Diagrammatic Monte Carlo: Ideas & Examples

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Special Lecture 1
TALENT School on Nuclear Quantum Monte Carlo
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Bit of History…

Goes back to the Swendsen-Wang Algorithm
for the Ising model from the late 1980's

Extensions to the O(N) models by Wolf.

Loop Cluster Algorithm for the quantum SU(2) spin
model by Evertz, Lana, Marcu in the early 1990's

Stochastic Series Methods by Sandvik in the mid 1990's

Worm Algorithms and Diagrammatic Methods
by Prokofev and Svistunov, in the late 1990's
and early 2000.

Including Fermions…
SC and Wiese 1999,
Rubtsov and Lichtenstein 2001,
Prokofev and Svistunov, 2005

It is unclear if these methods are better than the traditional auxiliary field methods…

Perhaps for some problems they are…

Basic Idea:

Diagrammatic expansions are often used for analytic work.

1. Strong coupling expansions (High T expansions)
2. Weak coupling expansions (Feynman diagrams)

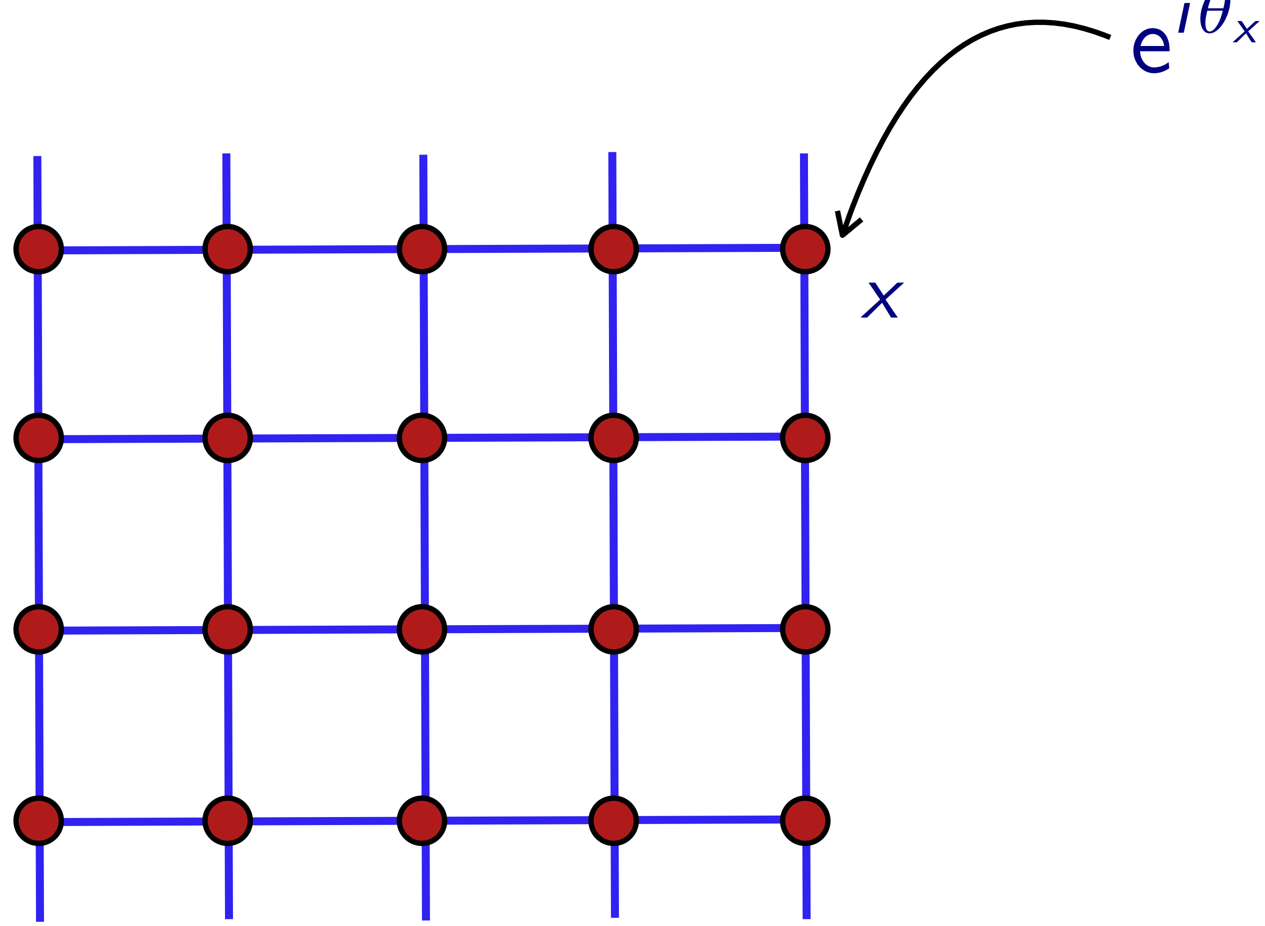
Why not combine such expansions with Monte Carlo methods?

In some cases this approach has helped solve problems that were unsolvable earlier.

These lectures will discuss these developments using four examples

XY Model with a chemical potential

A Lattice Model



Action

$$S([\theta]) = -\beta \sum_{x,\alpha} \cos(\theta_{x+\alpha} - \theta_x - ia\mu\delta_{\alpha,0})$$

inverse coupling

chemical potential

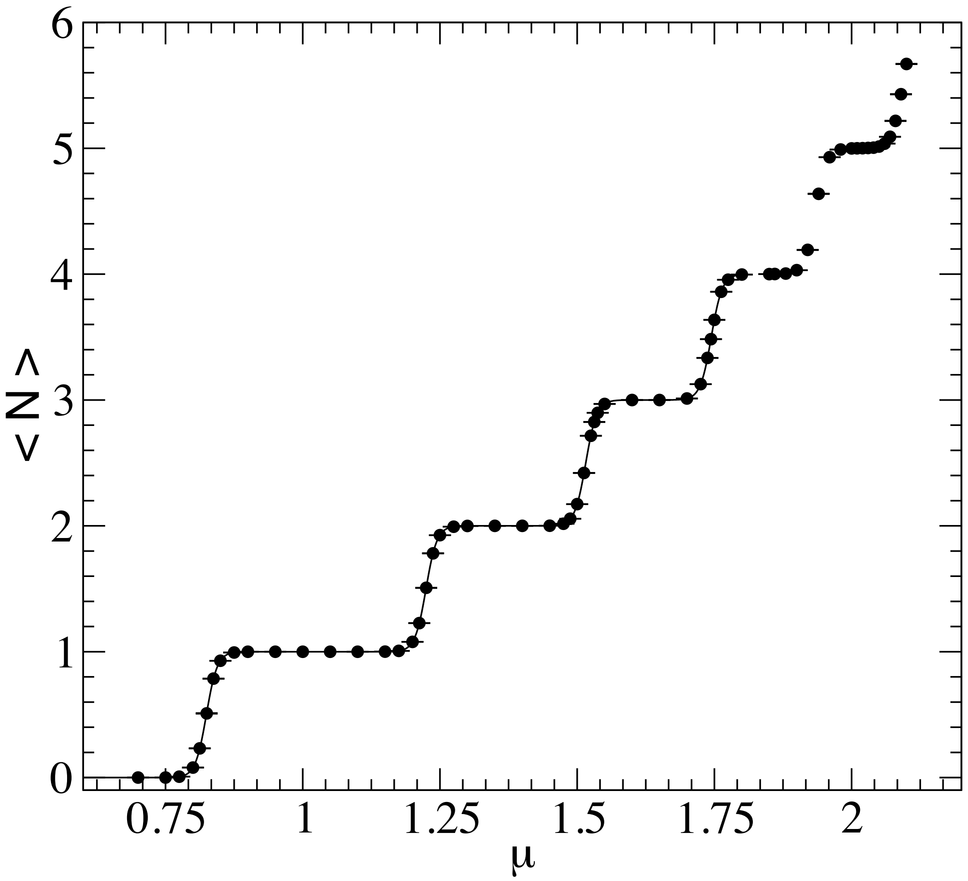
Partition function

$$Z = \int [d\theta]\ \mathrm{e}^{-S([\theta])}$$

Observables

$$\langle N \rangle = \frac{1}{T}\frac{1}{Z}\frac{\partial}{\partial\mu}Z$$

Traditional methods do not work, since the action is complex!



Results from a diagrammatic method

Diagrammatic Approach (strong coupling expansion)

Expand in powers of β

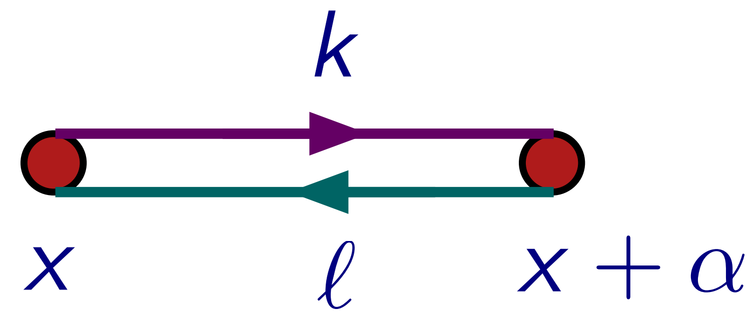
$$e^{-S([\theta])} = \prod_{x,\alpha} e^{\beta \cos(\theta_{x+\alpha} - \theta_x - ia\mu\delta_{\alpha,0})}$$

$$e^{\beta \cos(\theta_{x+\alpha} - \theta_x - ia\mu\delta_{\alpha,0})}$$

$$= \sum_k \frac{\beta^k}{2^k k!} e^{ik(\theta_{x+\alpha} - \theta_x) + a\mu\delta_{\alpha,0}} \sum_\ell \frac{\beta^\ell}{2^k \ell!} \; e^{-i\ell(\theta_{x+\alpha} - \theta_x) - a\mu\ell\delta_{\alpha,0}}$$

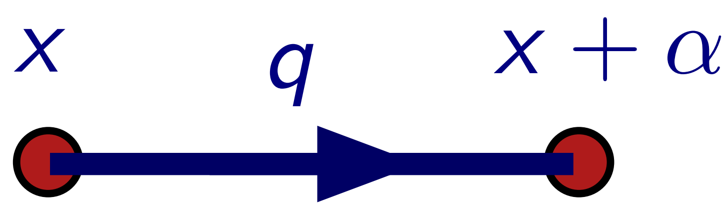
$$= \sum_q \; \mathrm{I}_q(\beta/2) \; e^{iq(\theta_{x+\alpha} - \theta_x) + a\mu q\delta_{\alpha,0}}$$

