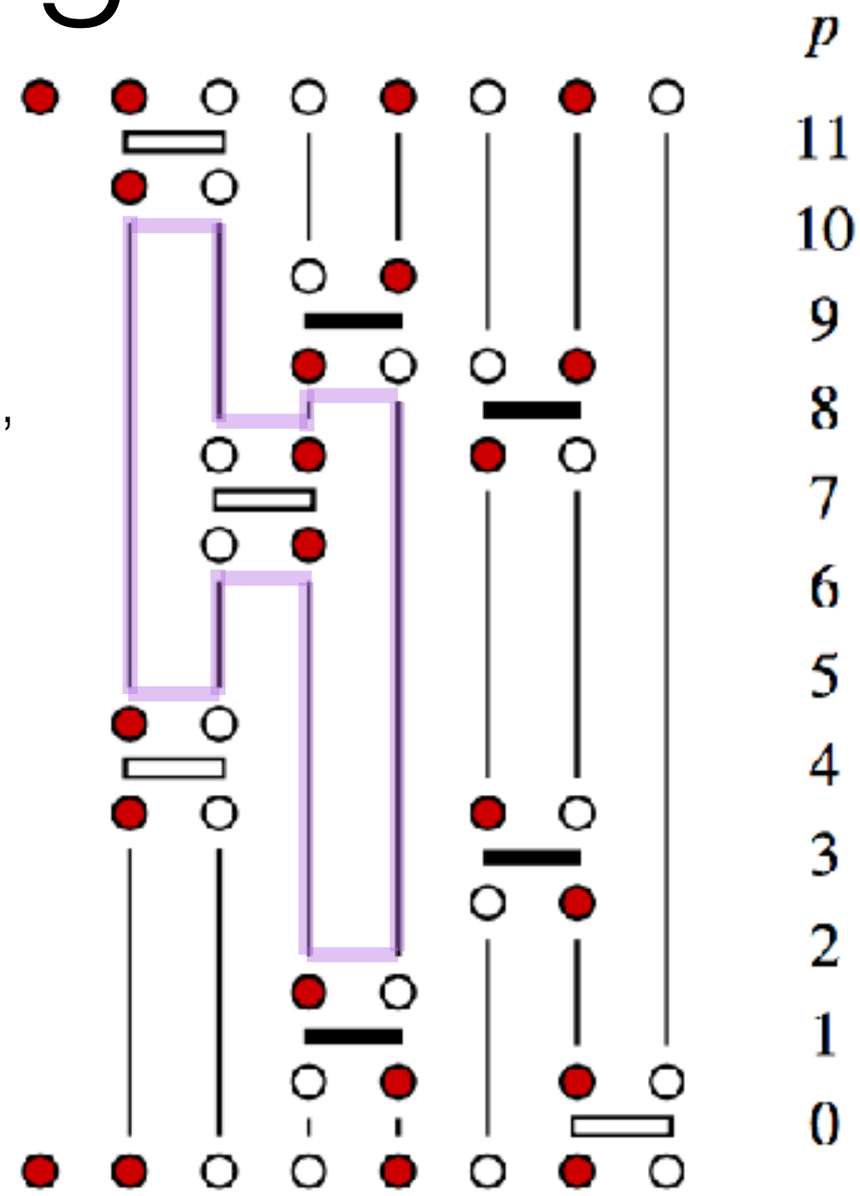
# The SSE representation of the Heisenberg model

very naturally leads to a loop algorithm!

the inverse temperature leads to another ‘classical’ dimension

$$W(\beta, n) = \left(\frac{\beta J}{2}\right)^n \frac{1}{n!}$$

(all configurational bond weights are 1/2 for this particular case; an energy shift has been applied)




see: A. Sandvik, Computational Studies of Quantum Spin systems, AIP Conf.Proc. 1297:135,2010, arXiv:1101.3281

