The Sign problem and Computational Complexity of Quantum Many Body Systems

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January 30, 2018

Supported by:
US Department of Energy, Nuclear Physics Division

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Introduction

Observables in quantum many body physics: $\langle O \rangle = \frac{Z_O}{Z}$

$$Z = \sum_{\mathcal{C}} W(\mathcal{C})) \qquad Z_O = \sum_{\mathcal{C}} O(\mathcal{C})\, W(\mathcal{C})$$

The configuration space $\mathcal{C}$ is exponetially large in system size V

Real time problems: $W(\mathcal{C}) \sim \exp\left(iS(\mathcal{C})\right)$

Imaginary time problems: $W(\mathcal{C}) \sim \exp\left(-S(\mathcal{C})\right)$

The "action" $S(\mathcal{C})$ can be complex in general, and scales with system size.

Quantum many body problems are computationally difficult in general!

Sign Problem: Definition

Consider computing the observable $\langle O \rangle = \dfrac{\sum_{\mathcal{C}} O(\mathcal{C})\ W(\mathcal{C})}{\sum_{\mathcal{C}} W(\mathcal{C})}$

Result: $\langle O \rangle \approx O_\varepsilon \qquad \delta\langle O \rangle \sim \varepsilon$

Time to answer: $\tau_{\mathrm{ans}} \sim \dfrac{V^\omega}{\varepsilon^{\omega'}}$ no sign problem!

Otherwise the observable suffers from a sign problem!

$$\tau_{\mathrm{ans}} \sim \exp\left(A\ V^\omega\right)\ \exp\left(\frac{B}{\varepsilon^{\omega'}}\right)$$

Practically we want not only to solve the sign problem but also have small values for the powers $\omega,\ \omega'$

Challenge: Solve sign problems!

Analytic methods: Perturbation expansion, resurgence theory,….

Monte Carlo Methods: $$\langle O \rangle = \frac{\sum_{\mathcal{C}} O(\mathcal{C})\ W(\mathcal{C})}{\sum_{\mathcal{C}} W(\mathcal{C})}$$

If the "Boltzmann weight" is $W(\mathcal{C}) \geq 0$ and computable in polynomial time, then can use Monte Carlo important sampling method.

Monte Carlo Result: $$\langle O \rangle \approx \frac{1}{N} \sum_{i=1}^{N} O(\mathcal{C}_i)$$

For efficient algorithms $N \sim \dfrac{1}{\varepsilon^2}$

(not guaranteed for generic algorithms!)

In efficiencies in algorithms come from two sources:

A. Autocorrelation times:

The formula $\langle O \rangle \approx \frac{1}{N} \sum_{i=1}^{N} O(\mathcal{C}_i)$ assumes that we have

"N" de-correlated equilibrium Monte Carlo samples.
The algorithm may take a "long time" to produce them.

B. There can be a very bad signal to noise ratio.

For example $\langle O \rangle \sim \exp(-Mt), \qquad O(\mathcal{C}_i) \sim e^{i\varphi},$

In this case the sign problem is back through the observable!

Such problems can sometimes be tackled through "multi-level" algorithms.

Luscher, Weisz (2001)

For quantum many body problems it is more common that

$W(\mathcal{C})$ is negative or complex!

Then the Monte Carlo method is not even applicable "naively"!

A. In real time this is obvious.

$$W(\mathcal{C}) \sim \exp\left(iS(\mathcal{C})\right)$$

B. In imaginary time also, many interesting problems have complex action!

$$W(\mathcal{C}) \sim \exp\left(-S(\mathcal{C})\right)$$

We will learn more about the origin of this problem.

This leads to the so called computational complexity of quantum many body problem.

What can we do?

Consider $\langle O \rangle = \dfrac{\sum_{\mathcal{C}} \; O(\mathcal{C}) \; W(\mathcal{C})}{\sum_{\mathcal{C}} \; W(\mathcal{C})}$

This representation is NOT unique! (room for creativity!)

A. Find a representation where $W(\mathcal{C}) \geq 0$ and computable in polynomial time.

Technically this first step itself can be called a solution to the sign problem!

B. Find an efficient Monte Carlo algorithm to compute the observable.

Origin of the Sign Problems and Solutions

Example 1

Consider quantum mechanics of a charge Q and its conjugate angle variable θ.

Operators:

$$\hat{Q} \qquad \hat{\Phi} = e^{i\hat{\theta}} \qquad \hat{\Phi}^{\dagger} = e^{-i\hat{\theta}}$$

$$[Q, \Phi] \ = \ \Phi, \quad [Q, \Phi^{\dagger}] \ = \ \Phi^{\dagger}$$

Two obvious basis states:

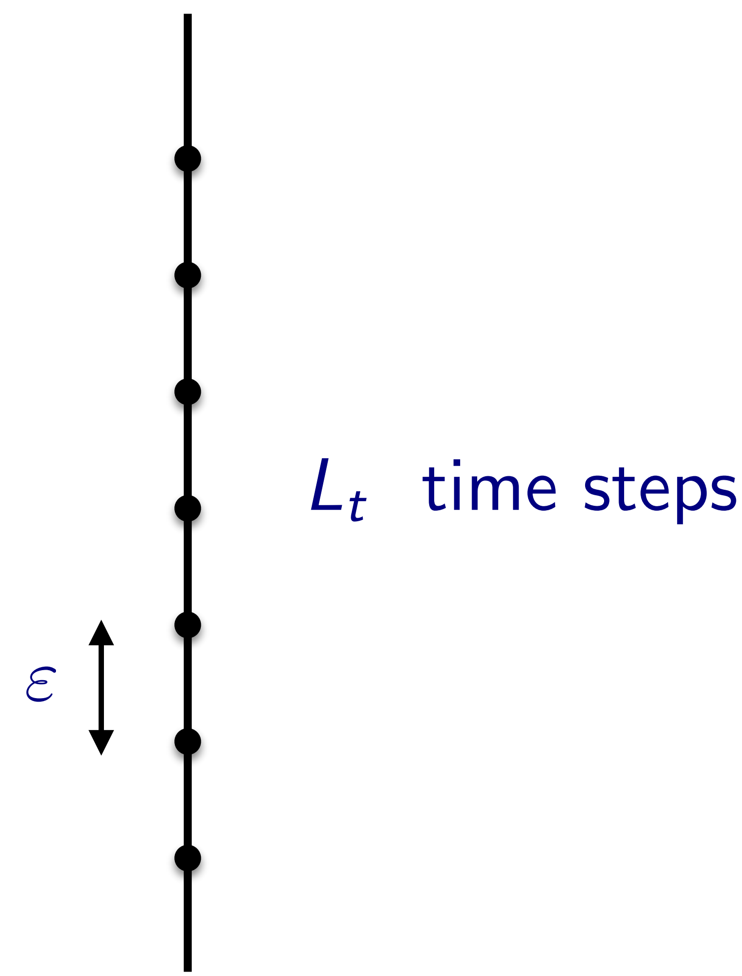
charge	phase
$Q \ \vert q\rangle \ = \ q \ \vert q\rangle,$	$\Phi\vert\theta\rangle \ = \ e^{i\theta} \ \vert\theta\rangle$
$q \ = \ ... -2, -1, 0, 1, 2, ...$	$-\pi < \theta \ \leq \ \pi$
$\langle q\vert q'\rangle \ = \ \delta_{q,q'}$	$\langle\theta\vert\theta'\rangle \ = \ \delta(\theta - \theta')$

Consider the lattice partition function $(\beta = L_t \, \varepsilon)$

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

Continuum limit:

$$\varepsilon \to 0$$
$$L_t \to \infty$$
$$L_t \, \varepsilon = \beta$$



H describes the energy of a charge

$$E_q \sim \lambda \, q^2$$

Let us we choose the lattice Hamiltonian such that

$$\mathrm{e}^{-\varepsilon H} \;=\; \sum_q \mathrm{e}^{-1/\lambda\varepsilon}\,\sqrt{\frac{2\pi}{\lambda\varepsilon}}\,I_q\Big(\frac{1}{\lambda\varepsilon}\Big)\;|q\rangle\langle q|$$

This gives
$$\lim_{\varepsilon\to 0}\;H \;=\frac{1}{2}\Big(\lambda q^2\;-\frac{\lambda}{4}\Big)|q\rangle\langle q|$$

Let us construct the partition function in the charge basis

$$Z \;=\; \sum_q\; W(q)$$

where we see that
$$W(q)\;=\;\left(\mathrm{e}^{-1/\lambda\varepsilon}\,\sqrt{\frac{2\pi}{\lambda\varepsilon}}\,I_q\Big(\frac{1}{\lambda\varepsilon}\Big)\right)^M \;>\; 0$$

The sign problem is absent!