Diagrams and Weights



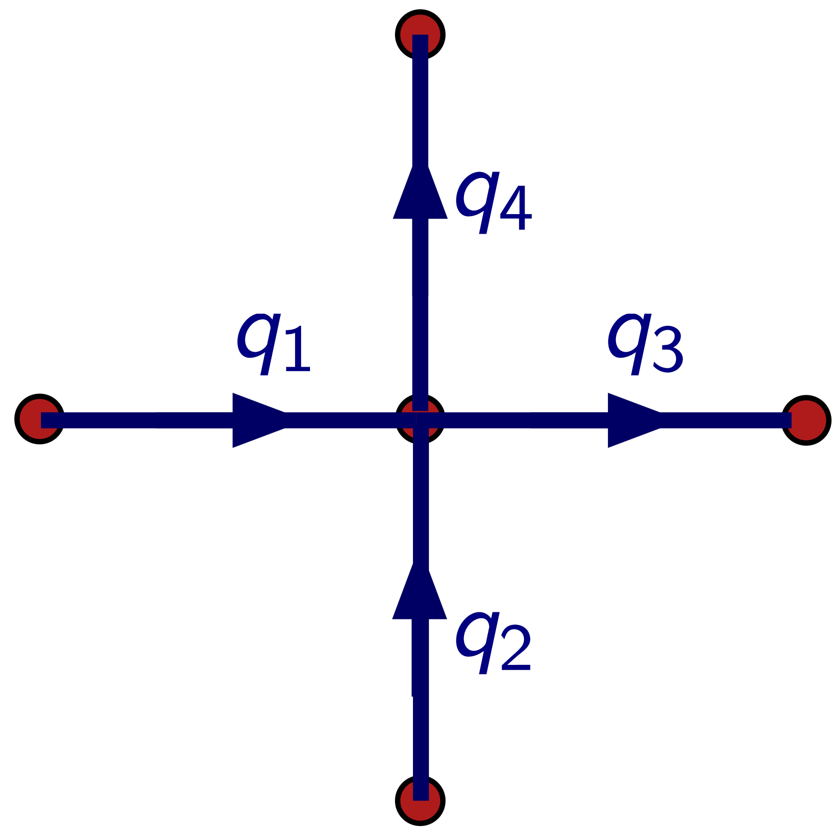
$$e^{\beta\cos(\theta_{x+\alpha}-\theta_x-ia\mu\delta_{\mu,0})}$$

$$\frac{\beta^{k+\ell}}{2^{k+\ell}k!\ell!}e^{i(k-\ell)(\theta_{x+\alpha}-\theta_x)+a\mu(k-\ell)\delta_{\mu,0}}$$



$$\mathrm{I}_q(\beta/2)\ e^{iq(\theta_{x+\alpha}-\theta_x)+a\mu q\delta_{\alpha,0}}$$

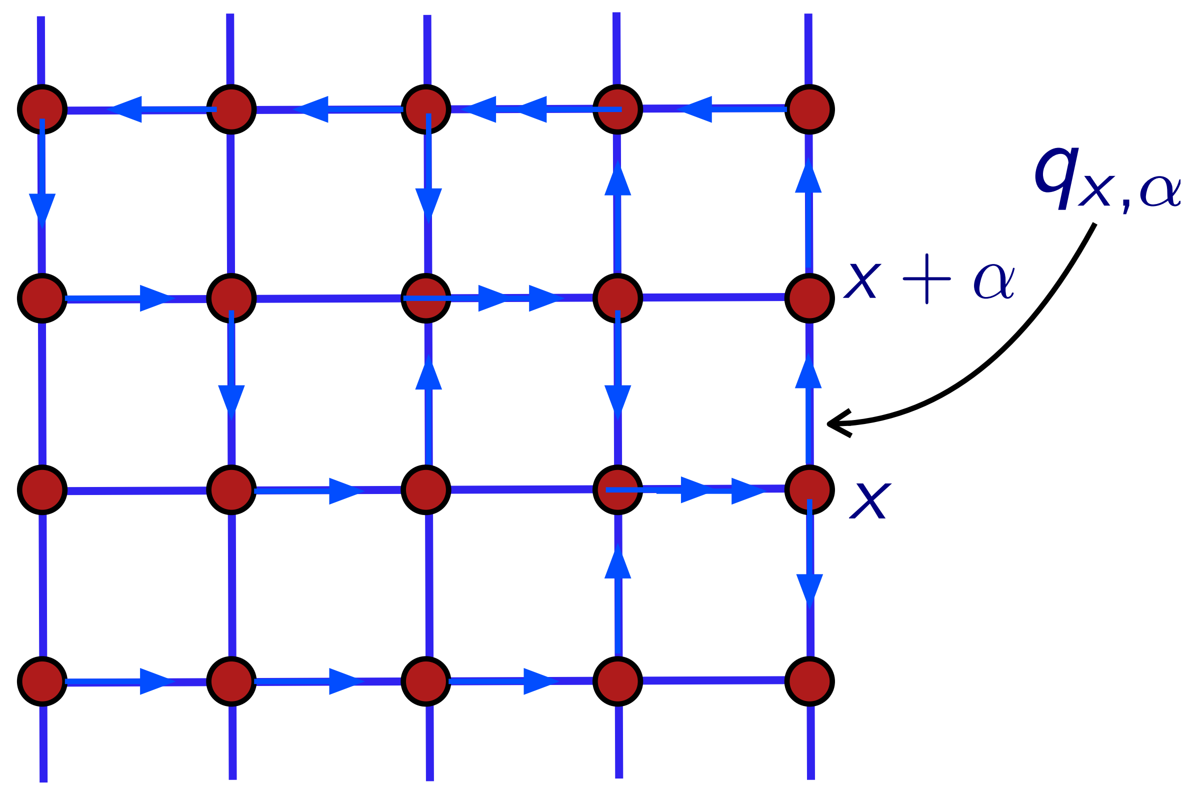
current conservation



$$\frac{1}{2\pi} \int d\theta_x e^{i(q_1+q_2-q_3-q_4)\theta_x} = \delta_{q_1+q_2,q_3+q_4}$$

Diagrammatic Representation of the partition function

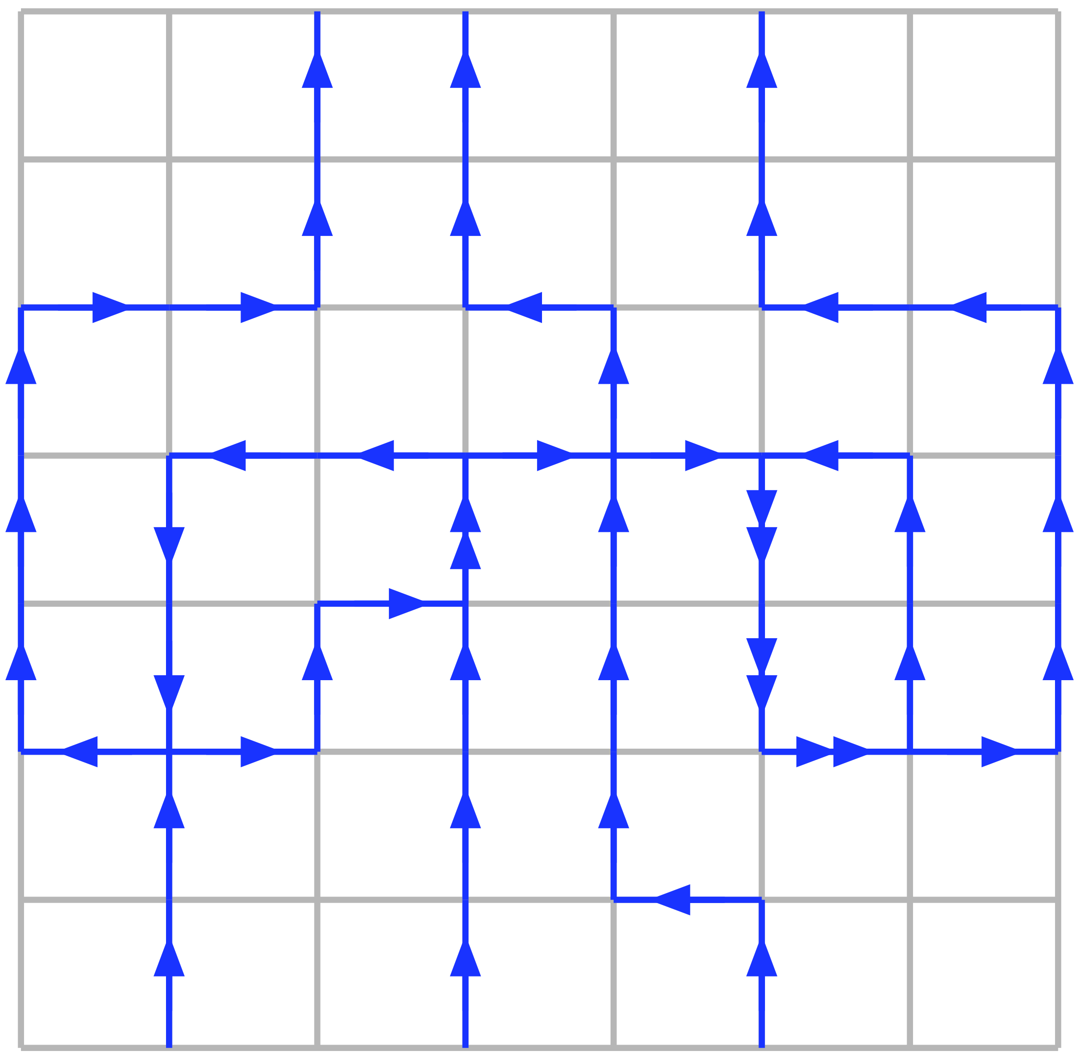
$$Z = \sum_{[q]} \left(\prod_{x,\alpha} I_{q_{x,\alpha}}(\beta/2)\, e^{a\mu q_{x,\alpha}\delta_{\alpha,0}} \right) \left(\prod_{x} \delta\Big(\sum_{\alpha} (q_{x,\alpha} - q_{x-\alpha,\alpha}) \Big) \right)$$



