Fermion Bags: Tutorial

Outline

A.The idea of Fermion Bags.

B.Applications in Lattice Field Theory.

C.Fermion world-lines in Hamiltonian lattice field theory.

D.Spatial Fermion Bags

A. The idea of Fermion Bags

Generic partition function in lattice field theory:

$$Z = \int [d\sigma]\ \int [d\overline{\psi}\ d\psi]\ \mathrm{e}^{-S_b[\sigma]\ -\ \sum_{i,j} \overline{\psi}_i\ M_{ij}[\sigma]\ \psi_j}$$

Traditional Approach: Integrate over the fermions

$$Z\ =\ \int [d\sigma]\ \mathrm{e}^{-S_b[\sigma]}\ \mathrm{Det}(M[\sigma])$$

negative

STOP

positive

Develop a QMC!

Fermion Bag Idea:

(i) Express the Grassman path integral in terms of fermion world lines.

(ii) Group the world lines into “fermion bags” so that we can integrate over the bosonic field and sum over fermion world lines within each bag.

(iii) Find the grouping so that the sum over weights of fermion world lines and the bosonic integral gives positive weight within each bag.

$$Z = \int [d\sigma] \sum_{C} W(C,\sigma) = \text{``}\sum_{B} \Omega(B)\text{''}$$

Hope: Local physics of the problem lends itself to this description.

Pros:
(i) New solutions to sign problems can emerge.
(ii) Faster algorithms can be designed.
(iii) Weights of fermion bags are smaller and less singular.

Cons:
(i) No simple recipe that is widely applicable. Each problem needs to be thought through carefully.
(ii) May require modifications to the action (“designer models”).
(iii) An area of research in itself.

In traditional lattice field theory this has yielded a new class of fermion Monte Carlo algorithms.

We can study exactly massless fermions on large lattices, which continues to be difficult with traditional HMC.

Recently we have been able to extend these to Hamiltonian lattice field theories.

Worldlines from Grassmann Variables:

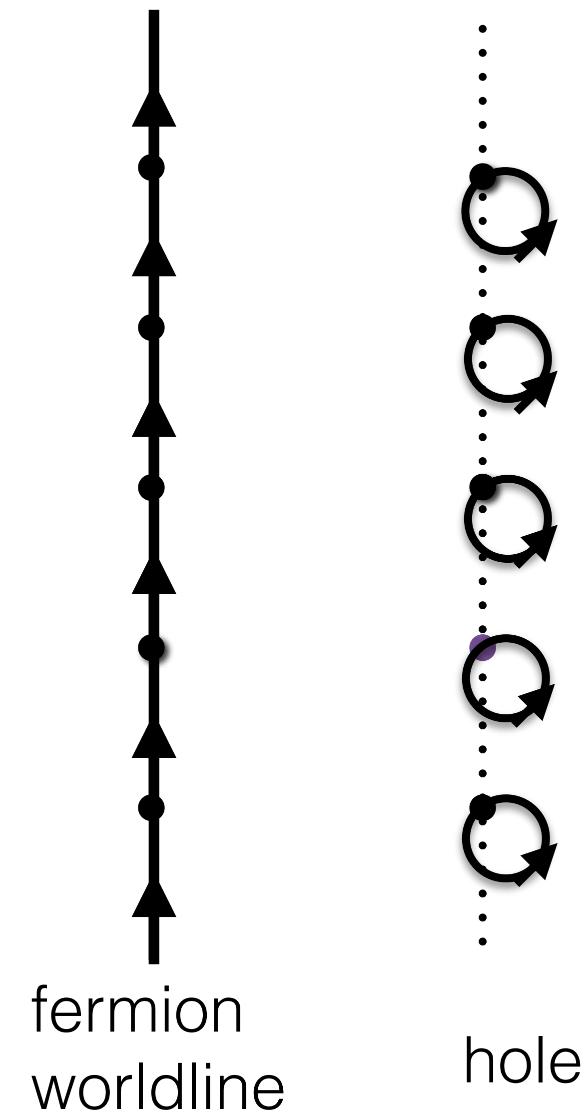
Single site example:

$$S_0 = -\sum_t \overline{\psi}_t \left(\psi_{t+1} - \psi_t\right)$$

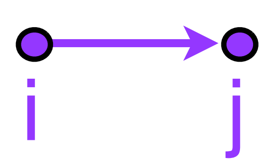
$$Z = \int \prod_t [d\overline{\psi}_t d\psi_t] \; e^{\sum_t \overline{\psi}_t (\psi_{t+1} - \psi_t)}$$

$$e^{\overline{\psi}_t \psi_{t+1}} = 1 + \overline{\psi}_t \psi_{t+1}$$

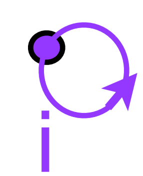
$$e^{-\overline{\psi}_t \psi_t} = 1 - \overline{\psi}_t \psi_{t+1}$$



$$\overline{\psi}_i \psi_j =$$

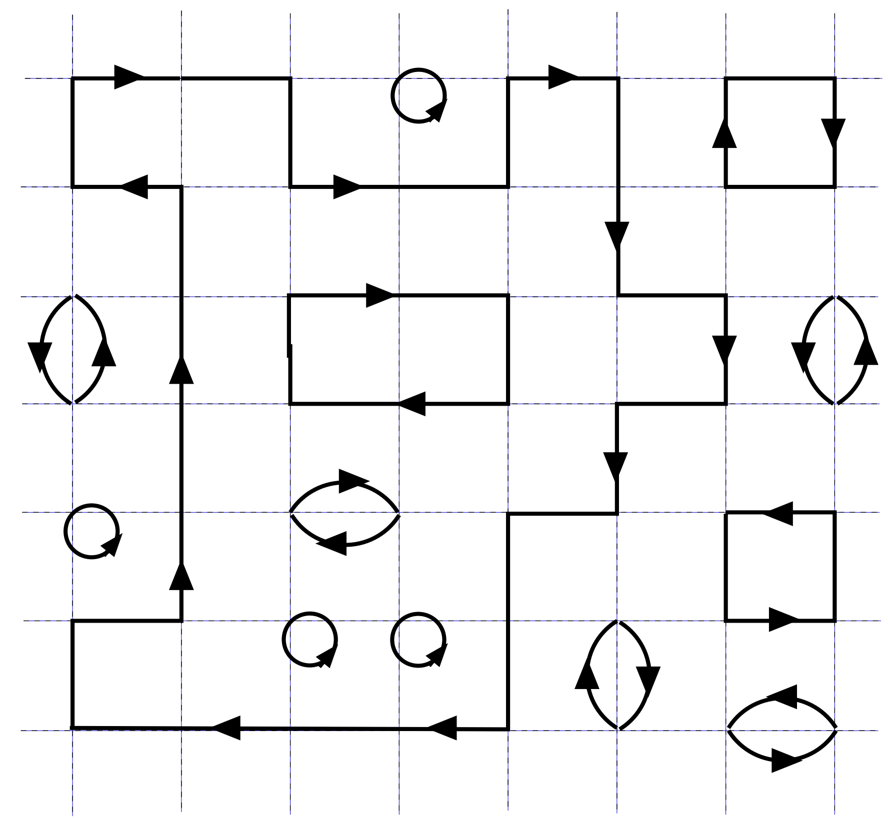


$$\overline{\psi}_i \psi_i =$$



In general

$$\int [d\overline{\psi}][d\psi]\mathrm{e}^{-\overline{\psi}_i M_{ij}(\sigma)\psi_j} = \sum_{[C]} W(C,\sigma)$$



Example of C

where the weight $W(C,\sigma)$

can be negative.

Here we expanded each term

$$\mathrm{e}^{-\overline{\psi}_i M_{ij}(\sigma)\psi_j} = 1 - \overline{\psi}_i M_{ij}(\sigma)\psi_j$$

and integrated over the
Grassmann variables.

If “M” is a “good” matrix then Det(M) is positive.
Usually this requires some “symmetry.”

B. Application in Lattice Field Theory

Lattice Yukawa Models

SC, PRD (2012)

Bosonic Action: $S_b[\theta] \;=\; -\kappa \sum_{x,\alpha} \left(\mathrm{e}^{i(\theta_x - \theta_{x+\alpha})} + \mathrm{e}^{-i(\theta_x - \theta_{x+\alpha})} \right)$

Fermion Action:

$$S_f[\overline{\psi}, \psi] \;=\; \sum_{x,\alpha} \frac{\eta_{x,\mu}}{2} \left(\overline{\psi}_x \; \psi_{x+\alpha} - \overline{\psi}_{x+\alpha} \; \psi_x \right) + g \sum_x \mathrm{e}^{i\varepsilon_x \theta_x} \overline{\psi}_x \psi_x$$

staggered fermions
(pi-flux)