$$W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

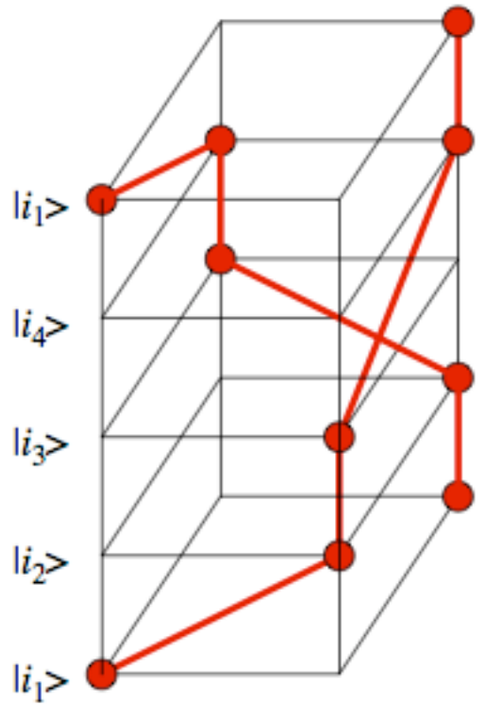
# fermions and sign problem

In mapping the quantum to the classical system

$$Z = \mathrm{Tr}\exp^{-\beta H} = \sum_i p_i$$

some of the $p_i$ may $p_i < 0$

e.g. 2 electrons might exchange places




Troyer and Wiese have shown that the sign problem is NP-hard

http://arxiv.org/abs/cond-mat/0408370; Phys.Rev.Lett. 94 (2005) 170201

consequence : exponential scaling

# Implications

(M.Troyer)

evaluation in case of negative weights:

$$\begin{aligned}\langle A\rangle &= \frac{\sum_c A(c)p(c)}{\sum_c p(c)} \\ &= \frac{\sum_c A(c)s(c)|p(c)|\,/\sum_c |p(c)|}{\sum_c s(c)|p(c)|\,/\sum_c |p(c)|} \equiv \frac{\langle As\rangle'}{\langle s\rangle'}.\end{aligned}$$

with $\langle s\rangle = Z/Z'$ the average sign given by

$Z = \sum_i p_i$ 'fermionic' system

$Z' = \sum_i |p_i|$ 'bosonic' system

$$Z/Z' = \exp(-\beta N \Delta f)$$

The variance can become exponentially large :

$$\frac{\Delta s}{\langle s\rangle} = \frac{\sqrt{\left(\langle s^2\rangle - \langle s\rangle^2\right)/M}}{\langle s\rangle} = \frac{\sqrt{1-\langle s\rangle^2}}{\sqrt{M}\langle s\rangle} \sim \frac{e^{\beta N \Delta f}}{\sqrt{M}}.$$

The sign problem is basis dependent : e.g., if we know the full spectrum, all weights are positive
However, still no solution
The situation is reminiscent of NP hard problems (no proof of exponential scaling, but no solution that scales polynomially is known)
A solution to the sign-problem is a solution that does not scale exponentially (stronger than positive weights) when the bosonic problem is easy (polynomial)

# Eulerian Circuit Problem

(M.Troyer)

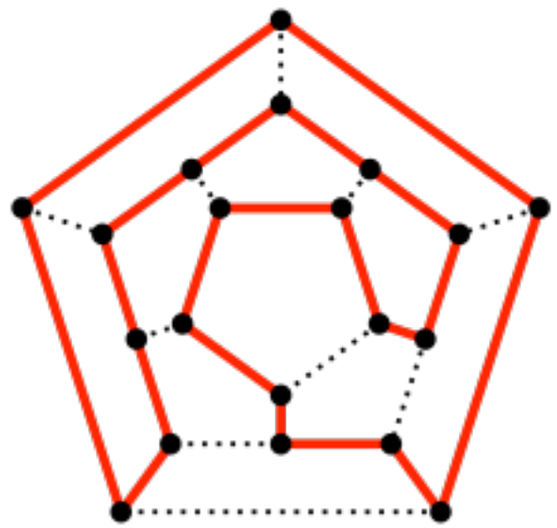
- 7 bridges of Königsberg
- is there a roundtrip that crosses each bridge exactly once?

•Euler (1735) : it exists if and only if the graph is connected and there are no nodes of odd degree at all

- can be evaluated in polynomial time; is in complexity class P

# Hamiltonian cycle problem

(M.Troyer)



- is there a path that crosses each *vertex* exactly once?
- expensive task by evaluating all paths
- no solution in polynomial time is known
- is NP-complete

# proof that sign problem is NP-hard

(M.Troyer)

consider 3d frustrated Ising model (glass)

$$H = -\sum_{\langle j,k \rangle} J_{jk}\sigma_j\sigma_k \qquad\qquad J_{j,k} = 0, \pm J$$

does there exist a state with energy less than a bound $E_0$?