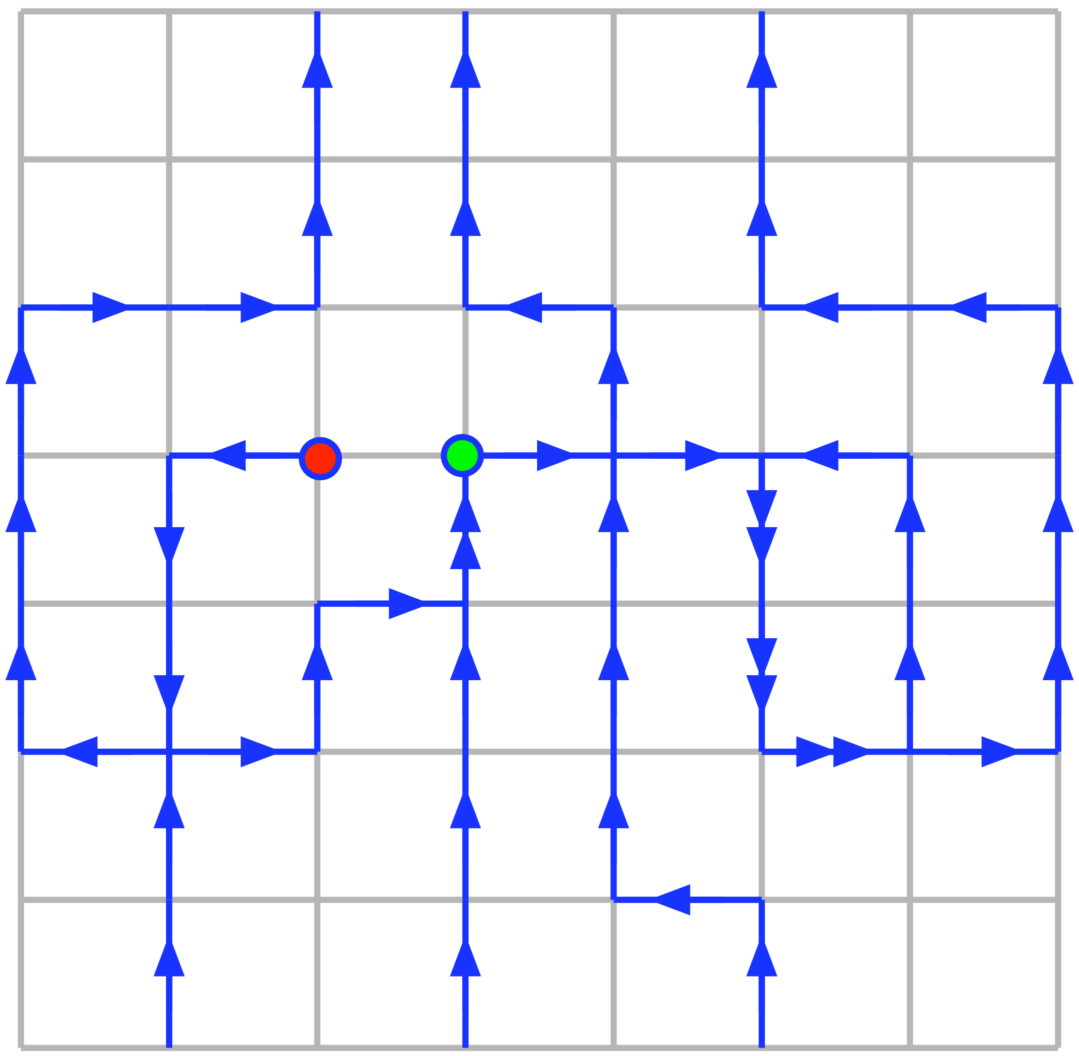
No complex weights, Monte Carlo is applicable!

Worm Algorithm

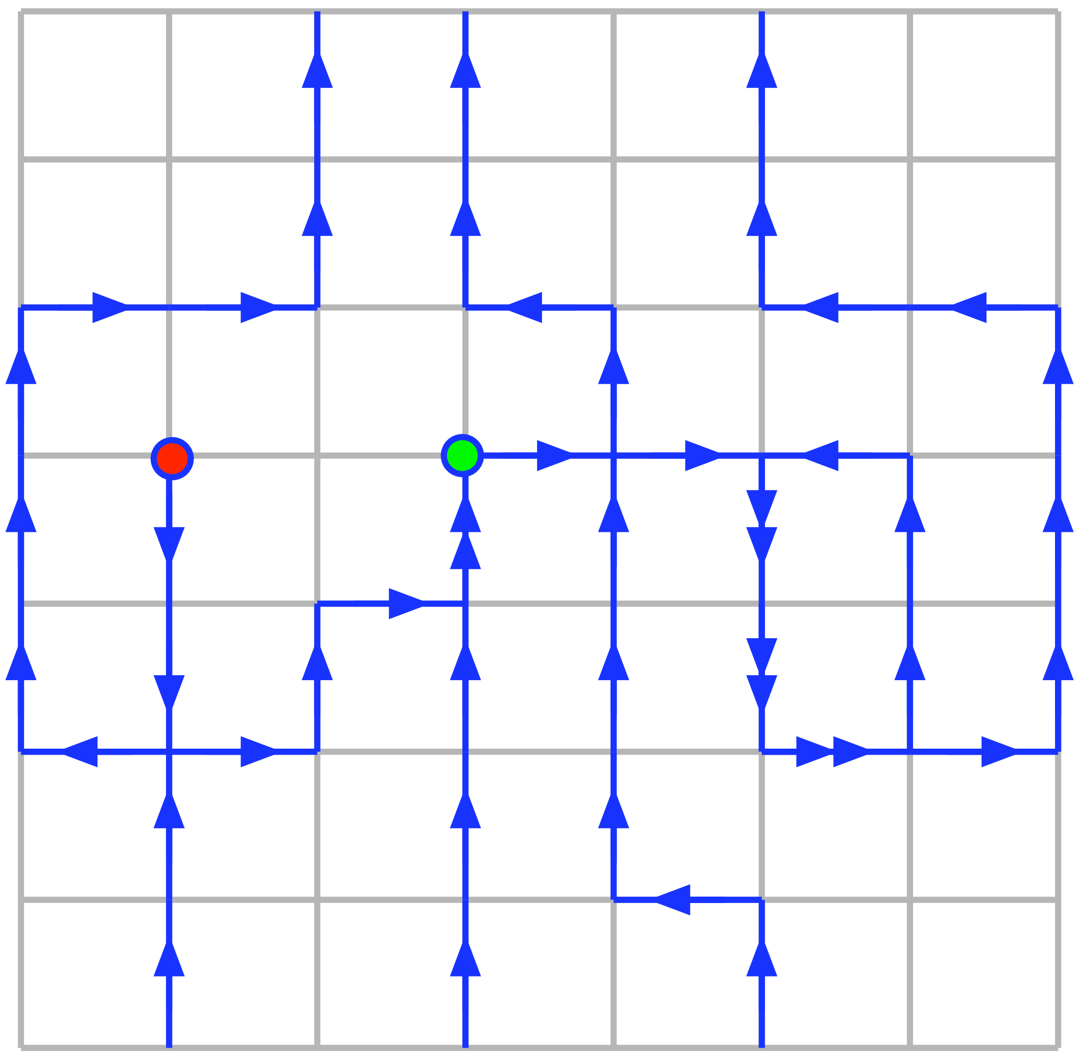
Prokofev & Svistunov
PRL, 87 (2001) 160601