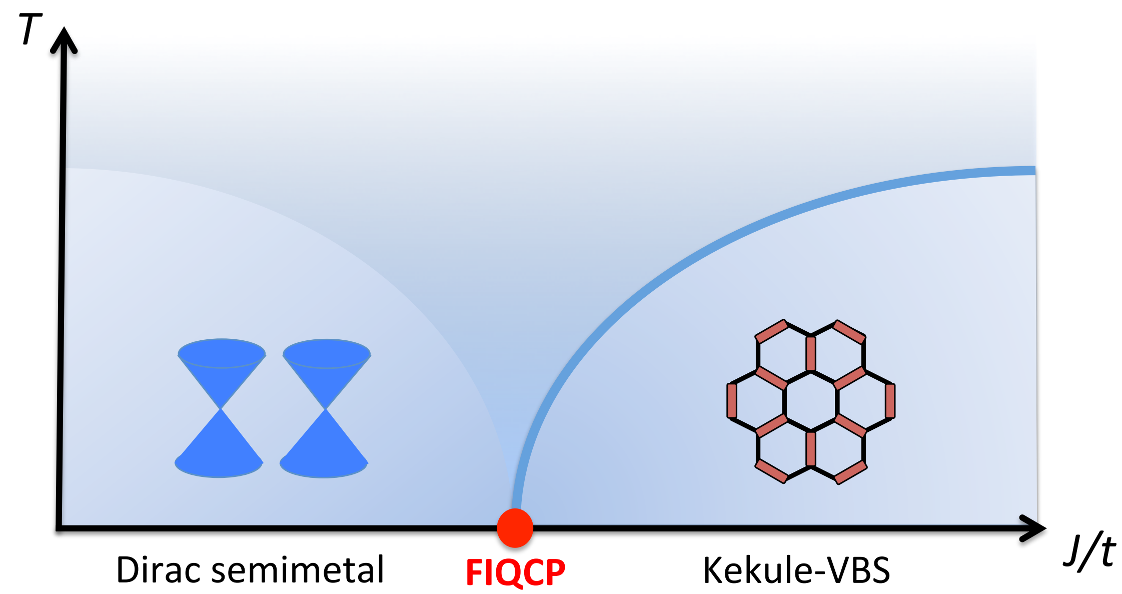
$$\varepsilon_x = \begin{cases} +1 & x \in \text{even} \\ -1 & x \in \text{odd} \end{cases}$$

The action is invariant under U(1) chiral transformations

Let us focus on the Z_3 symmetric case: $\theta_x = 0, 2\pi/3, -2\pi/3$

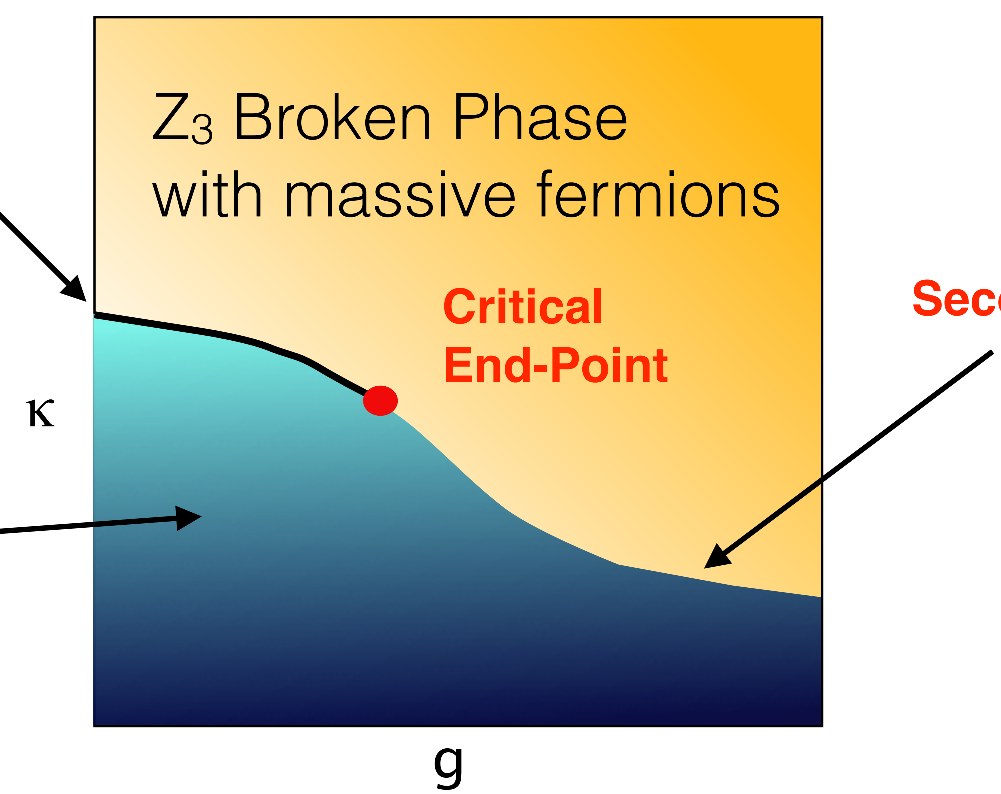
Recently the Z_3 model has become interesting, since it is related to the Semi-metal-Kekule VBS transition.

It has been proposed that fermions induce a quantum critical point in 2+1 dimensions.



First order

Phase Diagram of the lattice model:



Second order

Z_3 Symmetric Phase
with massless fermions

The traditional approach has a severe sign problem!

$$Z = \sum_{[z]} e^{\kappa \sum_{x,\alpha} (z_x z^*_{x+\alpha} + z^*_x z_{x+\alpha})}$$

$$\underbrace{\int [d\overline{\psi} d\psi] \; e^{-\sum_{x,\alpha} \frac{\eta_{x,\mu}}{2} \left(\overline{\psi}_x \; \psi_{x+\alpha} - \overline{\psi}_{x+\alpha} \; \psi_x\right) - \; g \sum_x (z_x)^{\varepsilon_x} \overline{\psi}_x \psi_x}}_{}$$

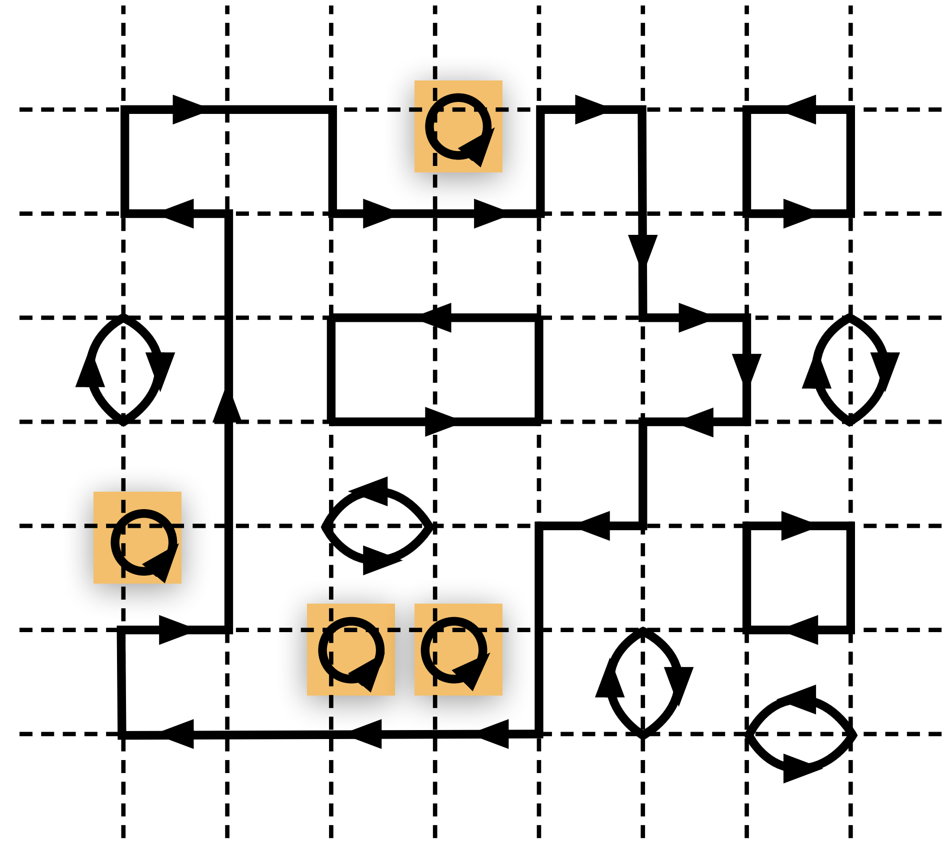
$\mathrm{Det}\big(A + D(z)\big)$ is complex

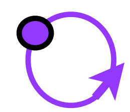
Antisymmetric matrix,
has positive determinant

source of the
sign problem!

Fermion Bag Approach:

$$e^{-g\,(z_x)^{\varepsilon_x}\,\overline{\psi}_x\psi_x} = 1 + g\,(z_x)^{\varepsilon_x}\,(-\overline{\psi}_x\psi_x)$$