Consider now the partition function in the phase basis!

$$Z \;=\; \int \left[d\theta_0 \; d\theta_2 ... d\theta_{L_t-1}\right] \langle\theta_0|\mathrm{e}^{-\varepsilon H}|\theta_{L_t-1}\rangle\langle\theta_{L_t-1}|...|\theta_2\rangle\langle\theta_2|\mathrm{e}^{-\varepsilon H}|\theta_0\rangle$$

Basis change

$$|q\rangle \;=\; \int \frac{d\theta}{\sqrt{2\pi}}\,\mathrm{e}^{iq\theta}\;|\theta\rangle\langle\theta| \qquad |\theta\rangle \;=\; \sum_q \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{-iq\theta}\;|q\rangle\langle q|$$

$$\langle\theta_{i+1}|\mathrm{e}^{-\varepsilon H}|\theta_i\rangle \;=\; \sum_q \langle\theta_{i+1}|\left(\mathrm{e}^{-1/\lambda\epsilon}\sqrt{\frac{2\pi}{\lambda\varepsilon}}\; I_q(\frac{1}{\lambda\varepsilon})\;|q\rangle\langle q|\right)\;|\theta_i\rangle$$

$$= \sqrt{\frac{1}{2\pi\lambda\varepsilon}}\,\mathrm{e}^{-1/\lambda\epsilon}\sum_q \; I_q(\frac{1}{\lambda\varepsilon})\;\mathrm{e}^{iq(\theta_{i+1}-\theta_i)}$$

$$= \sqrt{\frac{1}{2\pi\lambda\varepsilon}}\;\mathrm{e}^{\frac{1}{\lambda\varepsilon}\left(\cos(\theta_{i+1}-\theta_i)-1\right)}$$

No sign problem even in the phase basis!

Thus the temporal lattice partition function

$$Z = \int [d\theta]\, \mathrm{e}^{-S(\theta)} \qquad S(\theta) = \frac{1}{\lambda\varepsilon} \sum_i \left(\cos(\theta_{i+1} - \theta_i) - 1 \right)$$

XY model in 1d!

Consider the Grand canonical partition function!

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

charge basis

$$Z = \sum_q W(q)\, \mathrm{e}^{q\mu\beta}$$

no sign problem!

phase basis

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

$$S_\mu(\theta) = \frac{1}{\lambda\varepsilon} \sum_i \left(\cos(\theta_{i+1} - \theta_i - i\mu) - 1 \right)$$

sign problem at finite density!

Example 2

Consider two identical particles moving on a periodic lattice:

Fock space Hamiltonian:

$$H \;=\; \sum_i \left\{ \; c_i^\dagger c_i - \frac{1}{2}\left(c_i^\dagger c_{i+1} + c_j^\dagger c_{i-1}\right) \; \right\}$$

Two problems:

- Bosons (hard core) unique ground state
- Fermions doubly degenerate ground state

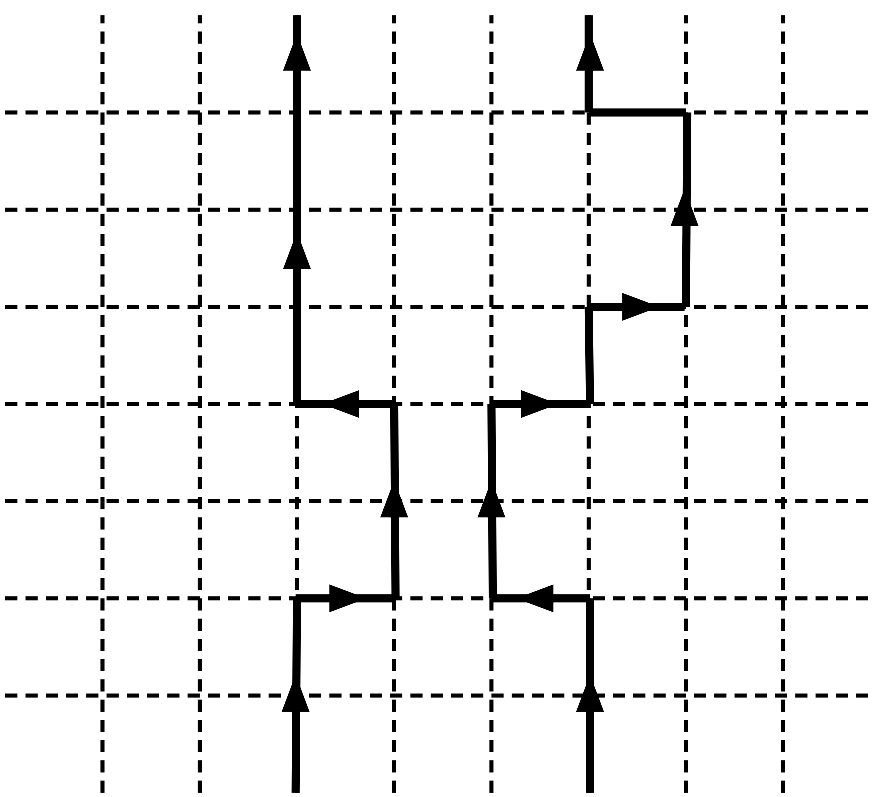
Feynman “world line path integral” can be easily constructed

$$Z \;=\; \mathrm{e}^{-\beta H} \;=\; \int \mathcal{D}(x_1(t)x_2(t))\; \mathrm{e}^{-S_E(x_1,x_2)}$$

Path integral almost entirely identical in the two cases!

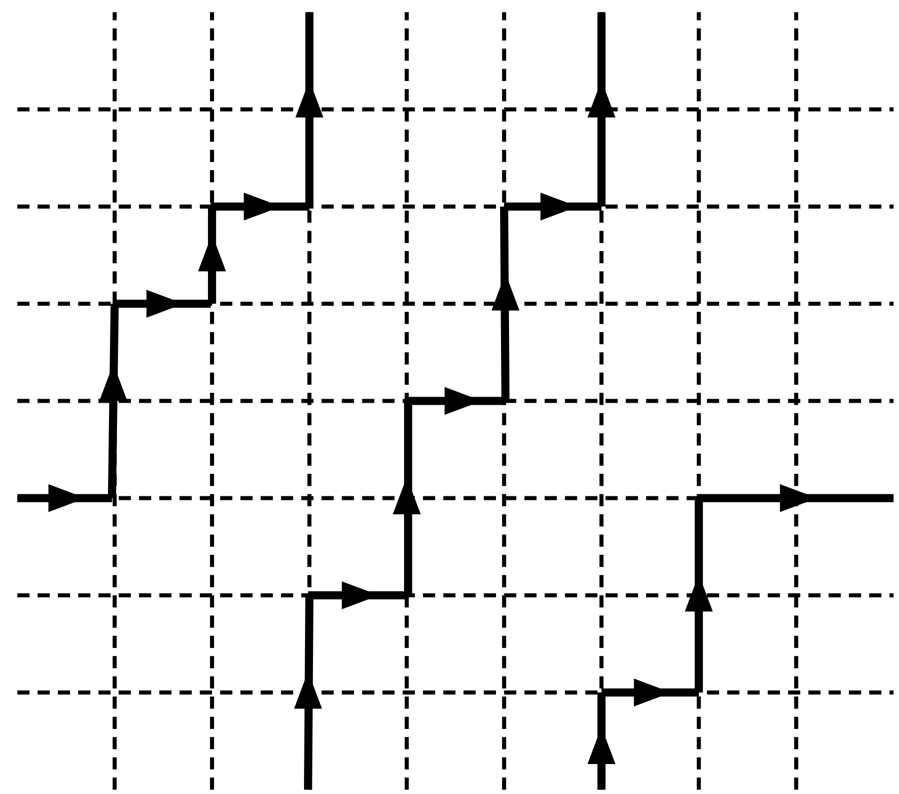
$$Z = e^{-\beta H} = \int \mathcal{D}(x_1(t)x_2(t))\ e^{-S_E(x_1,x_2)}$$

worldline configurations: self avoiding paths of equal weights



particles do not permute

positive weight



particles permute

fermion weight negative (Pauli principle)!