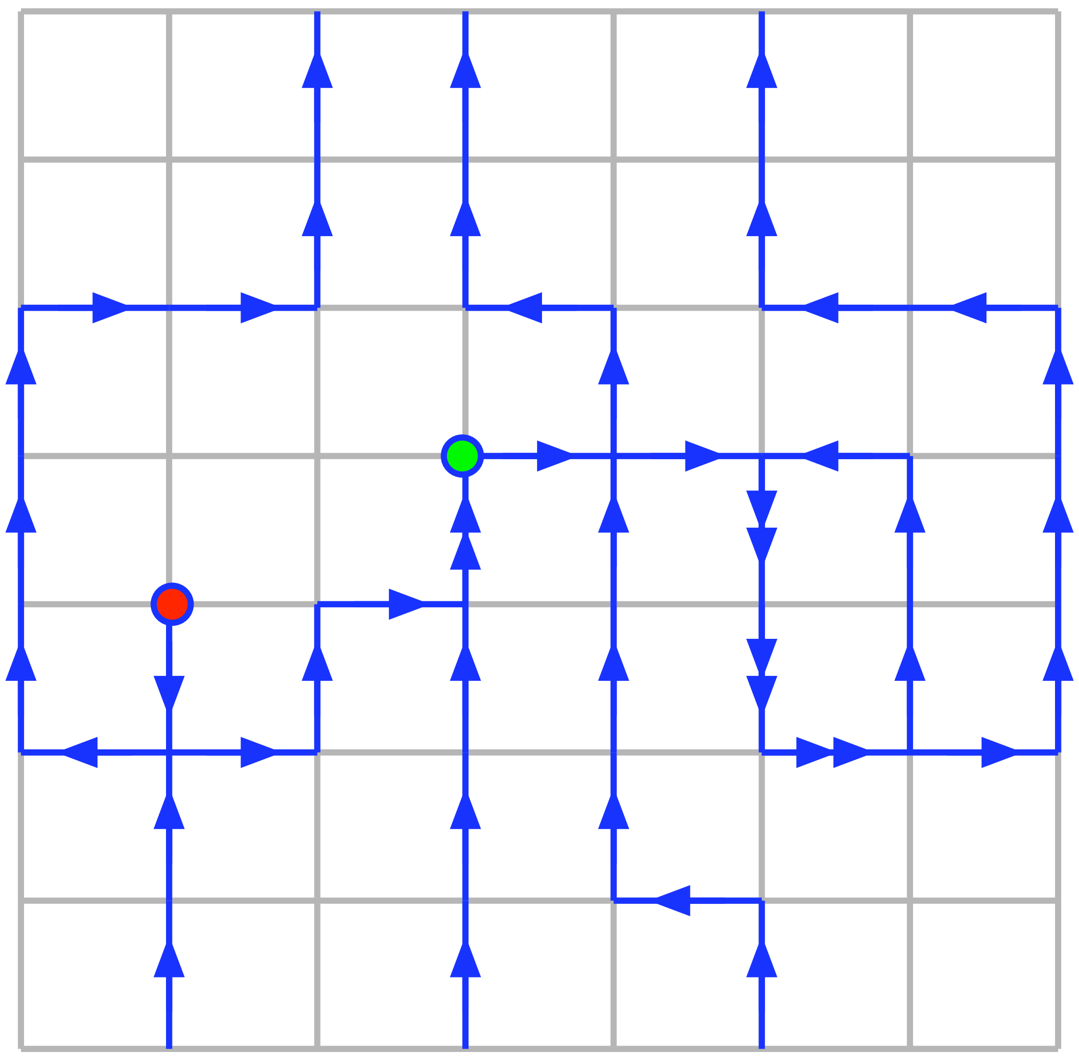
Worm Algorithm



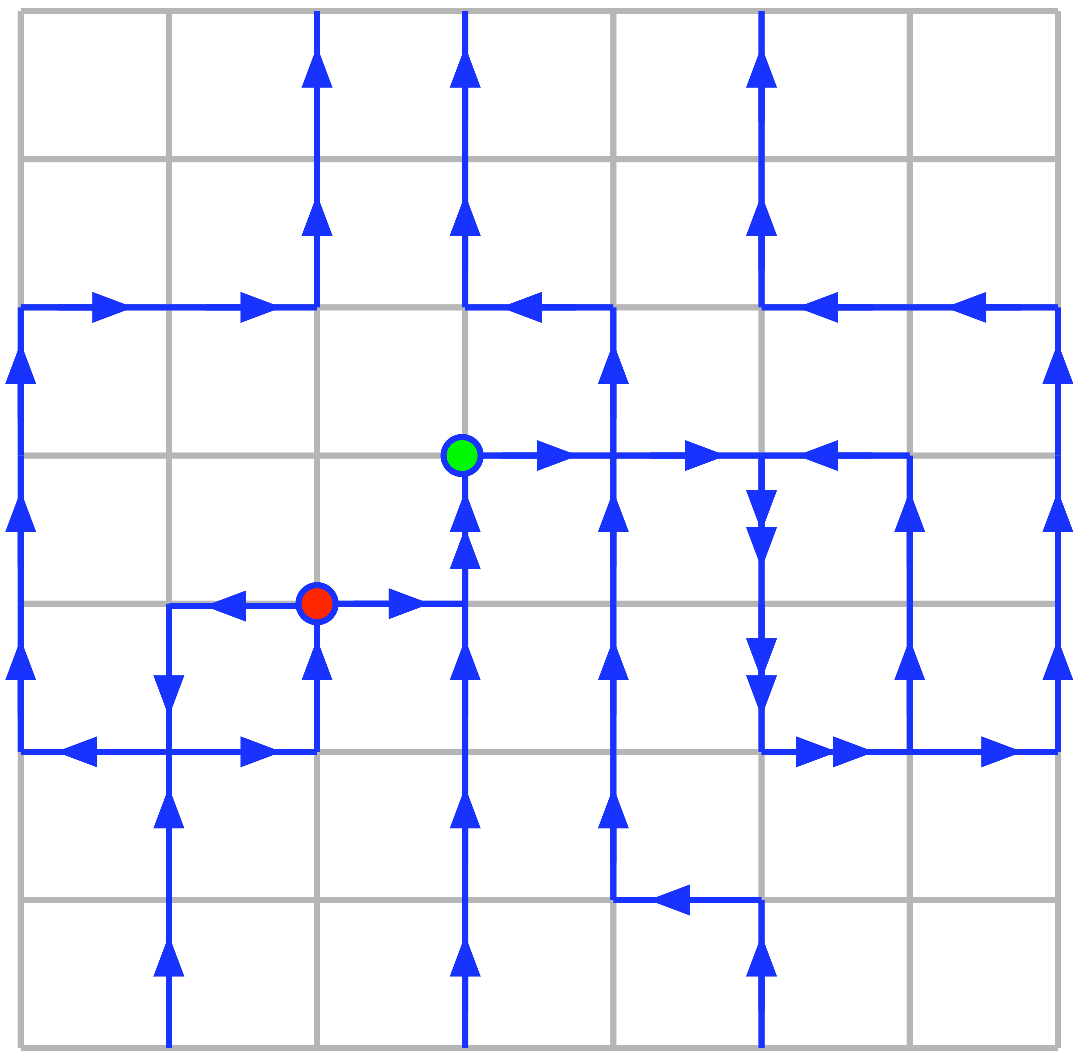
Worm Algorithm



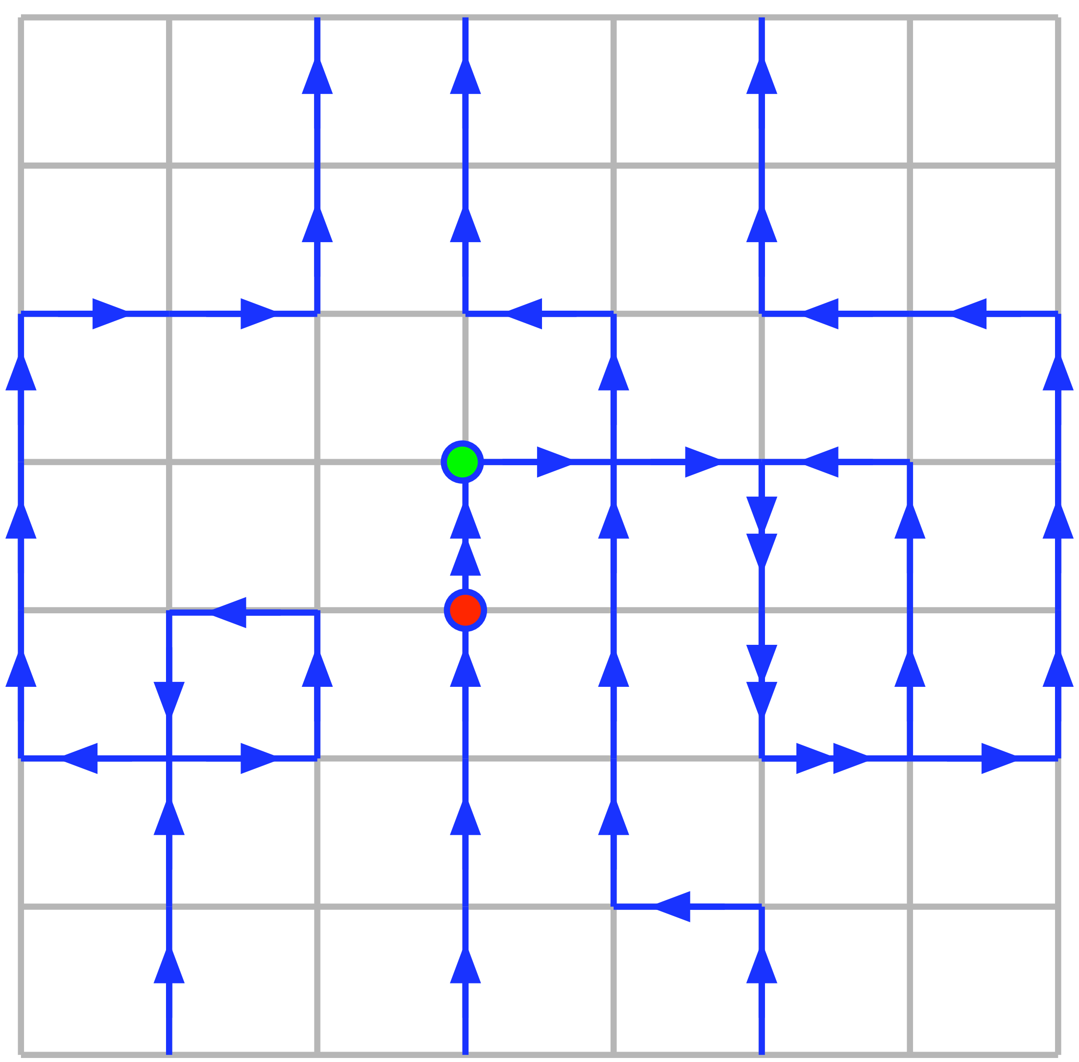
Worm Algorithm



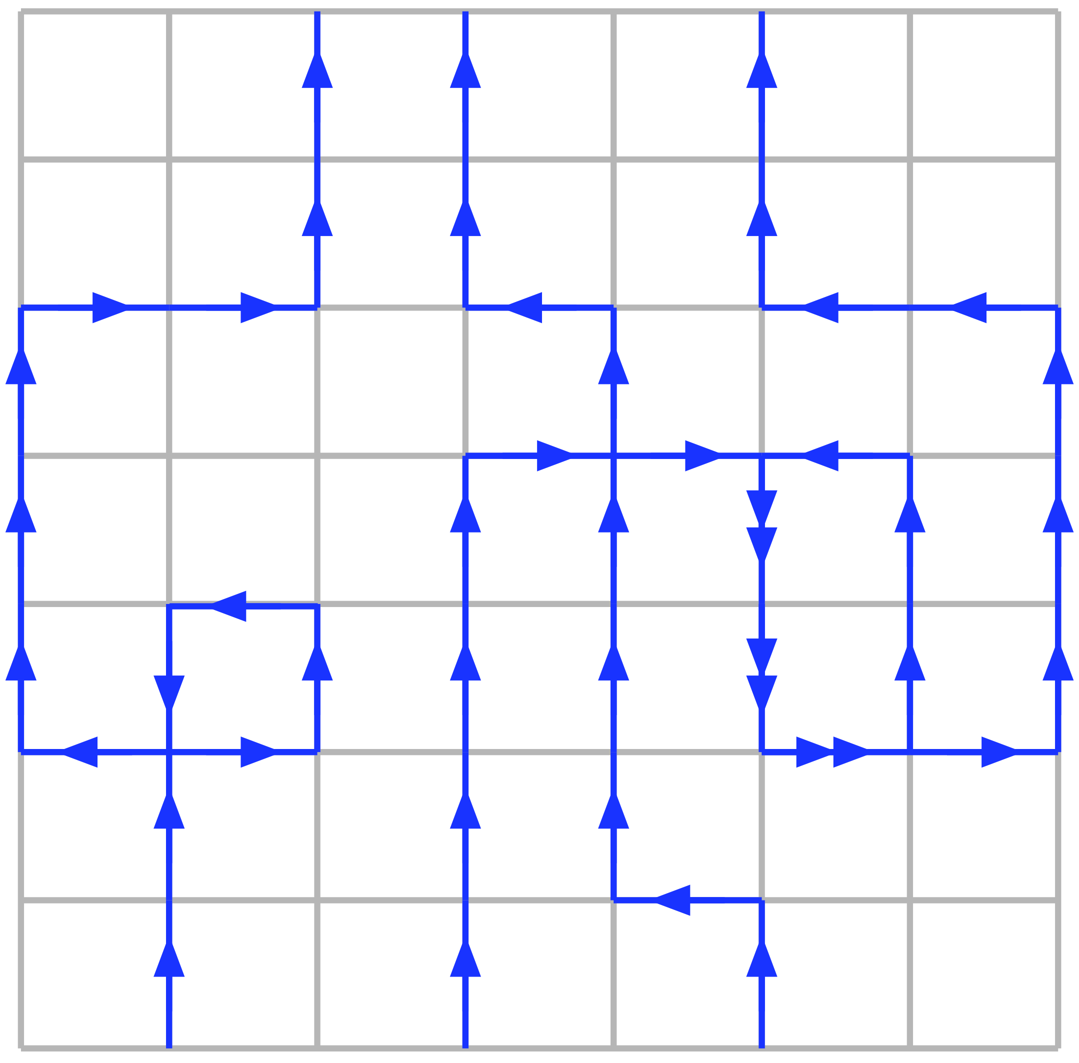
Worm Algorithm



Worm Algorithm



Worm Algorithm



Many applications to bosonic lattice field theories!

Application to variety of lattice field theory models

A New computational approach to lattice quantum field theories
SC, PoS LATTICE2008 (2008) 003

Strong coupling expansion Monte Carlo,
Ulli Wolff, PoS LATTICE2010 (2010) 020

New developments for dual methods in lattice field theory at non-zero density
Christof Gattringer, PoS LATTICE2013 (2014) 002

Continues to be interesting even today:

Dual lattice representations for O(N) and CP(N−1) models with a chemical potential
Falk Bruckmann, Christof Gattringer, Thomas Kloiber, Tin Sulejmanpasic.
Phys.Lett. B749 (2015) 495-501

Grand Canonical Ensembles, Multiparticle Wave Functions, Scattering Data, and Lattice Field Theories
Falk Bruckmann , Christof Gattringer, Thomas Kloiber, Tin Sulejmanpasic S
Phys.Rev.Lett. 115 (2015) no.23, 231601

What about fermions?

Fermions and Grassmann Variables

Partition function

$$Z = Tr\left(e^{-H/T}\right) = \int [d\overline{\psi}\ d\psi]\ e^{-S(\overline{\psi},\psi)}$$

How to deal with Grassmann integration in Monte Carlo?