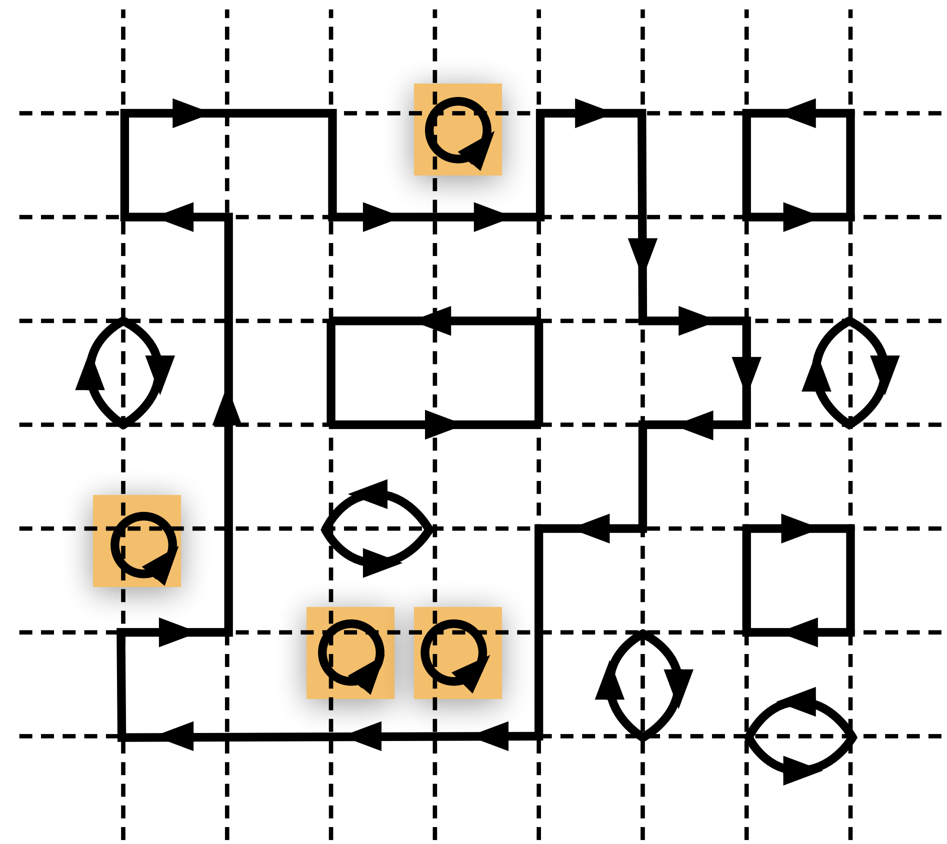
Introduce a monomer field [n]

$$Z = \sum_{[n]} g^k \sum_{[z]} e^{\kappa \sum_{x,\alpha}\,(z_x z^*_{x+\alpha} + z^*_x z_{x+\alpha})}\,(z_{x_1})^{\varepsilon_{x_1}} \ldots (z_{x_k})^{\varepsilon_{x_k}}$$

$$\int [d\overline{\psi} d\psi]\; e^{-\sum_{x,\alpha} \frac{\eta_{x,\mu}}{2}\left(\overline{\psi}_x\;\psi_{x+\alpha} - \overline{\psi}_{x+\alpha}\;\psi_x\right)}\;(-\overline{\psi}_{x_1}\psi_{x_1})\ldots(-\overline{\psi}_{x_k}\psi_{x_k})$$

Anti-symmetric matrix

We group the interaction sites first and perform the sum over Z_3 spins.

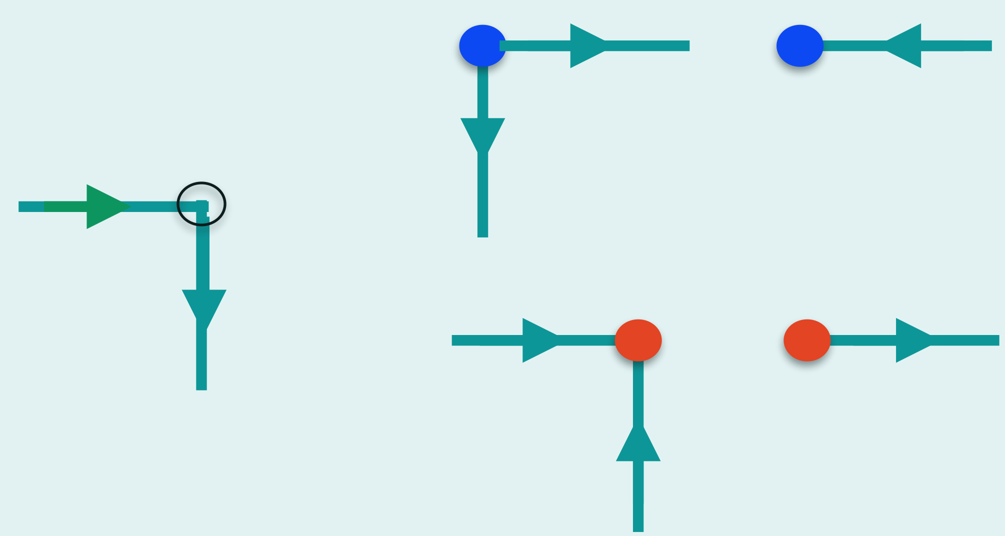


$$\sum_{[z]} e^{\kappa \sum_{x,\alpha} (z_x z^*_{x+\alpha} + z^*_x z_{x+\alpha})} \, (z_{x_1})^{\varepsilon_{x_1}} \ldots (z_{x_k})^{\varepsilon_{x_k}}$$

$$e^{\kappa (z_x z^*_{x+\alpha} + z^*_x z_{x+\alpha})} = f_0(\kappa) + f_1(\kappa) \left(z_x z^*_{x+\alpha} + z^*_x z_{x+\alpha}\right)$$

boson worldlines

Sum of Z_3 spins imposes constraints on boson worldlines.

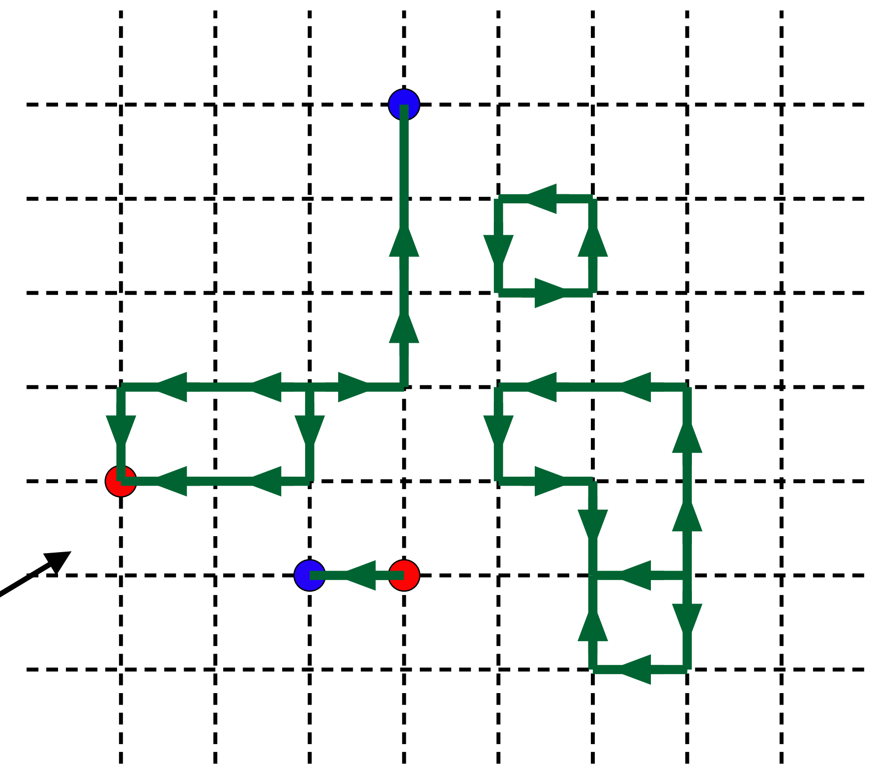


We can rewrite the spin partition function

$$\sum_{[z]} e^{\kappa \sum_{x,\alpha} (z_x z^*_{x+\alpha} + z^*_x z_{x+\alpha})} (z_{x_1})^{\varepsilon_{x_1}} \dots (z_{x_k})^{\varepsilon_{x_k}}$$

$$= \sum_{[q]}{}' \prod_{x,\alpha} f_{q_{x,\alpha}}(\kappa) \quad \Omega([q,n])$$

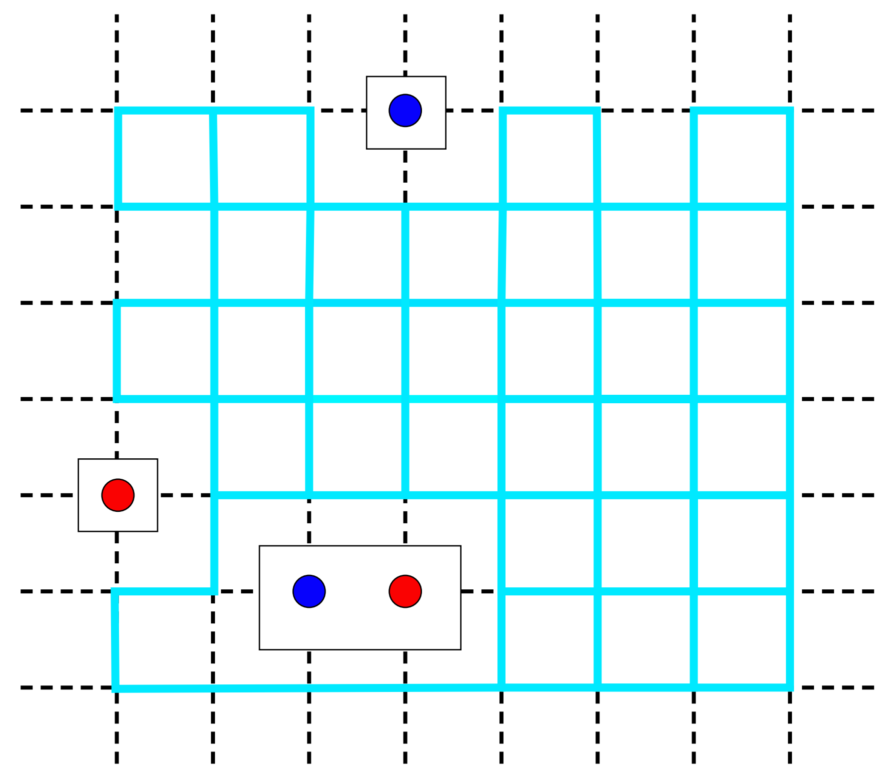
constrained Z_3 worldline configurations