(Similar to a Berry phase!)

Fermion worldlines configurations can create new sign problems due to the Pauli principle!

In one dimensional systems this sign problem can "often" be solved!

A. Open boundary conditions (fermions = hard core bosons)

B. Change of basis, especially at the boundaries.

C. Other ideas like DMRG, Tensor Network States,…

Excellent toy models for testing new ideas.

Example: Lattice Thirring Model with a Chemical Potential
Leftshitz Thimble Approach: Alexandru, Basar, Bedaque,Ridgeway, Warrington, PRD95 (2017)
Worldline approach: Ayyar, Rantaharju, SC arXiv:1711.07898

Example: Mass Imbalanced System of Fermions in 1D
Complex Langevin: Ramellmuller, Porter, Drut, Braun, PRD96 (2017)
Worldline approach: Singh, SC (in progress)

How are Grassmann variables related to all this?

Grassmann variables encode fermion worldlines!

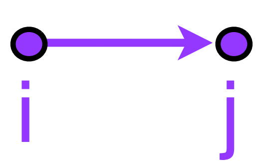
$$S_0 = -\sum_t \overline{\psi}_t \left(\psi_{t+1} - \psi_t\right)$$

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

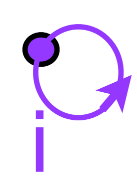
$$\mathrm{e}^{\overline{\psi}_t \psi_{t+1}} = 1 + \overline{\psi}_t \psi_{t+1}$$

$$\mathrm{e}^{-\overline{\psi}_t \psi_t} = 1 - \overline{\psi}_t \psi_t$$

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



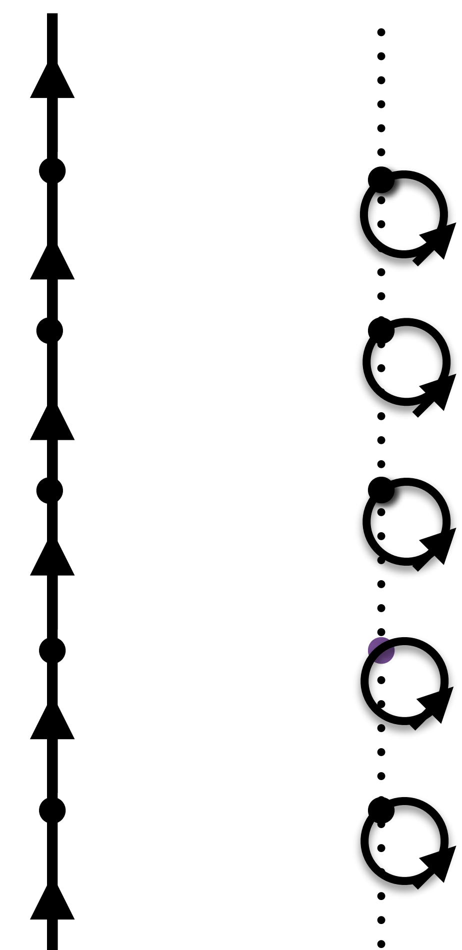
$\overline{\psi}_i \psi_i$ =



Single site example:

$$H = 0$$

$$Z = \mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right) = 2$$

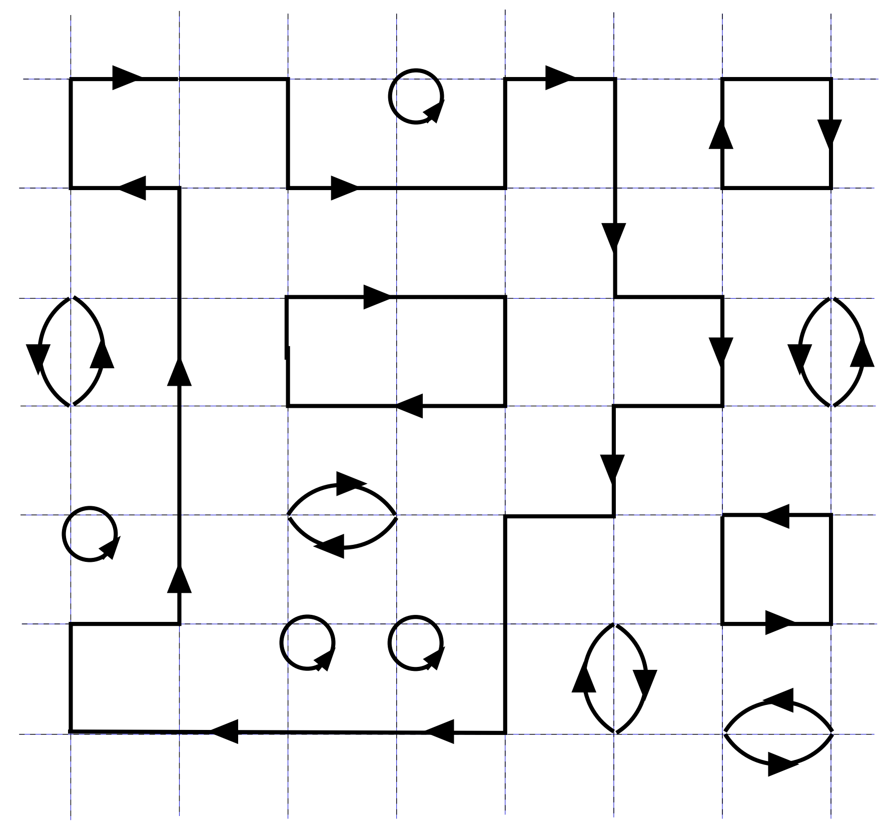


fermion worldline

hole

In general in the background of a bosonic field $[\sigma]$

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



Example of C

To see this we expand 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.

The weight $W(C,\sigma)$ can be negative.

Solution to sign problems in fermionic theories usually requires resummation of fermion worldlines.

Traditional Solution:

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

If “M” is a “good” matrix then Det(M) is positive.

Complex eigenvalues come in complex conjugate pairs and real eigenvalues come in pairs

This usually this some “symmetry.”

Fermion Bag Solution: SC, (2008)

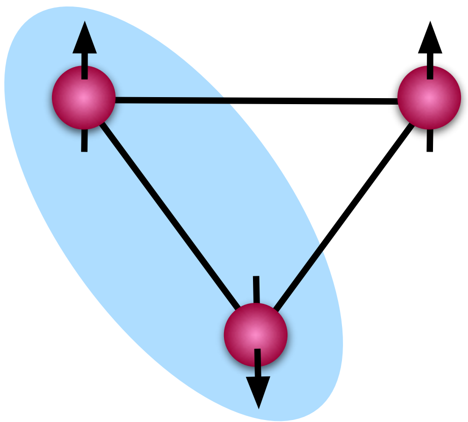
Consider the full partition function:

$$Z = \int [d\sigma]\, e^{-S_b(\sigma)} \sum_{C} W(C,\sigma) = \sum_{B} \Omega(B)$$

We are discovering that local physics often lends itself to this description.