Is a NP-complete problem. F. Barahona, J. Phys. A 15, 3241 (1982).

view it as a quantum problem in basis where H is not diagonal :

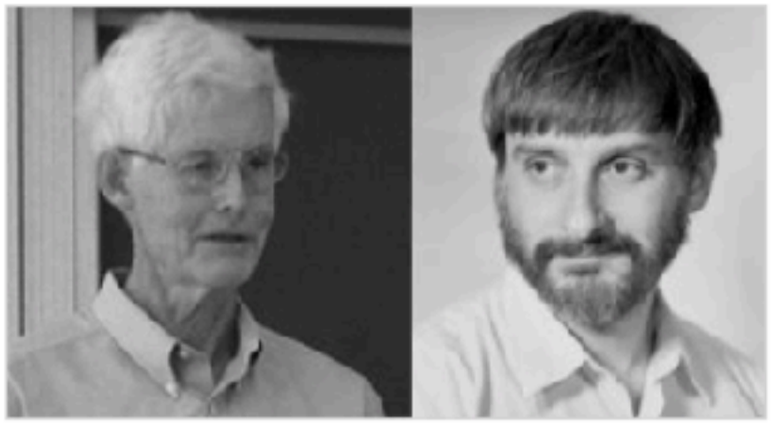
$$H = -\sum_{\langle j,k \rangle} J_{j,k}\sigma_j^x\sigma_k^x \qquad\qquad J_{j,k} = 0, \pm J$$

random signs appear in off-diagonal matrix elements

bosonic model (ferromagnet, $J_{jk} > 0$) easy to solve

Hence, the sign problem causes NP-hardness

# P vs NP Problem



Suppose that you are organizing housing accommodations for a group of four hundred university students. Space is limited and only one hundred of the students will receive places in the dormitory. To complicate matters, the Dean has provided you with a list of pairs of incompatible students, and requested that no pair from this list appear in your final choice. This is an example of what computer scientists call an NP-problem, since it is easy to check if a given choice of one hundred students proposed by a coworker is satisfactory (i.e., no pair taken from your coworker's list also appears on the list from the Dean's office), however the task of generating such a list from scratch seems to be so hard as to be completely impractical. Indeed, the total number of ways of choosing one hundred students from the four hundred applicants is greater than the number of atoms in the known universe! Thus no future civilization could ever hope to build a supercomputer capable of solving the problem by brute force; that is, by checking every possible combination of 100 students. However, this apparent difficulty may only reflect the lack of ingenuity of your programmer. In fact, one of the outstanding problems in computer science is determining whether questions exist whose answer can be quickly checked, but which require an impossibly long time to solve by any direct procedure. Problems like the one listed above certainly seem to be of this kind, but so far no one has managed to prove that any of them really are so hard as they appear, i.e., that there really is no feasible way to generate an answer with the help of a computer. Stephen Cook and Leonid Levin formulated the P (i.e., easy to find) versus NP (i.e., easy to check) problem independently in 1971.