Fermion partition function is a sum over all paths that does not contain the interaction sites.

$$\int{}' [d\overline{\psi} d\psi] \; e^{-\sum_{x,\alpha} \frac{\eta_{x,\mu}}{2} (\overline{\psi}_x \; \psi_{x+\alpha} - \overline{\psi}_{x+\alpha} \; \psi_x)}$$

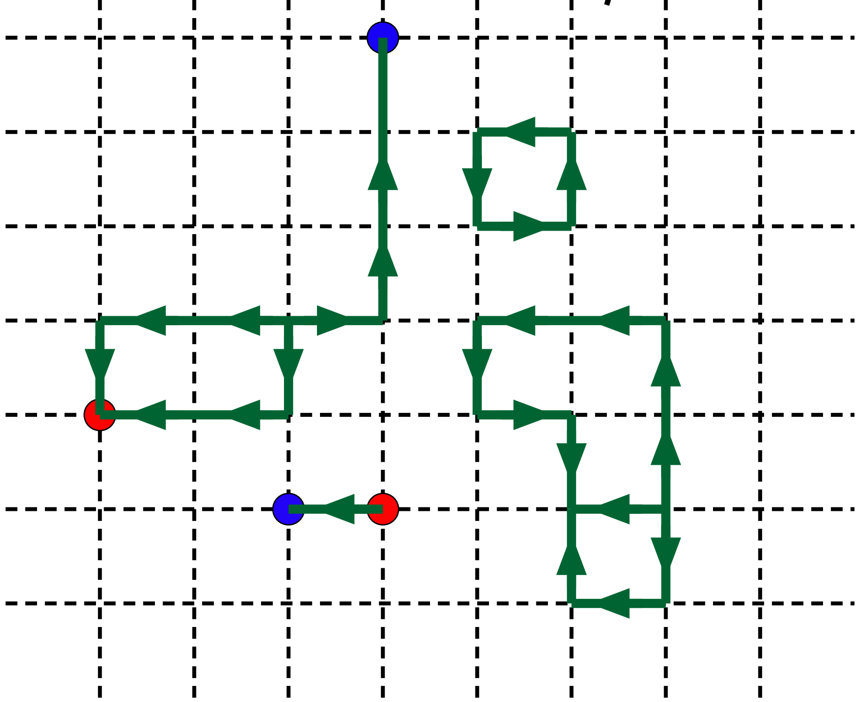
$$= \; \mathrm{Det}(W_k[n])$$

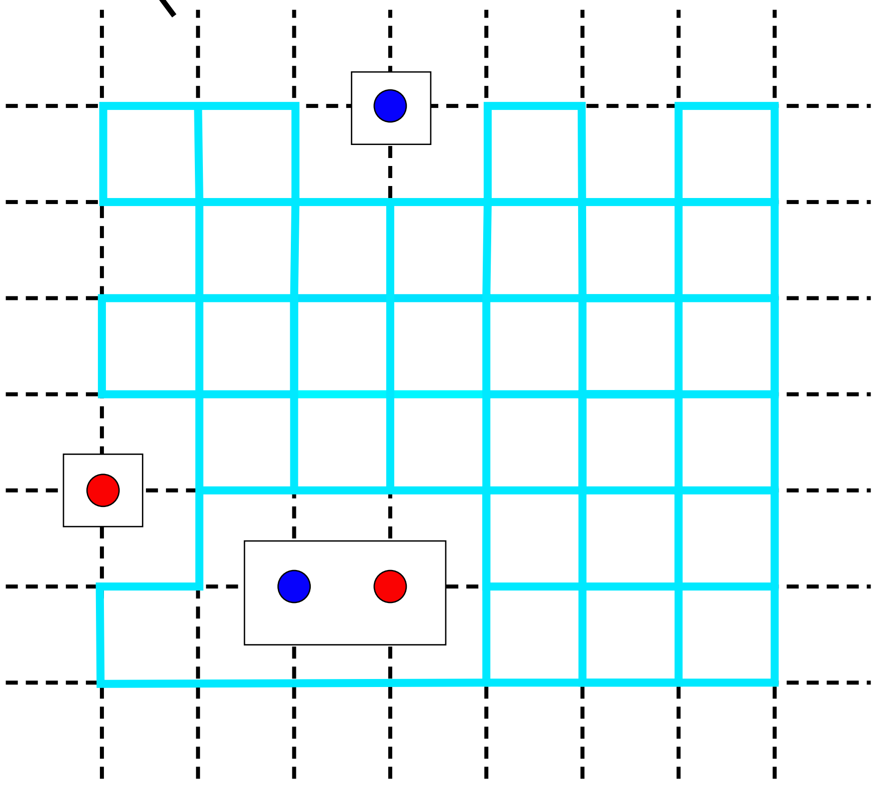


which is positive!

The partition function can be finally written without sign problems:

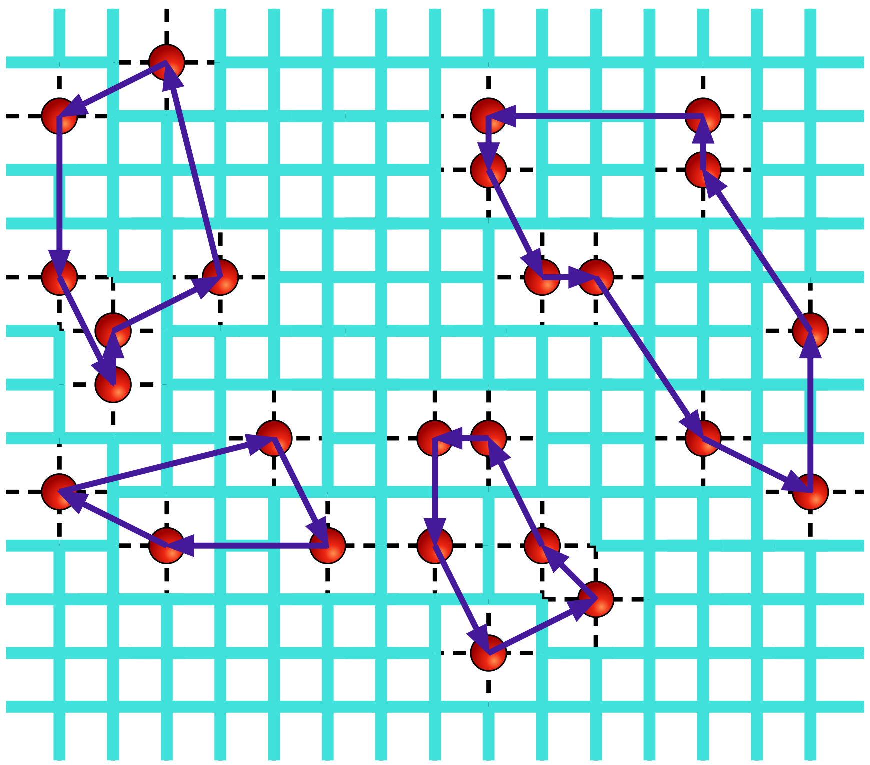
$$Z = \sum_{[n,q]} \Omega([q,n]) \, \mathrm{Det}(W_k[n])$$



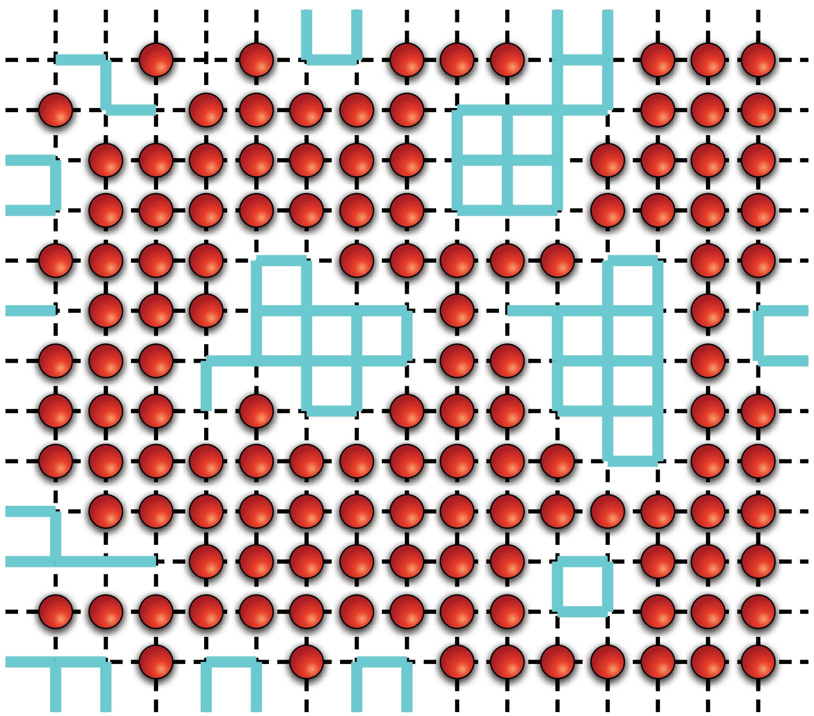


The boson and fermion sector talk to each other through the monomer field [n]

Weak coupling vs. Strong Coupling:



Weak Coupling



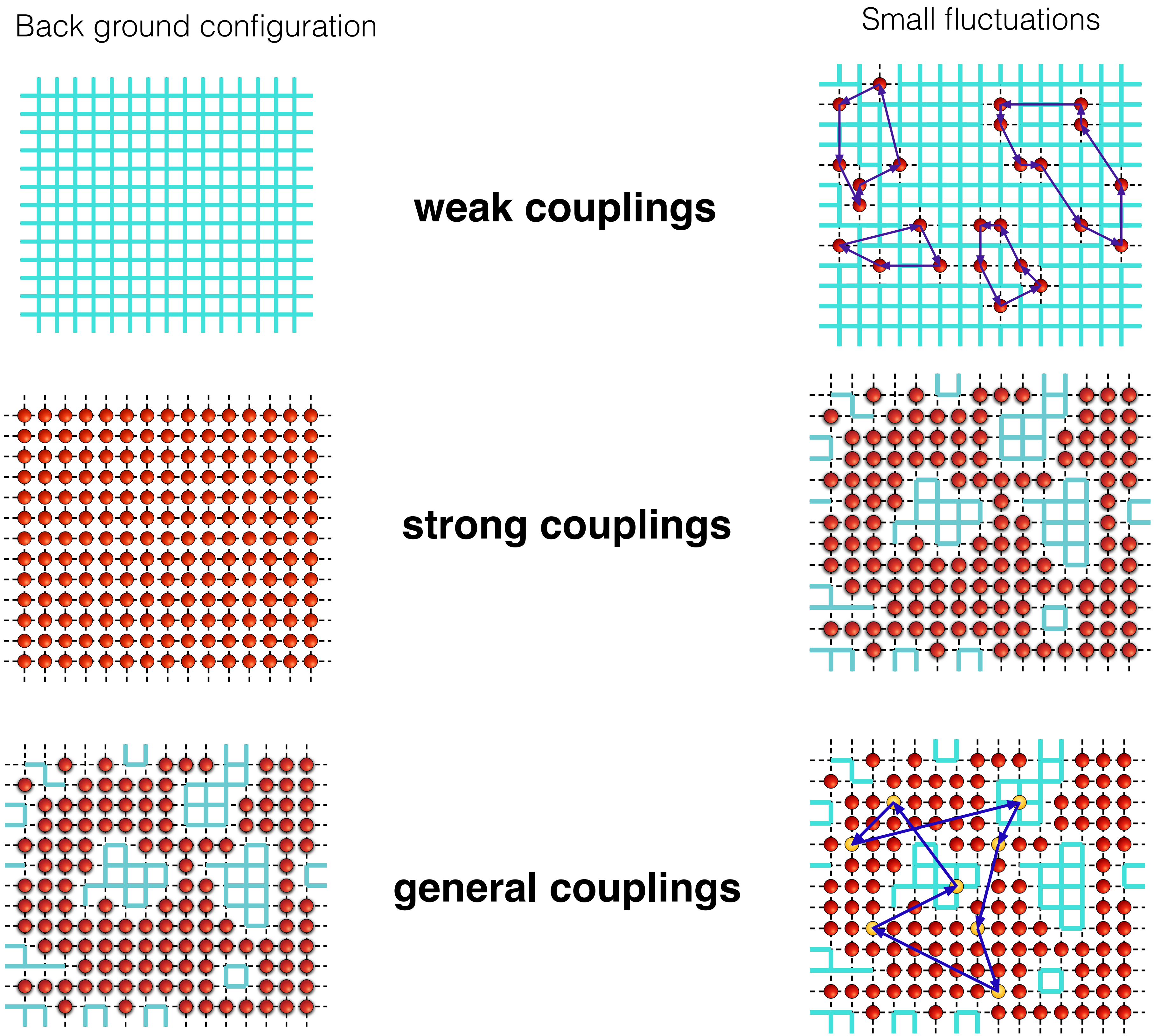
Strong Coupling

“A few small bags
and one big bag”

“Many small bags”

“Diagrammatic Determinantal
Monte Carlo.”

Background Fields: New definitions of fermion bags



C. Application in Hamiltonian Lattice Field Theory

Why think in terms of a Hamiltonian?

(i) Natural in condensed matter physics.

(ii) For lattice field theorists it eliminates an unnecessary fermion doubling and preserves some internal symmetries.

(iii) Some sign problems are easily solved.

(iv) Algorithms scale better.

In discrete time these formulations look like regular lattice field theories but without space-time rotation symmetries.

Partitio Function:

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right)$$

Where we will write the generic Hamiltonian as

$$H = H_0 + H_{\text{int}}$$

Discrete time approach:

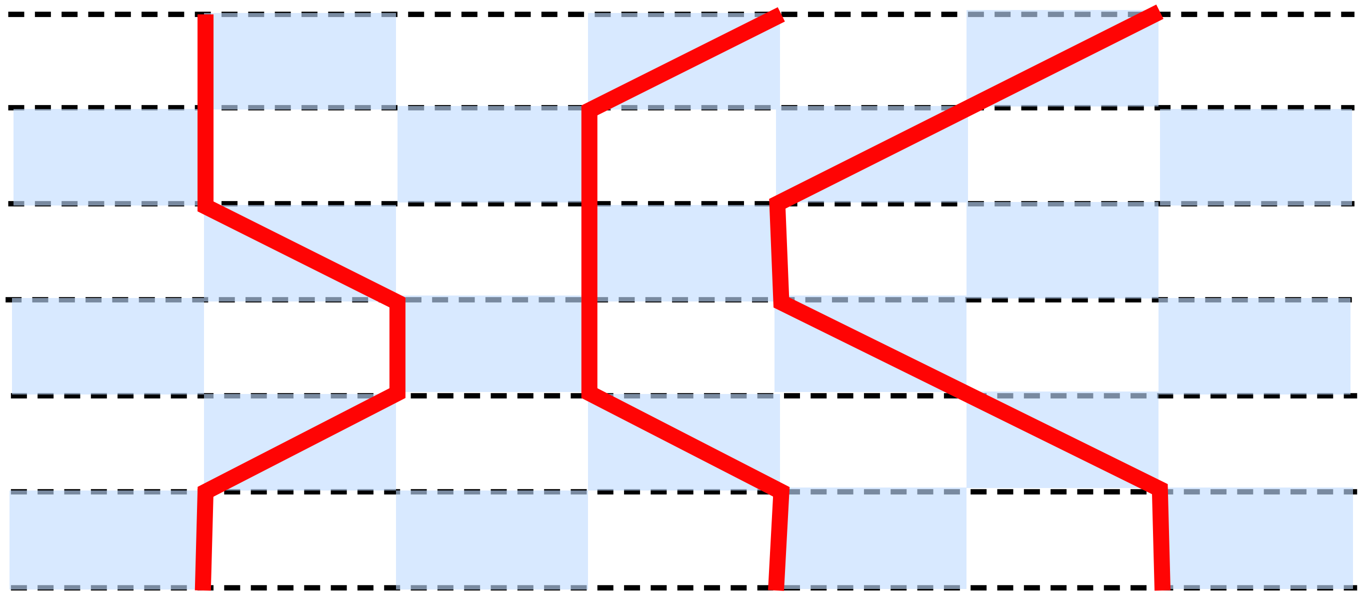
$$\mathrm{Tr}\left(e^{-\beta H}\right) = \mathrm{Tr}\left(e^{-\varepsilon H}\, e^{-\varepsilon H} \, ...e^{-\varepsilon H}\right)$$

Continuous time approach:

$$\mathrm{Tr}\left(e^{-\beta H}\right) = \sum_k \int [dt]\ \mathrm{Tr}\left(e^{-(\beta - t_k)H_0}(-H_{\text{int}})e^{-(t_k - t_{k-1})H_0}...H_{\text{int}}e^{-t_1 H_0}\right)$$

time ordered

Ideas of fermion bags should in principle extend to the discrete time approach for local Hamiltonians by using a "checkerboard" type space-time lattice.



Fermion world lines are simply the occupation number basis:

Problem:

In the auxiliary field approach each time step takes the form:

$$e^{-\varepsilon \; c_i^\dagger M_{ij}[\sigma] c_j}$$

In the continuous time limit the fermion bags are difficult to identify.

The partition function takes the form

$$Z \;=\; \int [d\sigma]\; \mathrm{Tr}\Big(...\mathrm{e}^{-\varepsilon\; c_i^\dagger M_{ij}^k[\sigma_k] c_j} ...\mathrm{e}^{-\varepsilon\; c_i^\dagger M_{ij}^{k'}[\sigma_{k'}] c_j} ... \Big)$$

We can define $\quad B_k(\sigma_k) \;=\; exp(-\varepsilon M^k(\sigma_k)) \quad$ then

$$Z \;=\; \int [d\sigma]\; \mathrm{Det}\Big(1 + B_{N_t}(\sigma_{N_t}) B_{N_t-1}(\sigma_{N_t-1}) .... B_1(\sigma_1)\Big)$$

Advantage: Determinants are spatial size x spatial size

Disadvantage: Difficult to identify fermion bags, except in the weak coupling language (?).

D. Spatial Fermion Bags

Challenge: How can we identify space-time fermion bags in the similar to the Lagrangian approach in continuous time?

A simple Idea: Choose $H_0 = 0$ and $H_{\rm int} = H$

Then the partition function is

$$\mathrm{Tr}\Big(\mathrm{e}^{-\beta H}\Big) \;=\; \sum_k \int [dt]\ \mathrm{Tr}\Big((-H_{\rm int})(-H_{\rm int})...(-H_{\rm int})\Big)$$

The at very high temperatures (no interactions) all spatial sites form fermions bags and are independent of each other!

What about lower temperatures?