Example 3

Consider three quantum spin-half particles with



$$H \;=\; J\big(\mathbf{S}_1\cdot\mathbf{S}_2+\mathbf{S}_2\cdot\mathbf{S}_3+\mathbf{S}_3\cdot\mathbf{S}_1\big)$$

Ground state is four-fold degenerate!

$$Z \;=\; \mathrm{Tr}\big(e^{-\beta H}\big) \;=\; \int d[s_1(t),s_2(t),s_3(t)]\; W([s])$$

Every spin-hop contributes a negative weight! $\langle\uparrow\downarrow|\, e^{-J\varepsilon\mathbf{S}_i\cdot\mathbf{S}_j}\,|\downarrow\uparrow\rangle<0$

This leads to a sign problem. $W([s])<0$

Solutions can be found by choosing a different basis!

Alet, Damle, Pujari, PRL117 (2016)

Current state of the art to solve sign problems:

Ideas:

No formal proof that these approach will work in general, but promising applications have been discovered.

Examples: Fixed Node Approximation, Complex Langevin Approach, Lefschetz Thimbles, ….

Solutions:

Based on discovering a new representation that is free of sign problems.

Examples: Worldlines, Fermion Bags, Meron Cluster, Multi-level algorithms, ….

A non-trivial solution to a sign problem in QFT

SC, PRD (2012)

Consider a lattice Yukawa model

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)

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

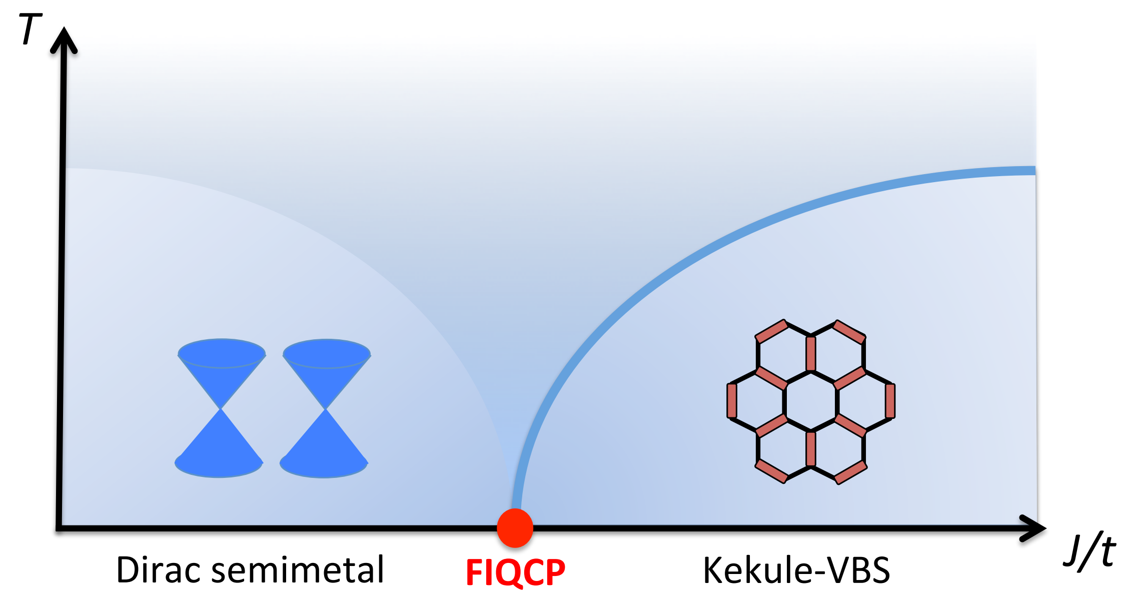
The action is invariant under U(1) chiral transformations

$$\psi_x \to \mathrm{e}^{i\varepsilon_x\alpha}, \quad \overline{\psi}_x \to \mathrm{e}^{i\varepsilon_x\alpha}, \quad \theta_x \to -2\alpha$$

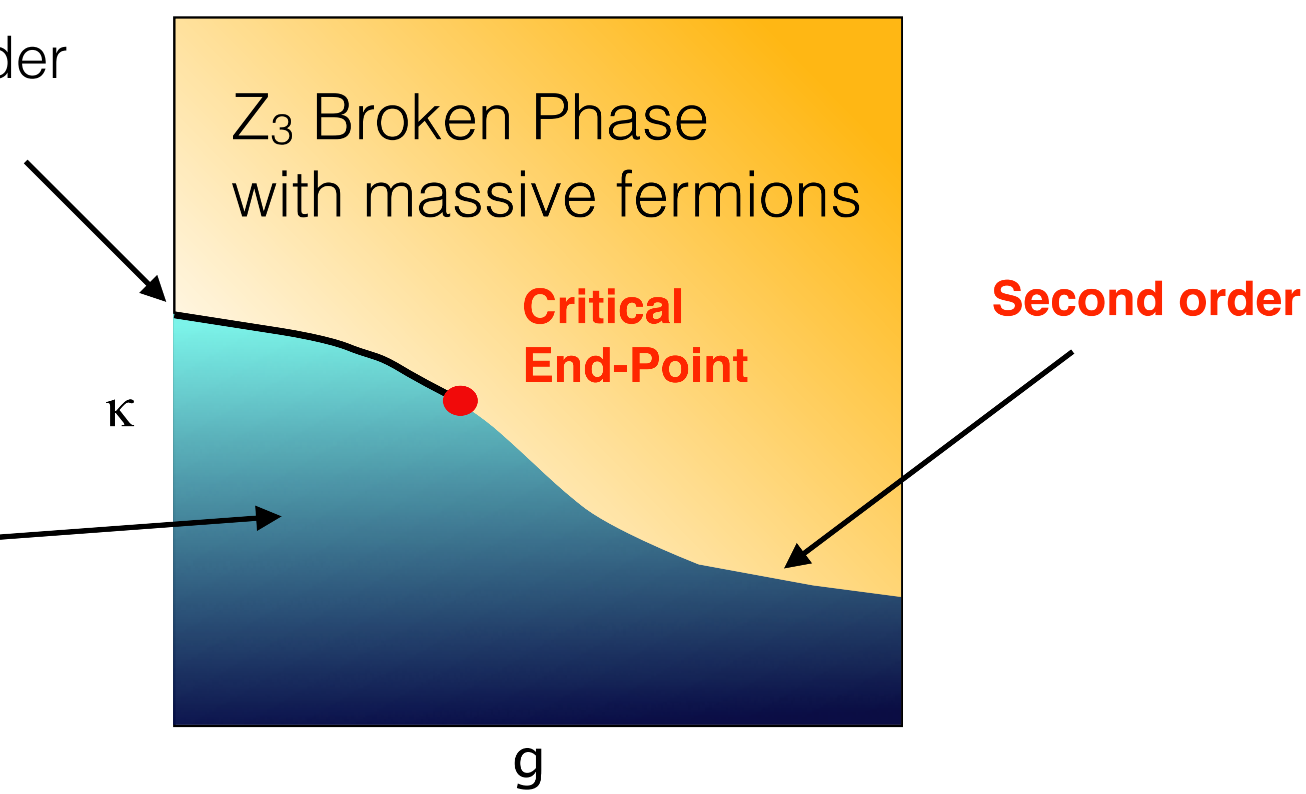
Let us focus on the Z_3 symmetric case: $\theta_x = 0, 2\pi/3, -2\pi/3$

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.



Phase Diagram of the lattice model:



Traditional Approach: Severe Sign Problem

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

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

Antisymmetric matrix,
has positive determinant

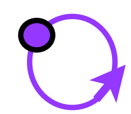
source of the
sign problem!