Grassmann variables $\Rightarrow$ Fermion Worldlines

Grassmann Integration $\Rightarrow$ Sum over fermion worldlines

Grassmann Calculus

Anti commutation $\psi_1\psi_2 = -\psi_2\psi_1 \longrightarrow \psi_1^2 = 0$

Integration rules $\int d\psi_1 \; \psi_1 = 1$ $\int d\psi_1 = 0$

$$\int d\psi_1 d\psi_2 \; \psi_1\psi_2 = -1$$

$$\int [d\overline{\psi}_1 \; d\psi_1][d\overline{\psi}_2 \; d\psi_2]...[d\overline{\psi}_k \; d\psi_k] = \mathrm{e}^{-\overline{\psi}_i M_{ij}\psi_j} = \mathrm{Det}(M)$$

Determinant

$$\int [d\psi_1] \; [d\psi_2][d\psi_3]...[d\psi_k] \; \mathrm{e}^{-\frac{1}{2}\psi_i M_{ij}\psi_j} = \mathrm{Pf}(M)$$

Pfaffian

worldline interpretation: free fermions

Action: $$S_0(\overline{\psi},\psi) \;=\; \sum_{x,y} \overline{\psi}_x M_{xy} \psi_y$$

$$e^{-S_0(\overline{\psi},\psi)} \;=\; \prod_{(x,y)} e^{M_{xy}\psi_y\overline{\psi}_x} = (1 + M_{xy}\psi_y\overline{\psi}_x)$$

$$= \prod_{(x,y)} \left(\overset{y}{\bullet} \qquad \overset{x}{\bullet} \;+\; \overset{y}{\bullet}\xrightarrow{\;M_{xy}\;}\overset{x}{\bullet} \right)$$

partition function = sum over world line configurations

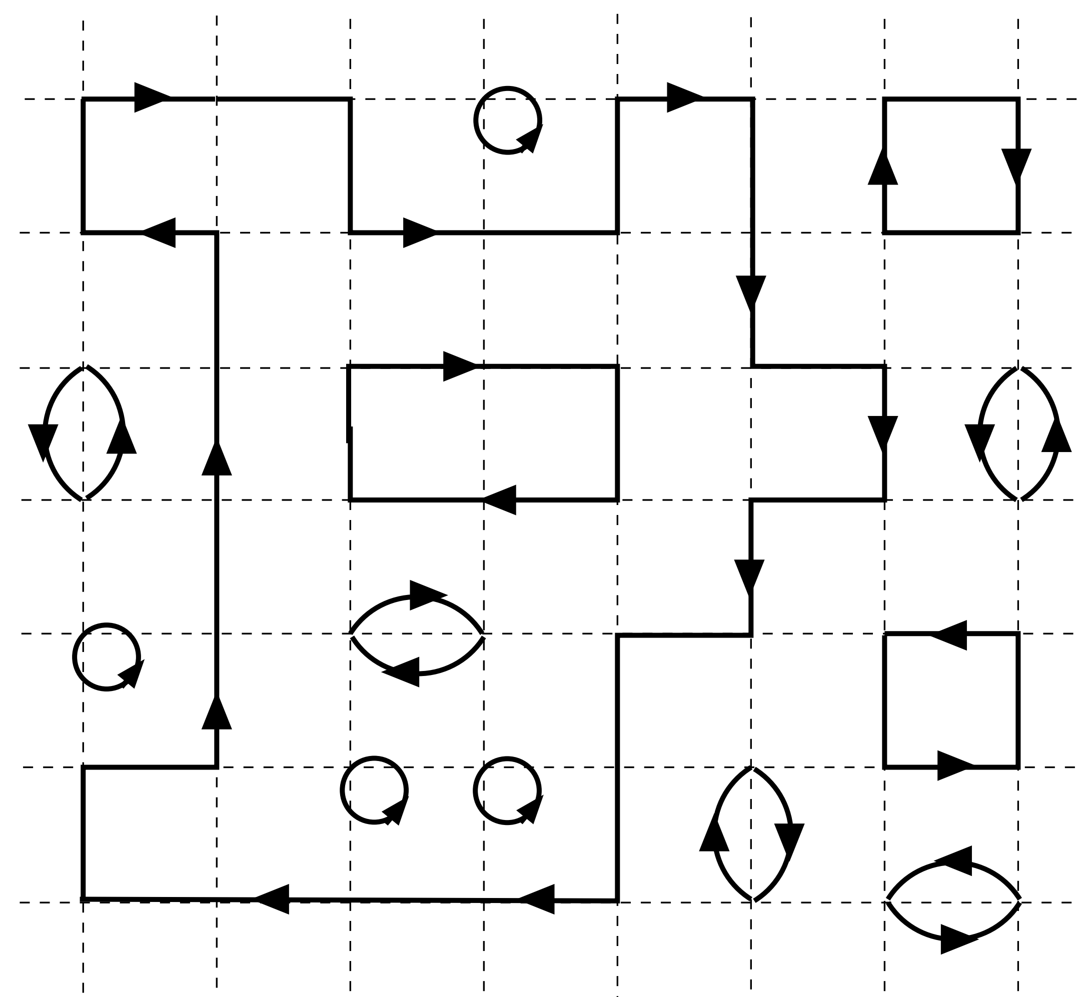
$$\int [d\overline{\psi}d\psi]\; e^{-S_0(\overline{\psi},\psi)} \;=\; \int [d\overline{\psi}d\psi] \prod_{(x,y)} \left(\overset{y}{\bullet} \qquad \overset{x}{\bullet} \;+\; \overset{y}{\bullet}\xrightarrow{\;M_{xy}\;}\overset{x}{\bullet} \right)$$

Every site has
one incoming and
one outgoing line

Every loop leads to a
negative sign

Every line has
local weights
that can be positive
or negative

An example of a fermion
world line configuration
with local hopping terms



Free "Dirac" fermions

$$Z = \int [d\overline{\psi}\; d\psi] e^{-\overline{\psi}\; M\; \psi} = \sum_{[C]} \mathrm{Sign(C)} W(C) = \mathrm{Det}(M)$$

Free "Majorana" fermions

$$Z = \int [d\psi]\; \mathrm{e}^{-\frac{1}{2}\; \psi^T M \psi} = \sum_{[d]} \mathrm{Sign}(d)\; W([d]) = \mathrm{Pf}(M)$$

Determinants and Pfaffians of a matrix can be interpreted as a sum over fermion world line configurations or vice versa

What about interacting fermions?

Lattice Thirring Model

Action

$$S = \sum_{x,\alpha} \left\{ \frac{1}{2}\eta_{x,\alpha}\left(\overline{\psi}_x \psi_{x+\alpha} - \overline{\psi}_{x+\alpha}\psi_x\right) + U\, \overline{\psi}_x \psi_{x+\alpha}\overline{\psi}_{x+\alpha}\psi_x \right\}$$

Free part describes massless staggered fermions

$$S_0 = \sum_{x,\alpha} \left\{ \frac{1}{2}\eta_{x,\alpha}\left(\overline{\psi}_x \psi_{x+\alpha} - \overline{\psi}_{x+\alpha}\psi_x\right) \right\} = \sum_{x,y} \overline{\psi}_x M_{xy} \psi_y$$

M is anti-symmetric $M = \begin{array}{cc} & \begin{array}{cc} \text{even} & \text{odd} \end{array} \\ & \left(\begin{array}{cc} 0 & A \\ -A^T & 0 \end{array} \right) \begin{array}{c} \text{even} \\ \text{odd} \end{array} \end{array}$

Traditional Approach: Auxiliary field method

$$e^{-U\,\overline{\psi}_x\psi_y\overline{\psi}_y\psi_x} = \frac{1}{2}\sum_{\sigma_{xy}=\pm 1} e^{\sigma_{xy}\overline{\psi}_x\psi_y - \sigma_{xy}\overline{\psi}_y\psi_x}$$

$$\begin{aligned} Z &= \int [d\overline{\psi}\; d\psi]\; e^{-S_0(\overline{\psi},\psi) - U\sum_{xy}\overline{\psi}_x\psi_y\overline{\psi}_y\psi_x} \\ &= \sum_{[\sigma]}\int [d\overline{\psi}\; d\psi]\; e^{-S_0(\overline{\psi},\psi) + U\sum_{xy}(\sigma_{xy}\overline{\psi}_x\psi_y - \sigma_{xy}\overline{\psi}_y\psi_x)} \\ &= \sum_{[\sigma]} \mathrm{Det}\big(\tilde{M}([\sigma])\big) \end{aligned}$$

$$\tilde{M}_{xy} = M_{xy} + \sigma_{xy}$$

no sign problem

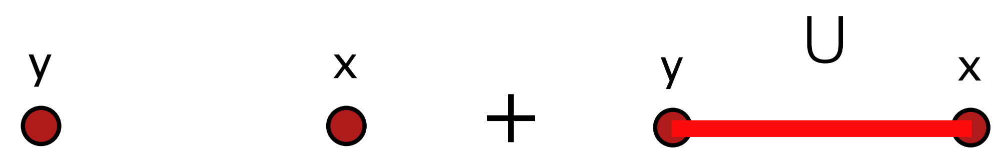
V x V anti-symmetric matrix

Diagrammatic Method (fermion bag approach)

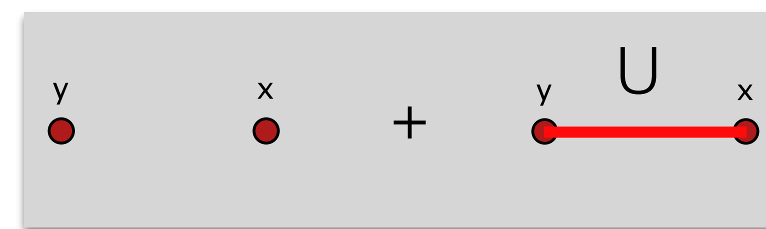
SC. Phys.Rev. D82 (2010) 025007

$$e^{-\ U\ \overline{\psi}_x \psi_y \overline{\psi}_y \psi_x} \ = \ 1 \ - \ U\ \overline{\psi}_x \psi_y \overline{\psi}_y \psi_x$$

=



$$Z \ = \ \int [d\overline{\psi}\ d\psi]\ e^{-S_0(\overline{\psi},\psi) - U \sum_{xy} \overline{\psi}_x \psi_y \overline{\psi}_y \psi_x}$$



$$= \ \int [d\overline{\psi}\ d\psi]\ e^{-S_0(\overline{\psi},\psi)} \prod_{(xy)} \left(1 \ - \ U\ \overline{\psi}_x \psi_y \overline{\psi}_y \psi_x\right)$$

$$= \sum_{[d]} \int [d\overline{\psi}\ d\psi]\ e^{-S_0(\overline{\psi},\psi)}\ U^{N_D} \prod_{(xy)} \left(-\overline{\psi}_x \psi_y \overline{\psi}_y \psi_x\right)^{d_{xy}}$$

$$d_{xy} = 0, 1$$

dimer field

$$Z = \sum_{[d]} U^{N_D} \int [d\overline{\psi}\ d\psi]\ e^{-S_0(\overline{\psi},\psi)}\ (-\overline{\psi}_{x_1}\psi_{y_1}\overline{\psi}_{y_1}\psi_{x_1})\ldots(-\overline{\psi}_{x_k}\psi_{y_k}\overline{\psi}_{y_k}\psi_{x_k})$$