Consider "local designer Hamiltonians" such that each insertion of the interaction gives a positive trace!

$$\mathrm{Tr}\Big((-H_{\mathrm{int}})(-H_{\mathrm{int}})\ldots(-H_{\mathrm{int}})\Big) \;\geq 0$$

The simplest example is

$$H \;=\; H_{\mathrm{int}} = \sum_{\langle ij\rangle} \delta e^{\alpha(c_i^\dagger c_j + c_j^\dagger c_i)}$$

which is equivalent to

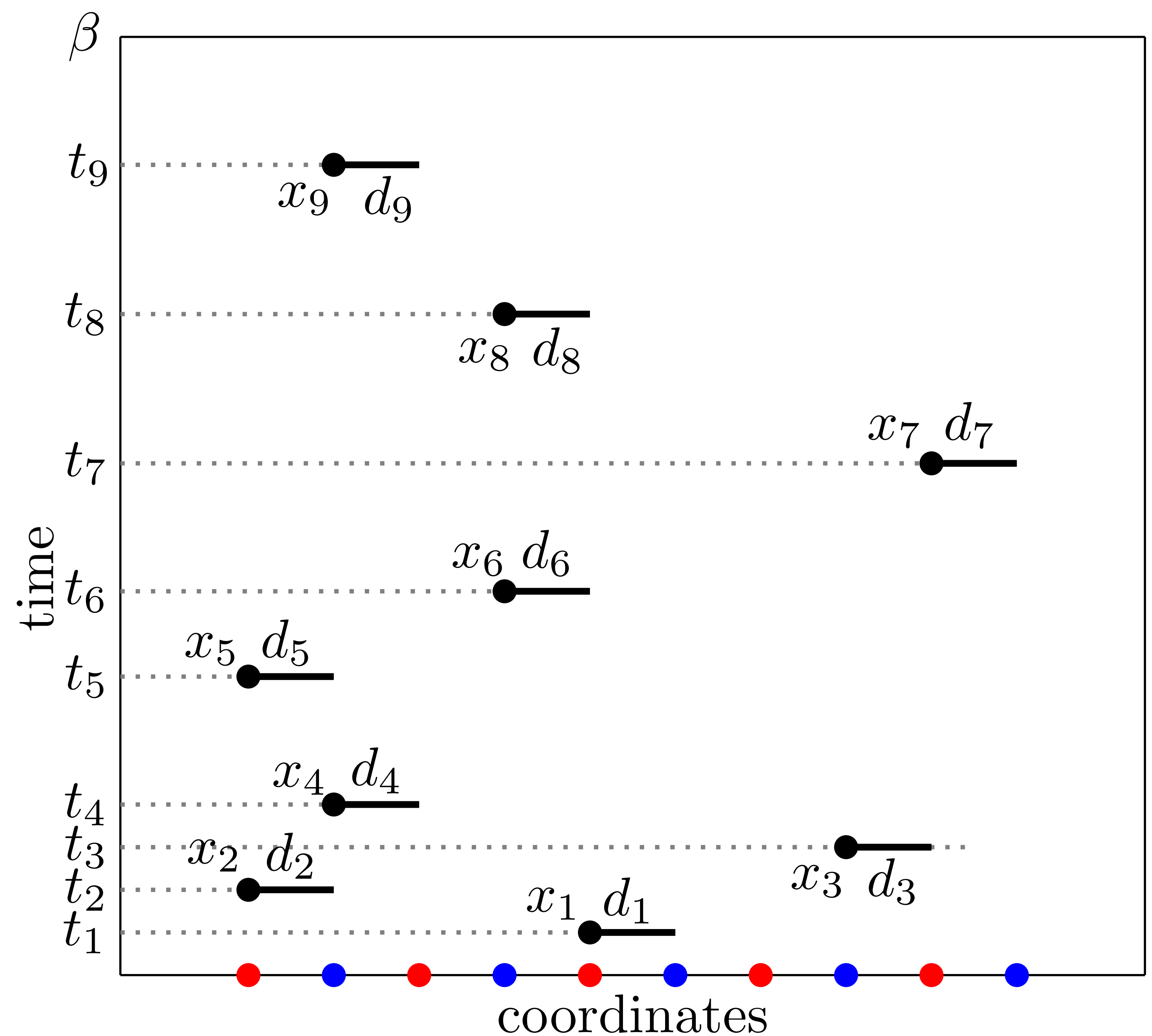
$$H \;=\; -t\sum_{\langle ij\rangle} \eta_{ij}\;(c_i^\dagger c_j + c_j^\dagger c_i) \;+\; V\;\sum_{\langle ij\rangle}\big(n_i - \frac{1}{2}\big)\;\big(n_j - \frac{1}{2}\big)$$

The partition function can be written as

$$Z \;=\; \int [dt] \sum_{[b,t]} \delta^k \;\mathrm{Tr}(\ldots(e^{\alpha(c_i^\dagger c_j + c_j^\dagger c_i)})\ldots.(e^{\alpha(c_i^\dagger c_j + c_j^\dagger c_i)})\ldots)$$