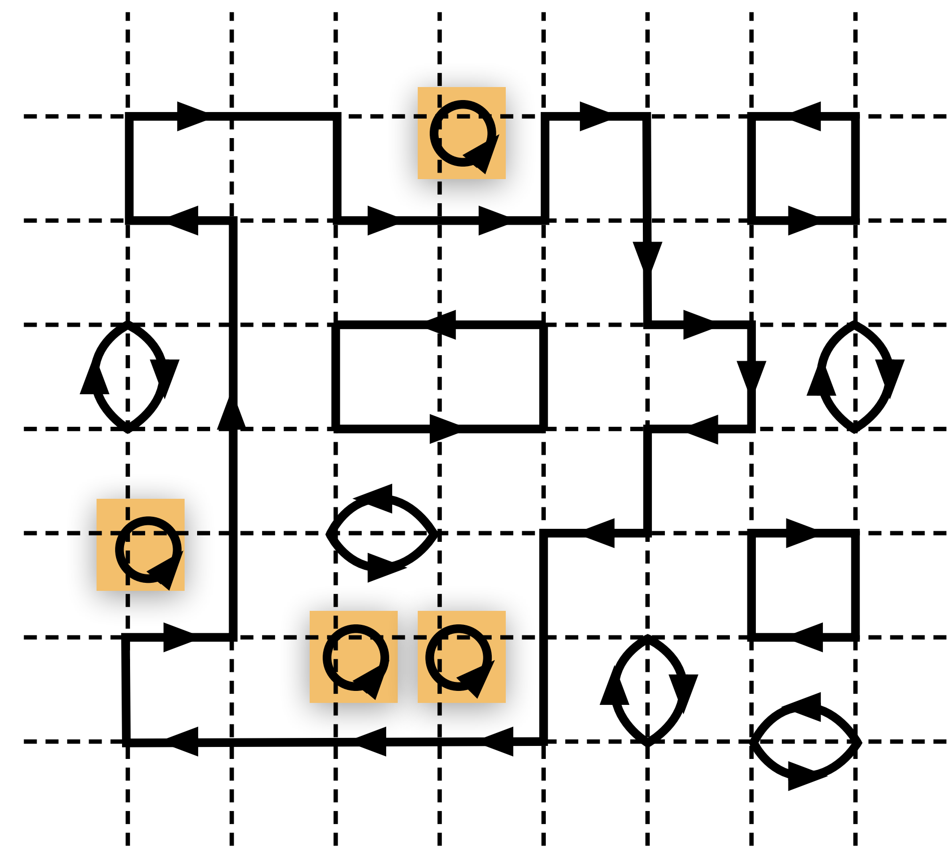
The sign problem "looks" as bad as in QCD!

Fermion Bag Approach:

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

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





Introduce a monomer field [n]

$$n_x = 0, 1$$

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

$$(z_{x_1})^{\varepsilon_{x_1}} \ldots (z_{x_k})^{\varepsilon_{x_k}}$$

The full path integral

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

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

Let us first perform Grassmann integration over the monomer sites!

We simply get a factor 1!

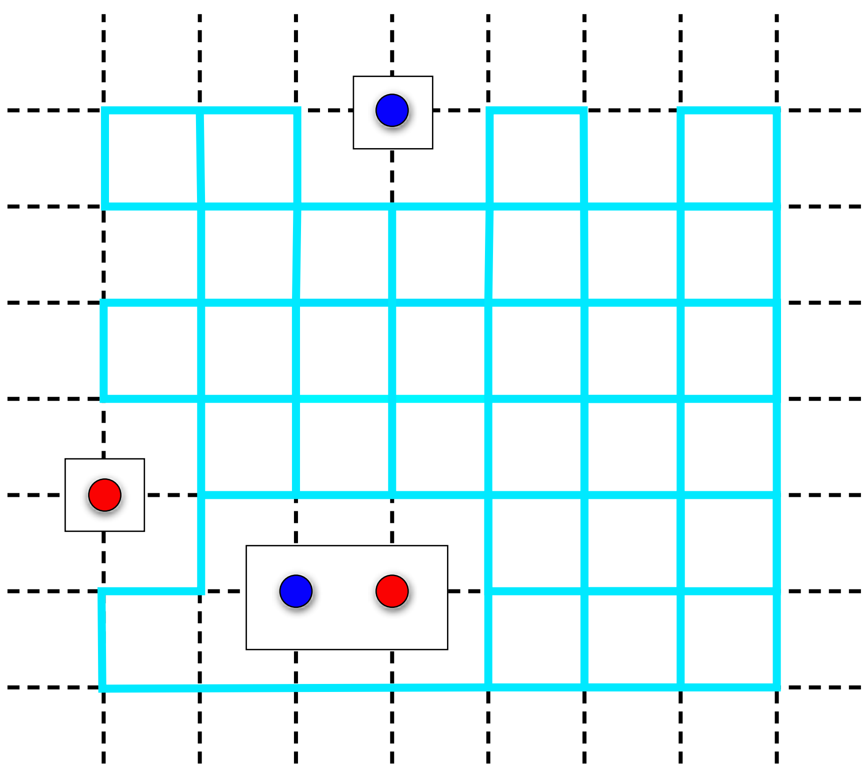
Each monomer site is a local fermion bag.

These sites should then be dropped when we perform the remaining Grassmann integrals

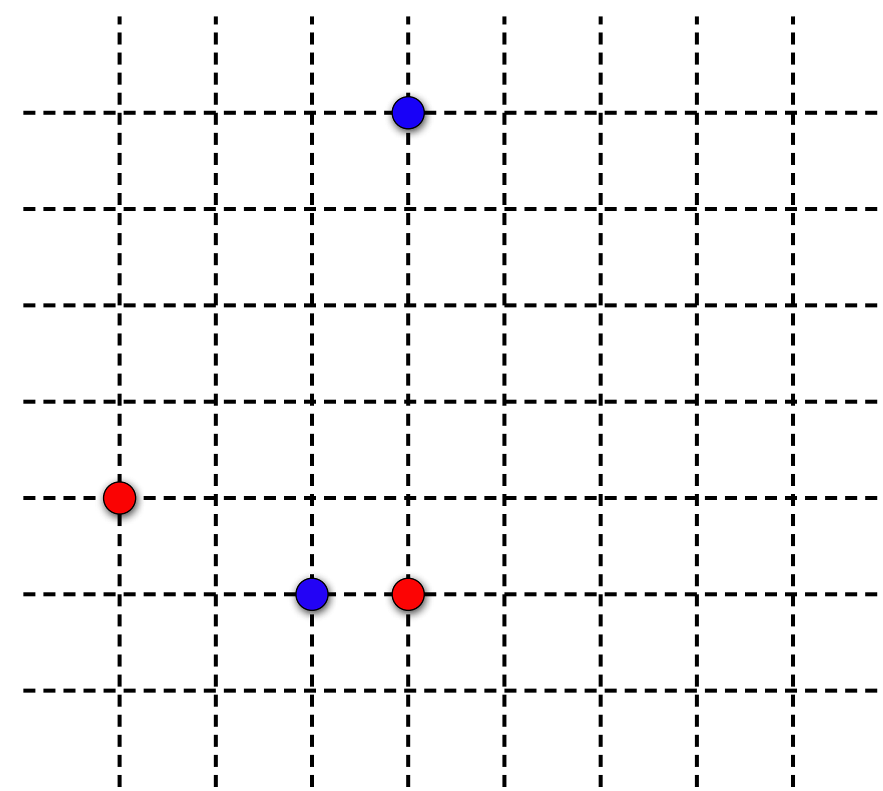
The full path integral

$$Z = \sum_{[n]} g^k \int' [d\bar{\psi} d\psi]\, e^{-\sum_{x,\alpha} \frac{\eta_{x,\mu}}{2}\left(\bar{\psi}_x\ \psi_{x+\alpha} - \bar{\psi}_{x+\alpha}\ \psi_x\right)}$$