Integrate over dimer
Grassmann variables first

$$Z = \sum_{[d]} U^{N_d} \prod_{\text{Bags}} \text{Det}(W_{\text{Bag}})$$

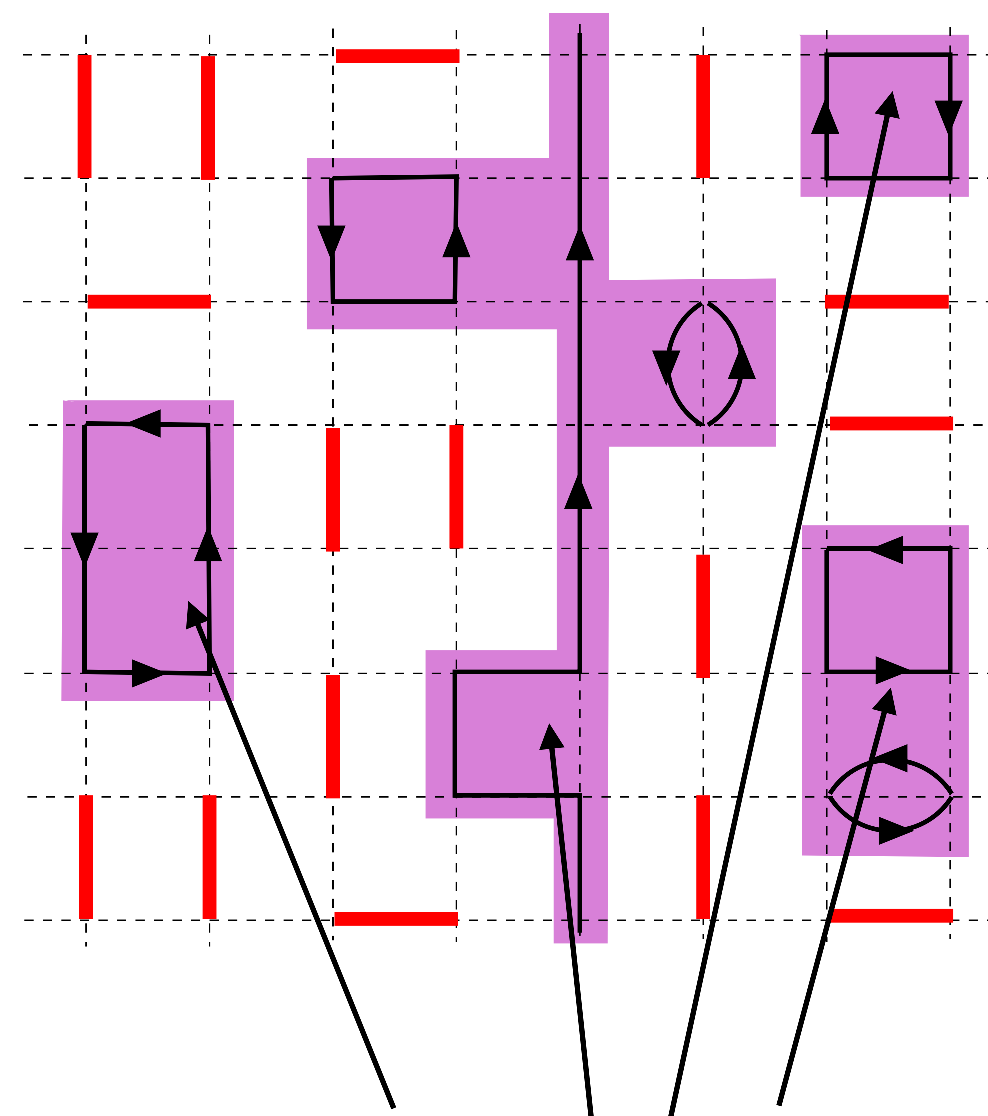
$$W_{\text{Bag}} = \begin{pmatrix} 0 & A_{\text{Bag}} \\ -A^T_{\text{Bag}} & 0 \end{pmatrix}$$

(V-2k) x (V-2k) matrix

$$\text{Det}(W_{\text{Bag}}) \geq 0$$

At strong couplings
free fermion bags
are small!

dimer configuration



free fermion bags

$$Z = \sum_{[d]} U^{N_D} \int [d\overline{\psi}\ d\psi]\ \mathrm{e}^{-S_0(\overline{\psi},\psi)}\ (-\overline{\psi}_{x_1}\psi_{y_1}\overline{\psi}_{y_1}\psi_{x_1})\ldots(-\overline{\psi}_{x_k}\psi_{y_k}\overline{\psi}_{y_k}\psi_{x_k})$$

Use Wick's theorem
to compute the 2k point correlation function

$$Z = \sum_{[d]} U^{N_D}\ \mathrm{Det}(M)\ \mathrm{Det}(G_{\mathrm{prop}})$$

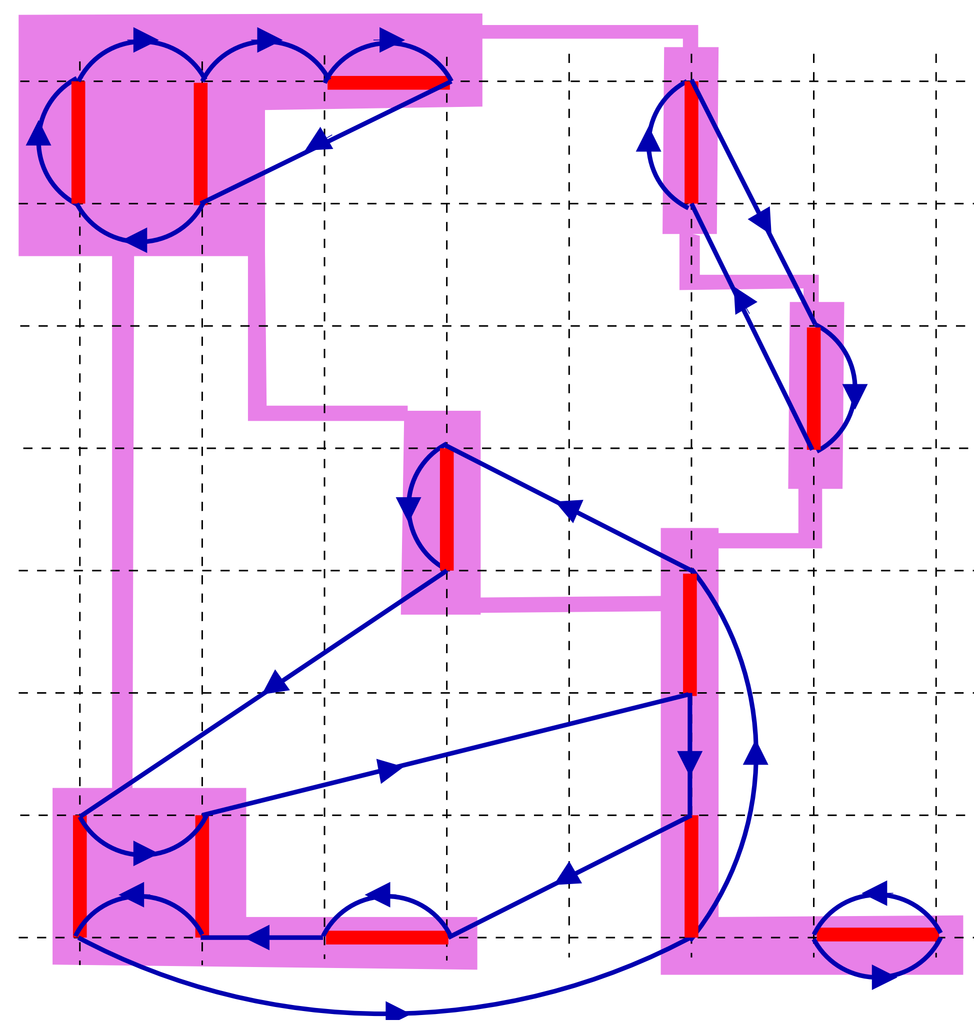
$$G_{\mathrm{prop}} = \begin{pmatrix} 0 & P \\ -P^T & 0 \end{pmatrix}$$

2k x 2k matrix

$$\mathrm{Det}(G_{\mathrm{prop}}) \geq 0$$

At weak couplings
k will be small

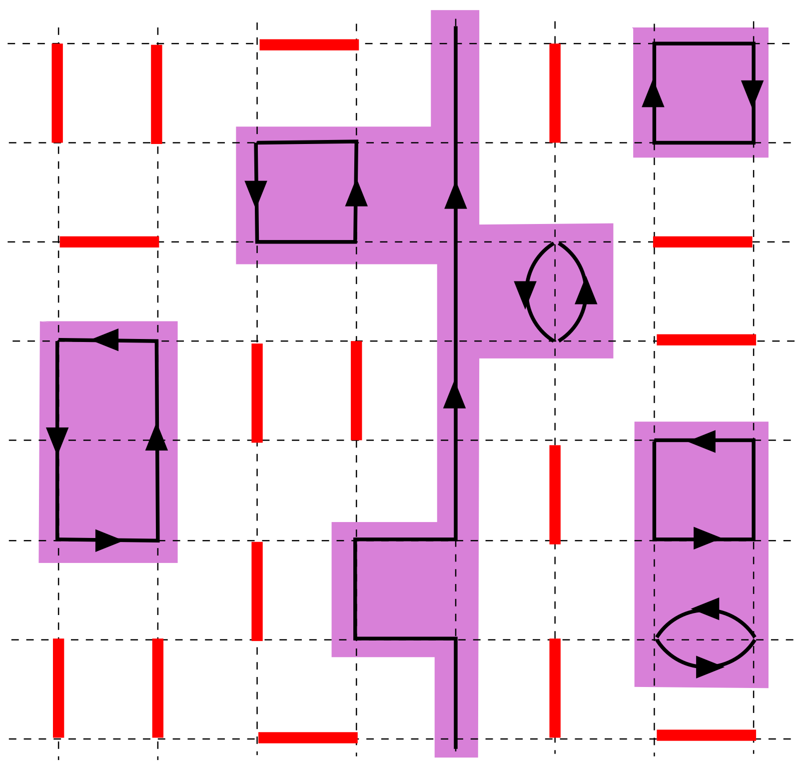
Feynman Diagram Configuration



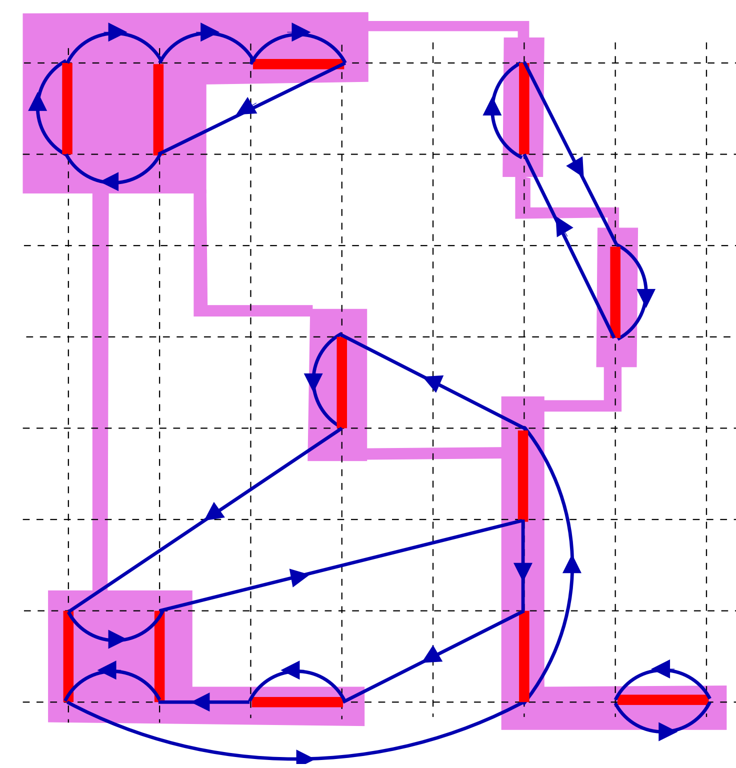
Duality: Weak Coupling versus Strong Coupling

$$Z = \sum_{[d]} U^{N_D} \int [d\overline{\psi}\ d\psi]\ \mathrm{e}^{-S_0(\overline{\psi},\psi)}\ (-\overline{\psi}_{x_1}\psi_{y_1}\overline{\psi}_{y_1}\psi_{x_1})\ldots(-\overline{\psi}_{x_k}\psi_{y_k}\overline{\psi}_{y_k}\psi_{x_k})$$

strong coupling



weak coupling



$$Z = \sum_{[d]} U^{N_d} \prod_{\mathrm{Bags}} \mathrm{Det}(W_{\mathrm{Bag}})$$

$$Z = \sum_{[d]} U^{N_D}\ \mathrm{Det}(M)\ \mathrm{Det}(G_{\mathrm{prop}})$$

A Lattice Yukawa Model

SC, PRD 86, (2012) 021701

Action

$$S \;=\; \sum_{x,y} \overline{\psi}_x \; M_{xy} \; \psi_y \;-\; g e^{i\varepsilon_x \theta_x} \overline{\psi}_x \psi_x \;-\; \beta \sum_{x,\alpha} \cos(\theta_{x+\alpha} - \theta_x)$$

M_{xy} is the massless fermions we discussed earlier.