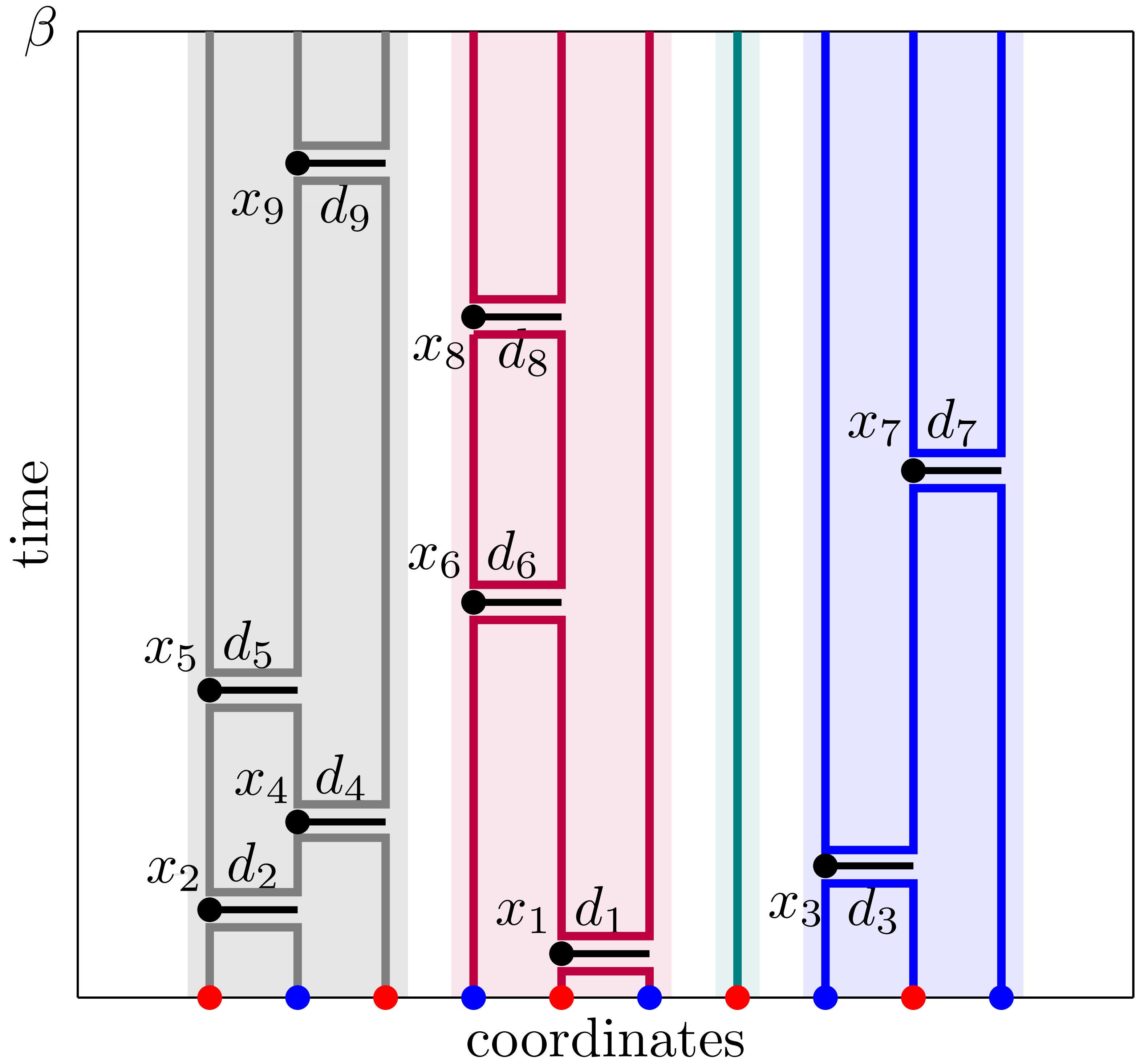
Positive

[b,t] configuration; k = 9



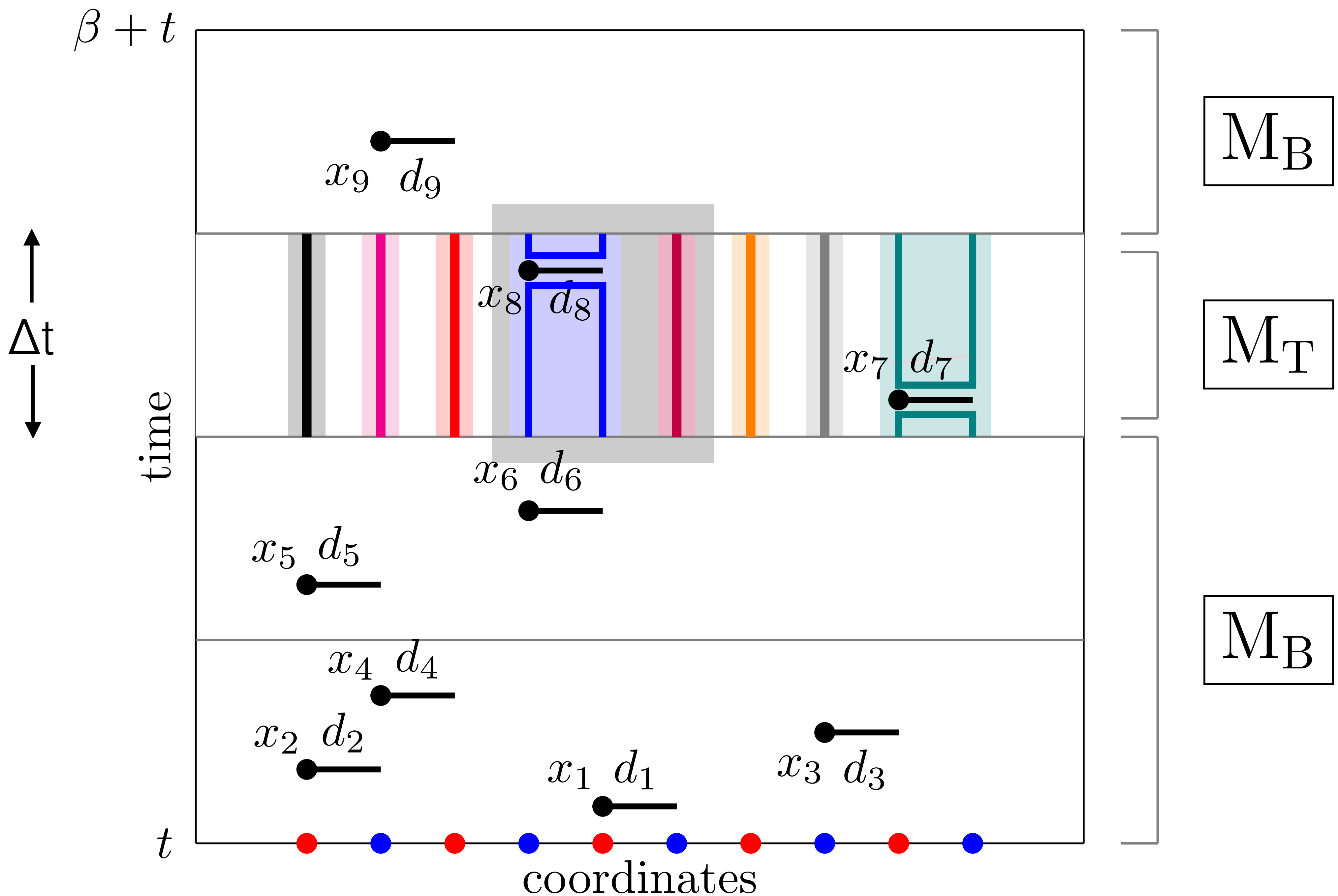
configuration weight $\Omega([b,t]) \; = \; \delta^k \; \mathrm{Tr}(\ldots(e^{\alpha(c_i^\dagger c_j + c_j^\dagger c_i})\ldots.(e^{\alpha(c_i^\dagger c_j + c_j^\dagger c_i)})\ldots)$

Fermion bags are “entangled” set of points!

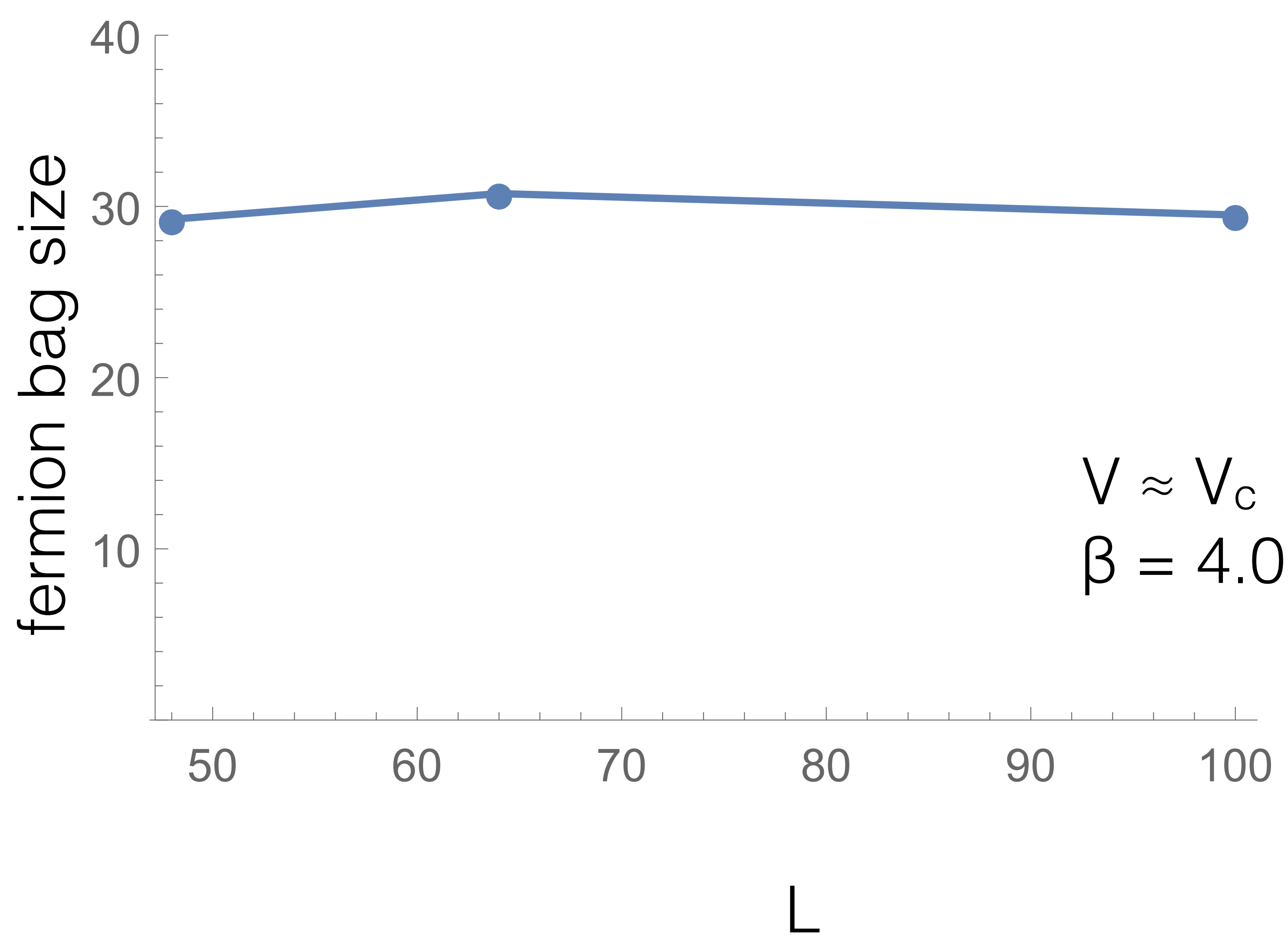


4 fermion bags!

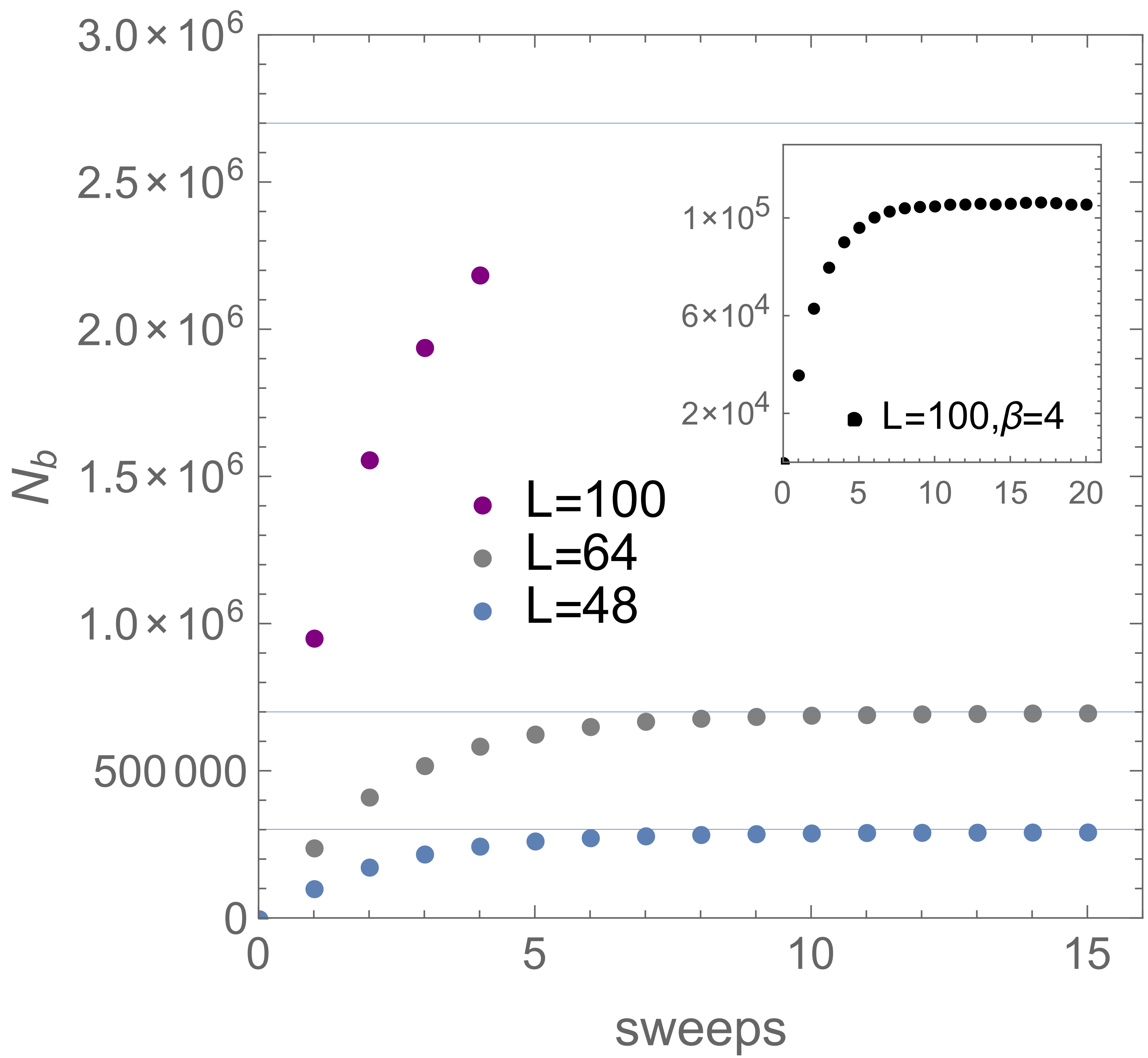
At high temperature fermion dynamics splits naturally into disconnected bags