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



fermion integration space



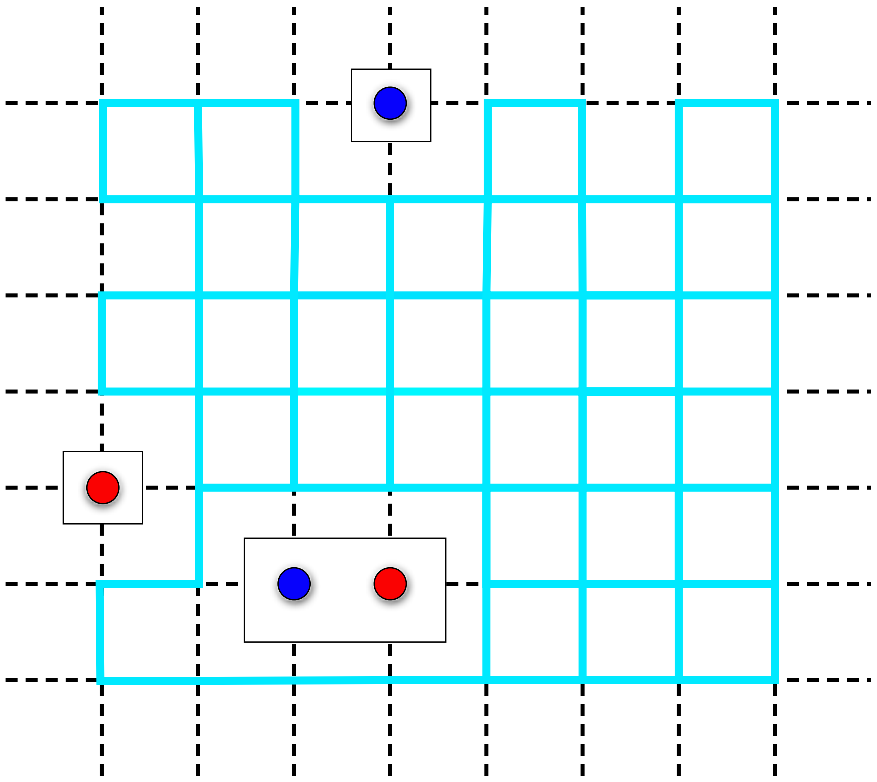
bosonic sum involves inclusion of sources!

The fermionic term now is positive!

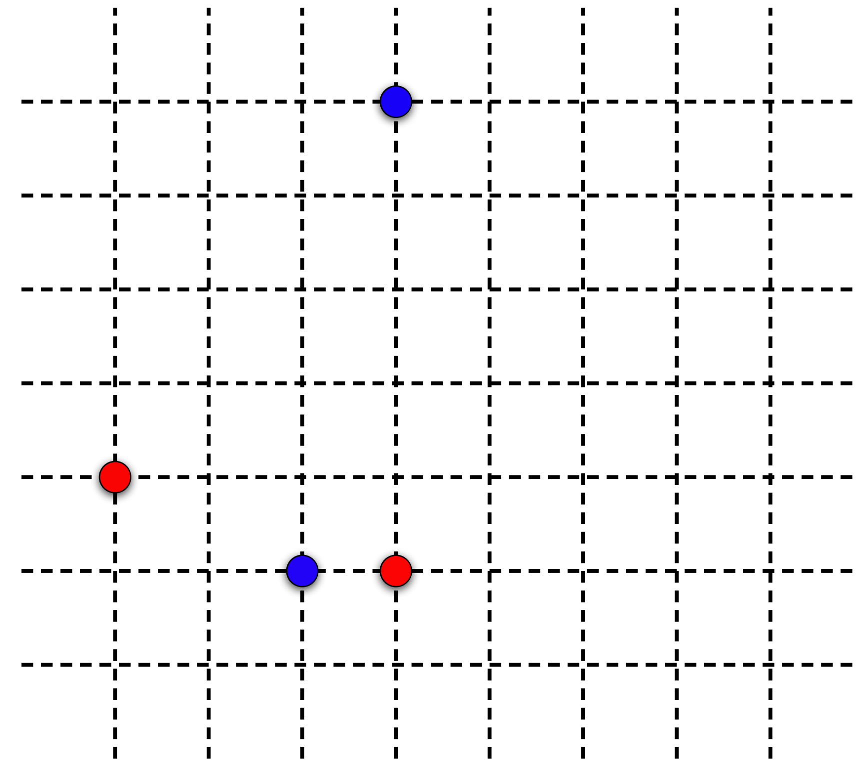
$$\int' [d\overline{\psi} d\psi]\ \mathrm{e}^{-\sum_{x,\alpha} \frac{\eta_{x,\mu}}{2}\left(\overline{\psi}_x\ \psi_{x+\alpha} - \overline{\psi}_{x+\alpha}\ \psi_x\right)}$$

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

Anti-symmetric matrix
which has a positive determinant



The sign problem is now shifted
into the bosonic theory!



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

Let us expand the exponential

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

boson worldlines

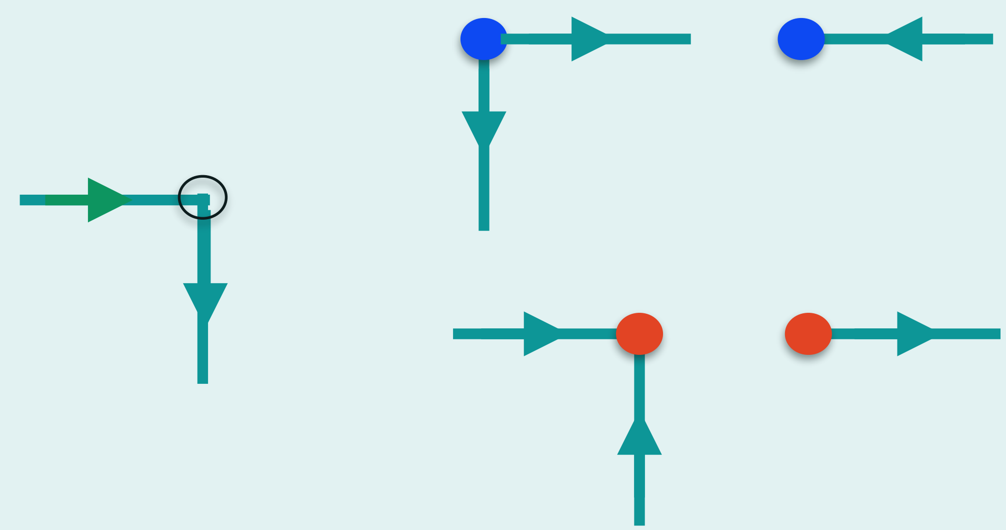
We introduce an integer bond field! $[q]$ $\qquad q_{x,\alpha} = 0, 1, -1$

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

$$= \sum_{[q]} \prod_{x,\alpha} f_{q_\alpha}(\kappa) \sum_{z} \prod_{x} (z_x)^{n_x + q_{x,1} + q_{x,-1} + q_{x,2} + q_{x,-2}}$$