Image credit: on the left, Stephen Cook by Jiří Janíček (cropped). CC BY-SA 3.0

**Rules:**

Rules for the Millennium Prizes

**Related Documents:**

Official Problem Description

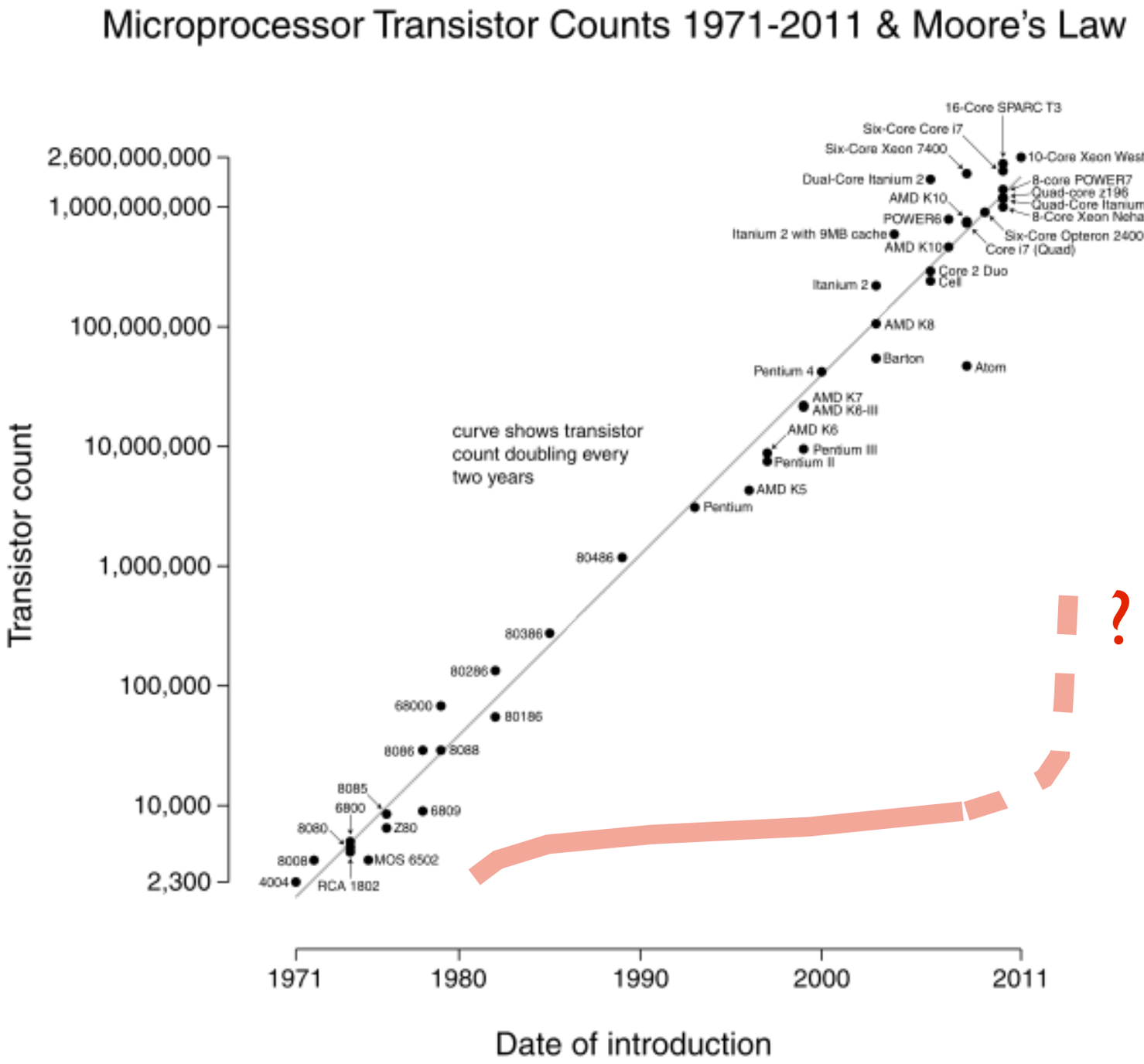
Minesweeper

**Related Links:**

Lecture by Vijaya Ramachandran

http://www.claymath.org/millennium-problems/p-vs-np-problem

# Moore's law for fermions




nr of fermions / complexity of problem

100
10
1

# Perturbative expansions

$$H = H_a + H_b$$

not talking about variational Monte Carlo, diffusion Monte Carlo, …

$$Z = \mathrm{Tr} T_\tau e^{-\beta H_a} \exp\left[ -\int_0^\beta d\tau H_b(\tau) \right]$$

$$= \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \mathrm{Tr}[e^{-\beta H_a} H_b(\tau_k) \times H_b(\tau_{k-1}) \cdots H_b(\tau_1)].$$

continuous time

**strong coupling expansions:**

two-body term is $H_a$; choose basis where this is diagonal

typically on finite system (requires finite size analysis), finite β

can be sign-free for bosons; spins with AF couplings on bipartite lattices, ...

**weak coupling expansions:**

one-body term is $H_a$; typically thermodynamic limit, can be ground state. Has Wick theorem, Dyson equation, etc

# Diagrammatic Monte Carlo

diagrammatic expansions:

sign ~ exp(- $\#_n$ n)  n = expansion order

no volume factors!

drawbacks

series usually asymptotic or worse (log Z instead of Z)

sign problem

multidimensional objects

active field of research; true challenge, many open questions

Thank you!