$\varepsilon_x = (-1)^{x_1 + x_2 + \ldots + x_d}$

xy-model

$$S \;=\; \sum_{x,y} \overline{\psi}_x \; D_{xy}([\theta]) \; \psi_y \;-\; \beta \sum_{x,\alpha} \cos(\theta_{x+\alpha} - \theta_x)$$

$$D_{xy}([\theta]) \;=\; M_{xy} - g e^{i\varepsilon_x \theta_x} \delta_{xy}$$

Partition function

$$Z = \int [d\theta] \prod_{x,\alpha} e^{\beta \cos(\theta_{x+\alpha} - \theta_x)} \int [d\overline{\psi}\ d\psi]\ e^{-\overline{\psi}\ D([\theta])\ \psi}$$

$$D_{xy}([\theta]) = M_{xy} - g e^{i\varepsilon_x \theta_x} \delta_{xy}$$

Traditional approach

$$Z = \int [d\theta] \prod_{x,\alpha} e^{\beta \cos(\theta_{x+\alpha} - \theta_x)}\ \mathrm{Det}\Big(D([\theta]) \Big)$$

complex!

Diagrammatic method offers a solution!

Diagrammatic Approach

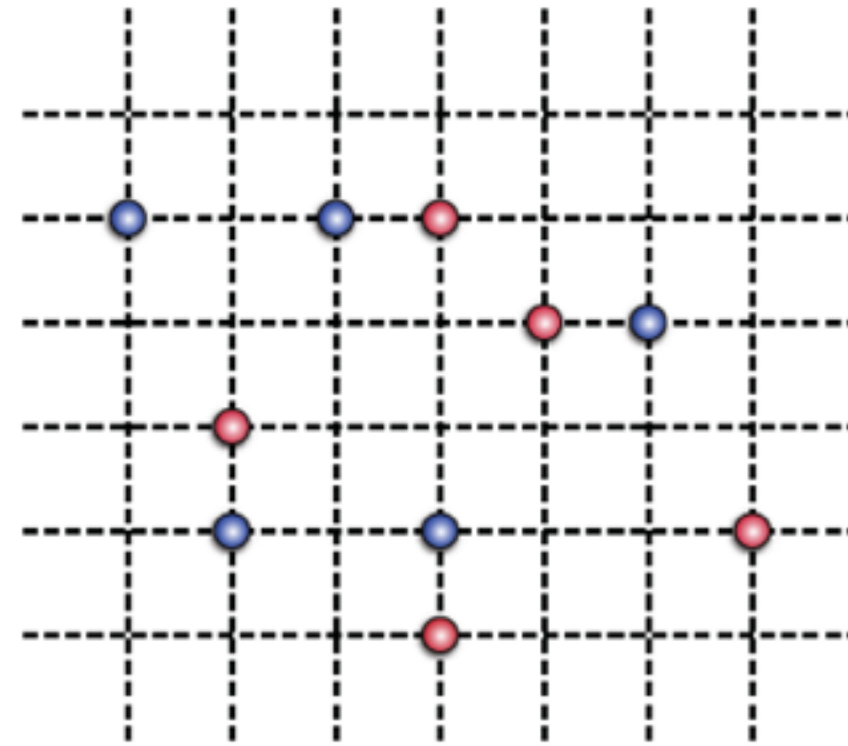
$$Z = \int [d\theta] \prod_{x,\alpha} \left(e^{\beta \cos(\theta_{x+\alpha} - \theta_x)} \right) \int [d\overline{\psi}\, d\psi]\, e^{-\overline{\psi}\ M\ \psi} \prod_{x} \left(e^{g e^{i\varepsilon_x \theta_x} \overline{\psi}_x \psi_x} \right)$$

$$e^{g e^{i\varepsilon_x \theta_x} \overline{\psi}_x \psi_x} = \left(1 + g e^{i\varepsilon_x \theta_x} \overline{\psi}_x \psi_x \right) = \sum_{n_x = 0,1} \left(g e^{i\varepsilon_x \theta_x} \overline{\psi}_x \psi_x \right)^{n_x}$$

$$Z = \sum_{[n]} \int [d\theta] \prod_{x,\alpha} \left(e^{\beta \cos(\theta_{x+\alpha} - \theta_x)} \right) \int [d\overline{\psi}\, d\psi]\, e^{-\overline{\psi}\ M\ \psi} \prod_{x} \left(g e^{i\varepsilon_x \theta_x} \overline{\psi}_x \psi_x \right)^{n_x}$$

monomer field

example of a monomer configuration



For a given configuration [n] let z_1 z_2 ... z_k be the k sites where n_x = 1 at all other sites n_x = 0.

$$Z = \sum_k g^k \int [d\theta] \left(\prod_{x,\alpha} e^{\beta \cos(\theta_{x+\alpha} - \theta_x)} \; e^{i\varepsilon_{z_1}\theta_{z_1}} \; e^{i\varepsilon_{z_2}\theta_{z_2}} \ldots e^{i\varepsilon_{z_k}\theta_{z_k}} \right)$$

$$\int [d\overline{\psi} \; d\psi] \; e^{-\overline{\psi} \; M \; \psi} \; \overline{\psi}_{z_1} \; \psi_{z_1} \ldots \overline{\psi}_{z_k} \; \psi_{z_k}$$

Bosonic term
(k-point correlation function)

Fermionic term
(k-point correlation function)

fermionic k-point correlation function

(strong coupling view point)

$$\int [d\overline{\psi}\ d\psi]\ e^{-\overline{\psi}\ M\ \psi}\ \overline{\psi}_{z_1}\ \psi_{z_1} \ldots \overline{\psi}_{z_k}\ \psi_{z_k}$$

integrate over monomers first

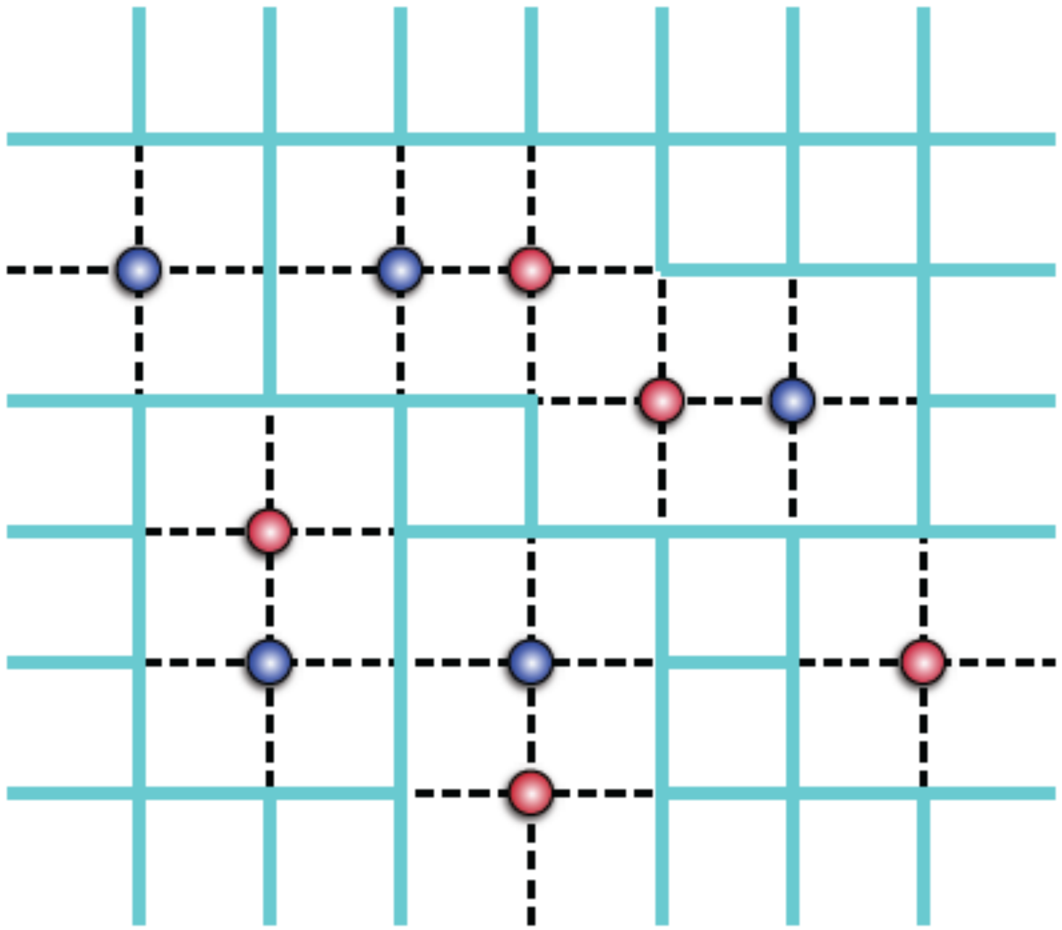
$$= \ \mathrm{Det}(W[n])$$

(V-k) x (V-k) matrix
obtained by dropping sites
z_1 ... z_k in M

$$W([n]) \ = \ \begin{pmatrix} 0 & A \\ -A^T & 0 \end{pmatrix}$$

$$\mathrm{Det}(W[n]) \ \geq 0$$

monomer configuration



fermionic k-point correlation function

(weak coupling view point)

$$\int [d\overline{\psi}\ d\psi]\ \mathrm{e}^{-\overline{\psi}\ M\ \psi}\ \overline{\psi}_{z_1}\ \psi_{z_1} \ldots \overline{\psi}_{z_k}\ \psi_{z_k}$$