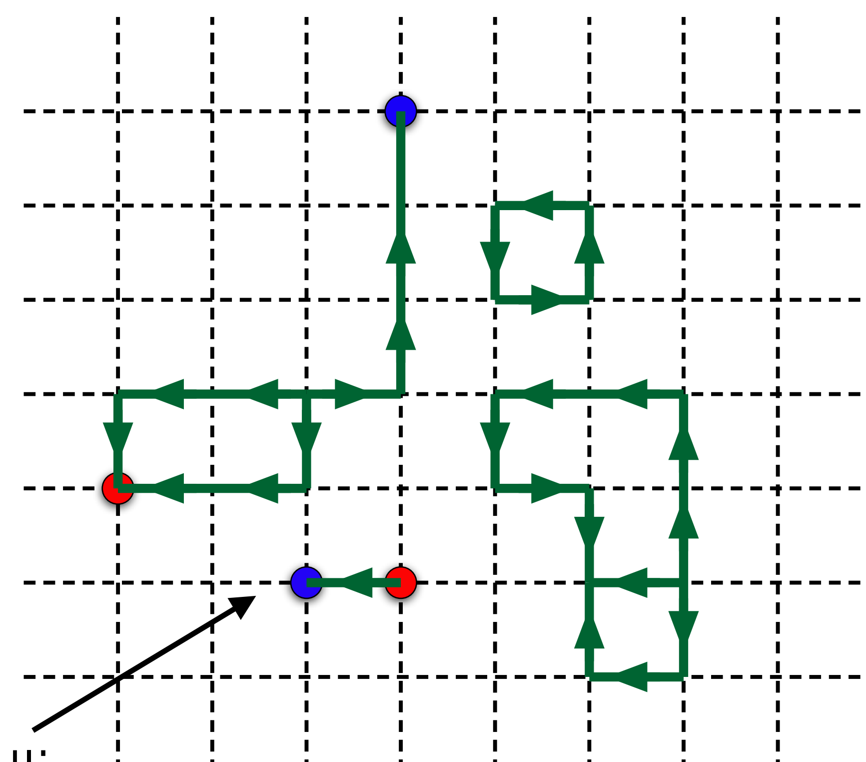
We can now perform the sum over z variables on each site

Sum of Z_3 spins imposes constraints on boson worldlines.



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

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

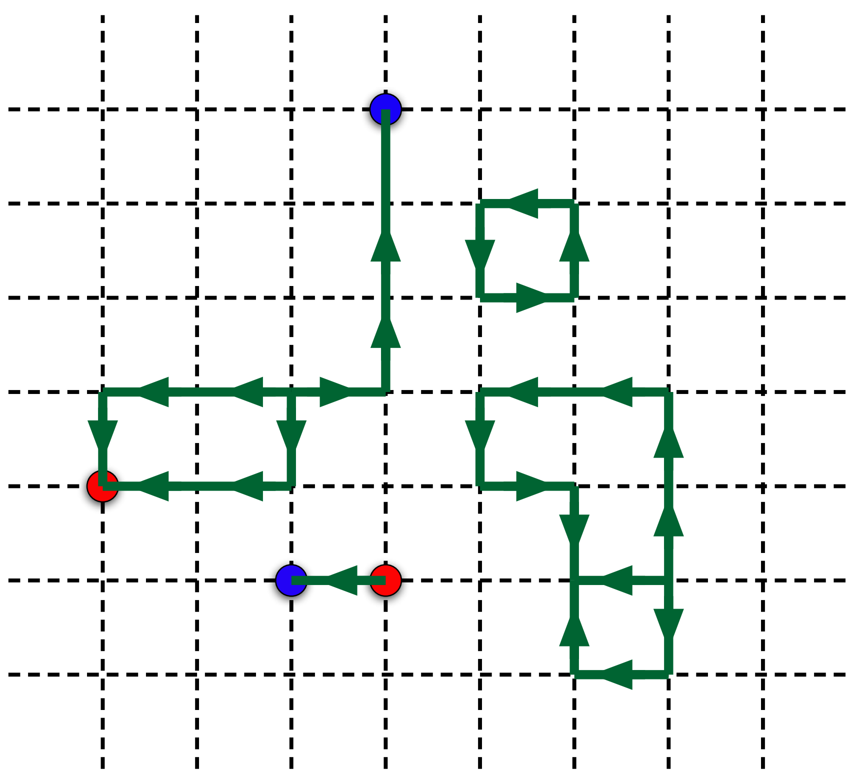


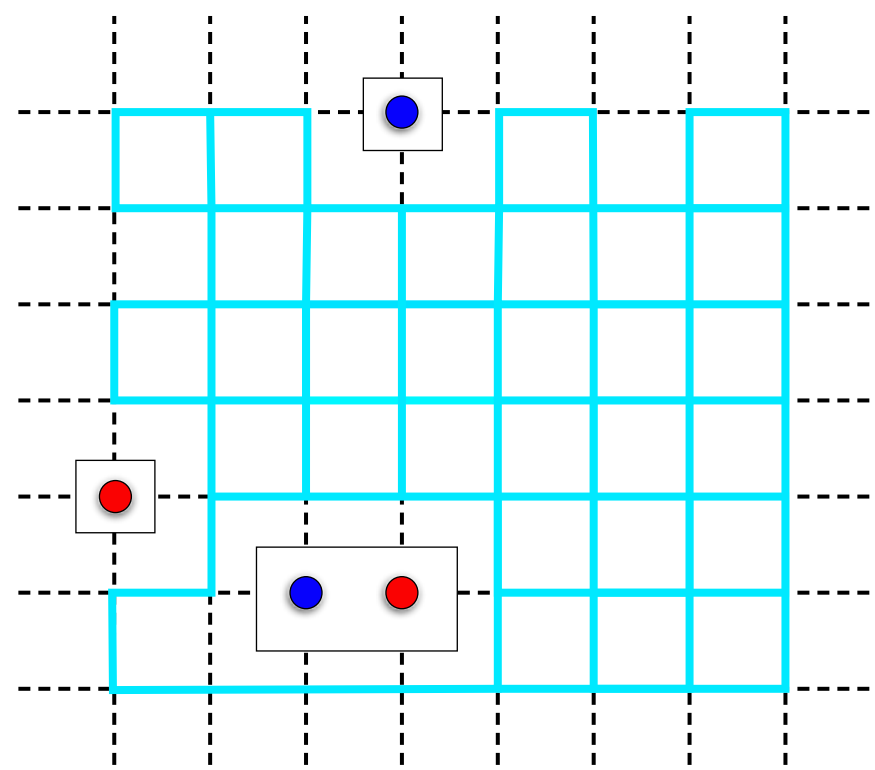
constrained Z_3 worldline configurations