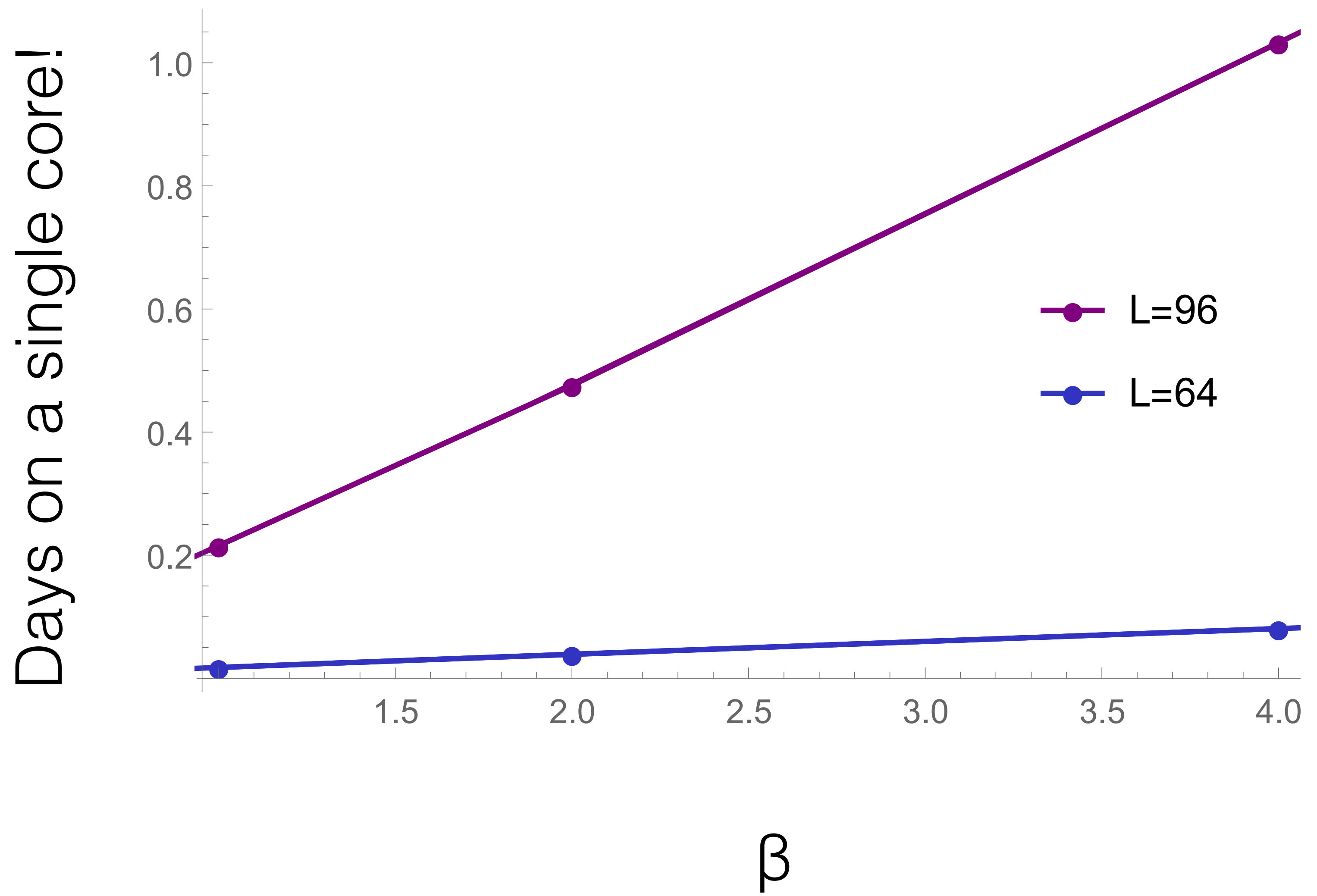
Fermion bag size as a function of spatial volume with $\Delta t = 0.25$



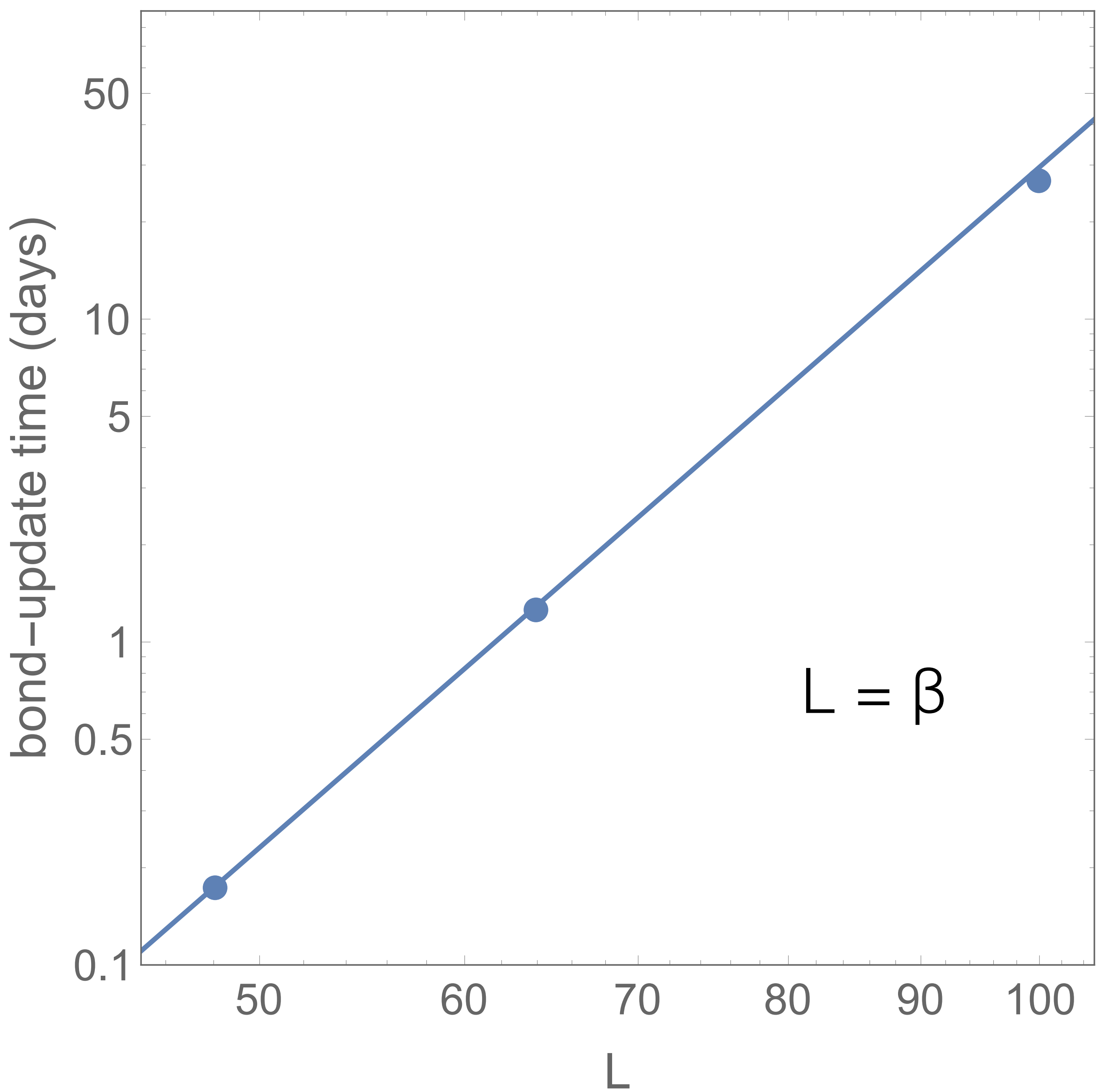
Equilibration



time to update bonds is linear in β



Scaling of the algorithm: $V^3 \beta$



We can accelerate the algorithm further if we abandon the continuous time approach, in line with the “Lattice Field Theory” paradigm!

Technical Details:
Emilie Huffman (Poster Next week!)