Use Wick's theorem
(Feynman diagrams)

$$= \ \mathrm{Det}(M)\ \mathrm{Det}(G_{\mathrm{prop}}([n]))$$

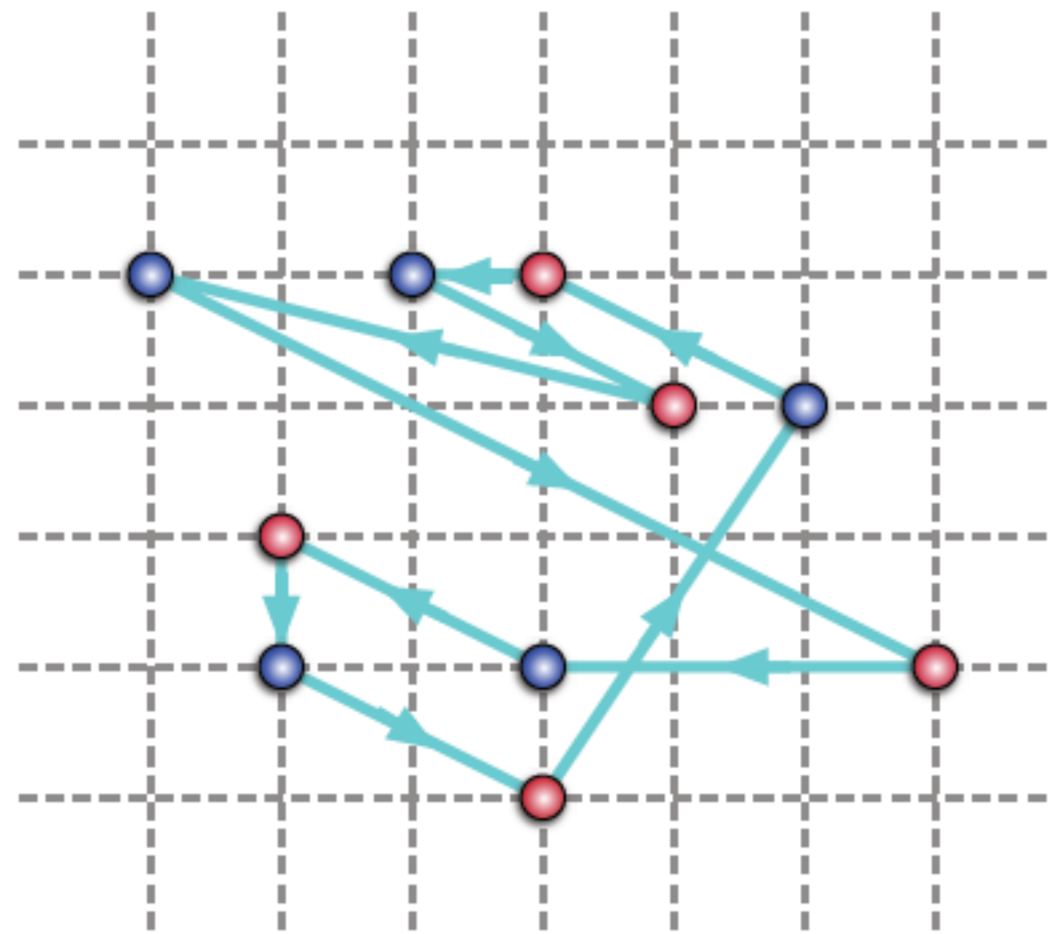
(k x k) matrix of propagators

$$\mathrm{Det}(W([n])) \ = \ \mathrm{Det}(M)\ \mathrm{Det}(G([n]))$$

strong coupling

weak coupling

monomer configuration

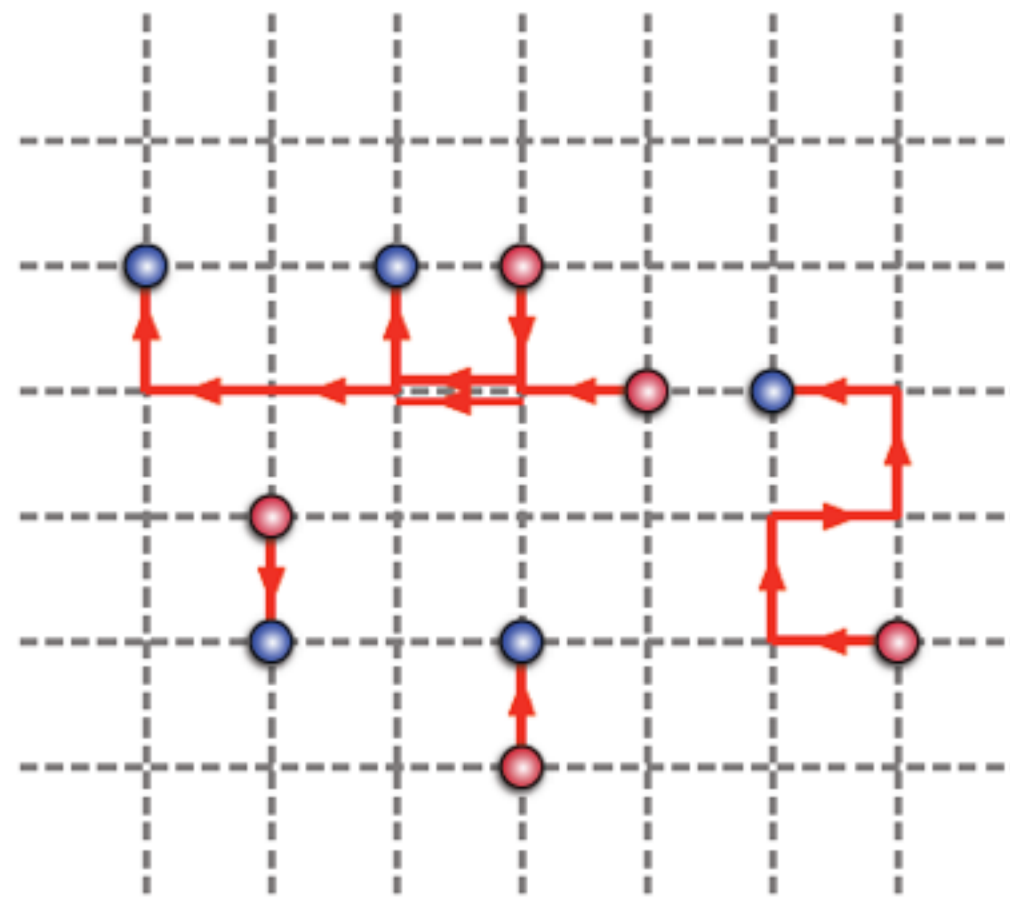


bosonic k-point correlation function

$$\int [d\theta] \left(\prod_{x,\alpha} e^{\beta \cos(\theta_{x+\alpha} - \theta_x)} \right. \left. e^{i\varepsilon_{z_1}\theta_{z_1}} \; e^{i\varepsilon_{z_2}\theta_{z_2}} \ldots e^{i\varepsilon_{z_k}\theta_{z_k}} \right)$$

$$= \sum_{[q]} \left(\prod_{x,\alpha} I_{k_{x,\alpha}}(\beta/2) \right) \left\{ \prod_x \delta\left(\varepsilon_x n_x + \sum_\alpha (q_{x,\alpha} - q_{x-\alpha,\alpha}) \right) \right\}$$

example of a [q] configuration consistent with [n]

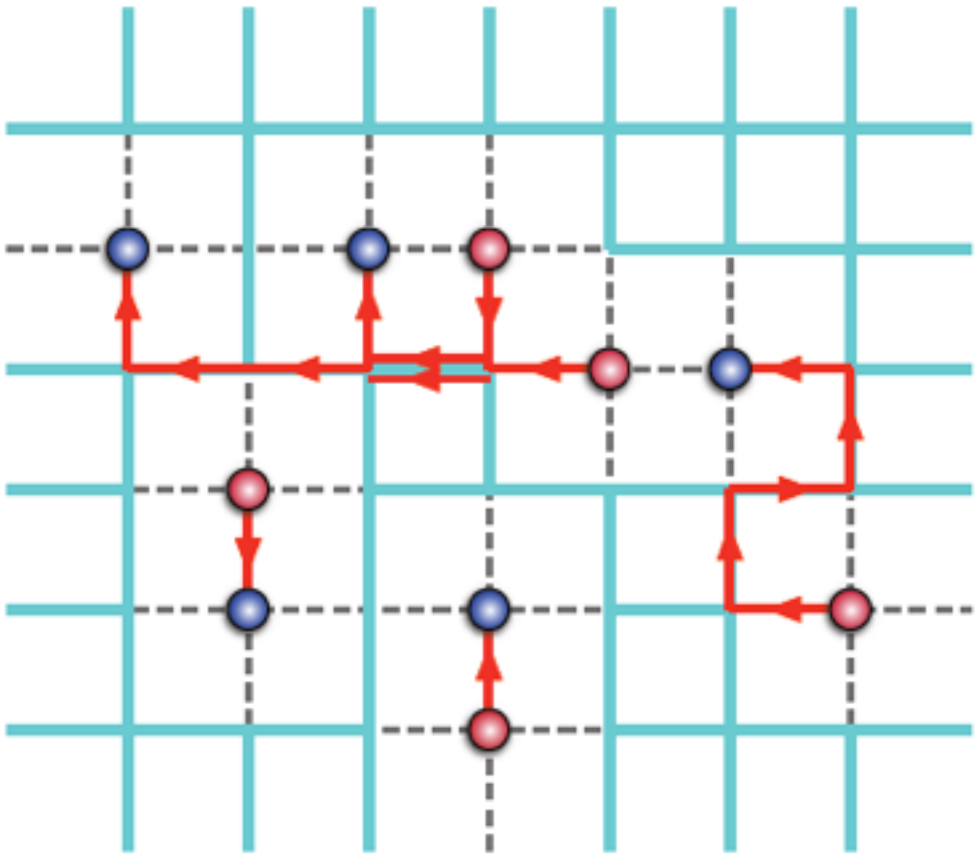


Final partition function of the lattice Yukawa model

$$Z = \sum_{[n],[q]} g^k \prod_{x,\alpha} I_{k_{x,\alpha}}(\beta/2)\, \mathrm{Det}(W([n])) \left\{ \prod_x \delta\Big(\varepsilon_x n_x + \sum_\alpha (q_{x,\alpha} - q_{x-\alpha,\alpha})\Big) \right\}$$

Sign problem solved!

[n,q] configurations



Other applications of diagrammatic ideas:

Many applications in the Hamiltonian formulation, used in CM physics.

Continuous-time Monte Carlo methods for quantum impurity models
Emanuel Gull, Andrew J. Millis, Alexander I. Lichtenstein, Alexey N. Rubtsov, Matthias Troyer, and Philipp Werner
Rev. Mod. Phys. 83, 349 (2011).

Application in infinite volume by computing “one-particle irreducible” vertices

Bold Diagrammatic Monte Carlo Technique: When the Sign Problem Is Welcome
Nikolay Prokof’ev and Boris Svistunov, Phys. Rev. Lett. 99, 250201 (2007).

Applications in real time are also being explored.

Taming the Dynamical Sign Problem in Real-Time Evolution of Quantum Many-Body Problems
Guy Cohen, Emanuel Gull, David R. Reichman, and Andrew J. Millis
Phys. Rev. Lett. 115, 266802

We are currently exploring application in nuclear physics.