The partition function can now be written as

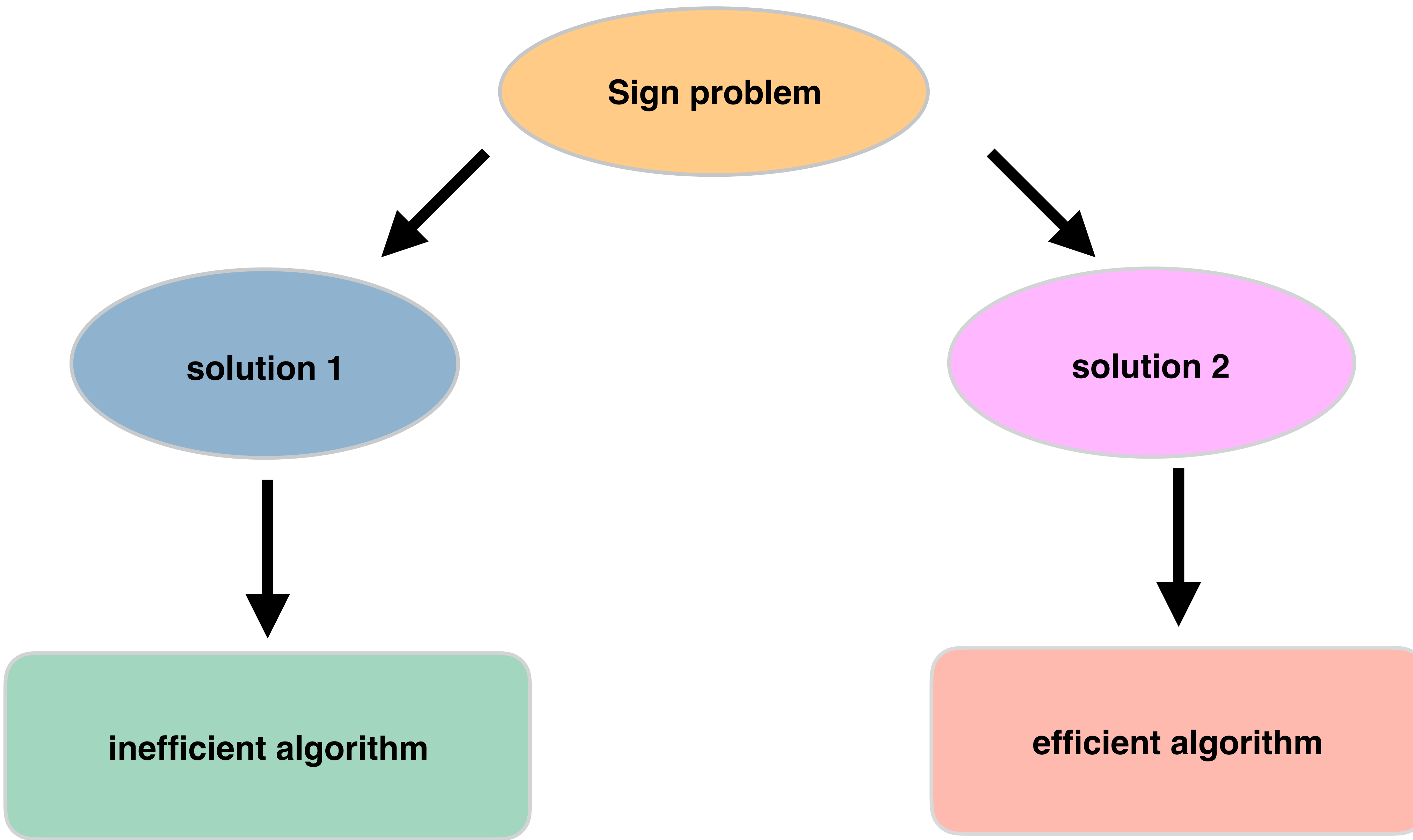
$$Z = \sum_{[n]} \sum_{[q]}{}' \left(\prod_{x,\alpha} f_{q_\alpha}(\kappa) \right) \mathrm{Det}(W_k[n])$$

sign problem is solved!





Two solutions with very different algorithms



Lattice Thirring Model

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

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 Solution: Auxiliary field method

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

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

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

$$= \sum_{[\sigma]} \mathrm{Det}\left(\tilde{M}([\sigma])\right)$$

At strong couplings very singular matrices, leads to very inefficient algorithms

no sign problem

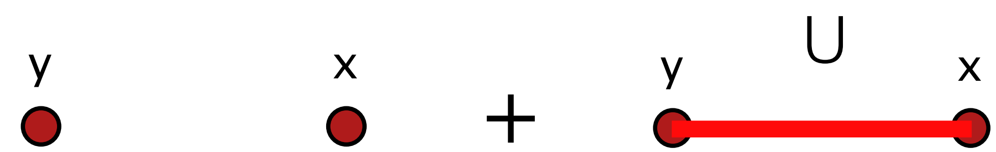
$$\tilde{M}_{xy} = M_{xy} + \sigma_{xy}$$

V x V anti-symmetric matrix

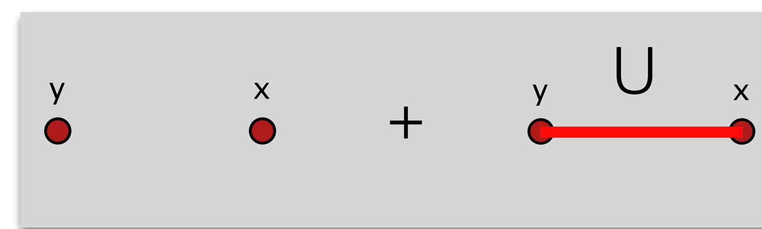
Fermion Bag Approach

SC. Phys.Rev. D82 (2010) 025007

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

$=$ 

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



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

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

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

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

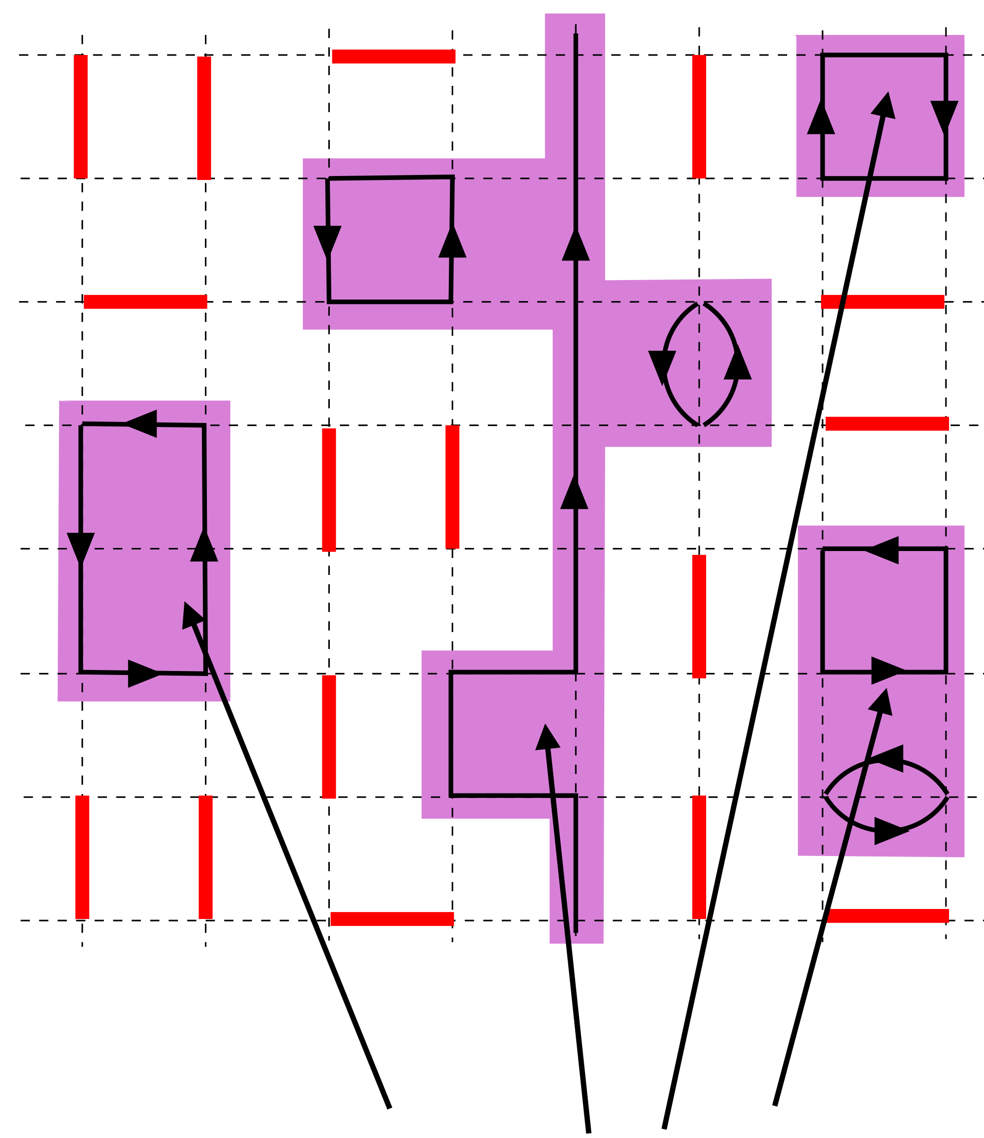
$$Z = \sum_{[d]} U^{N_d} \prod_{\text{Bags}} \mathrm{Det}(W_{\text{Bag}})$$

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

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

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

dimer configuration



free fermion bags

At strong couplings free fermion bags are small! The algorithm is very efficient

Weak coupling approach

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

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

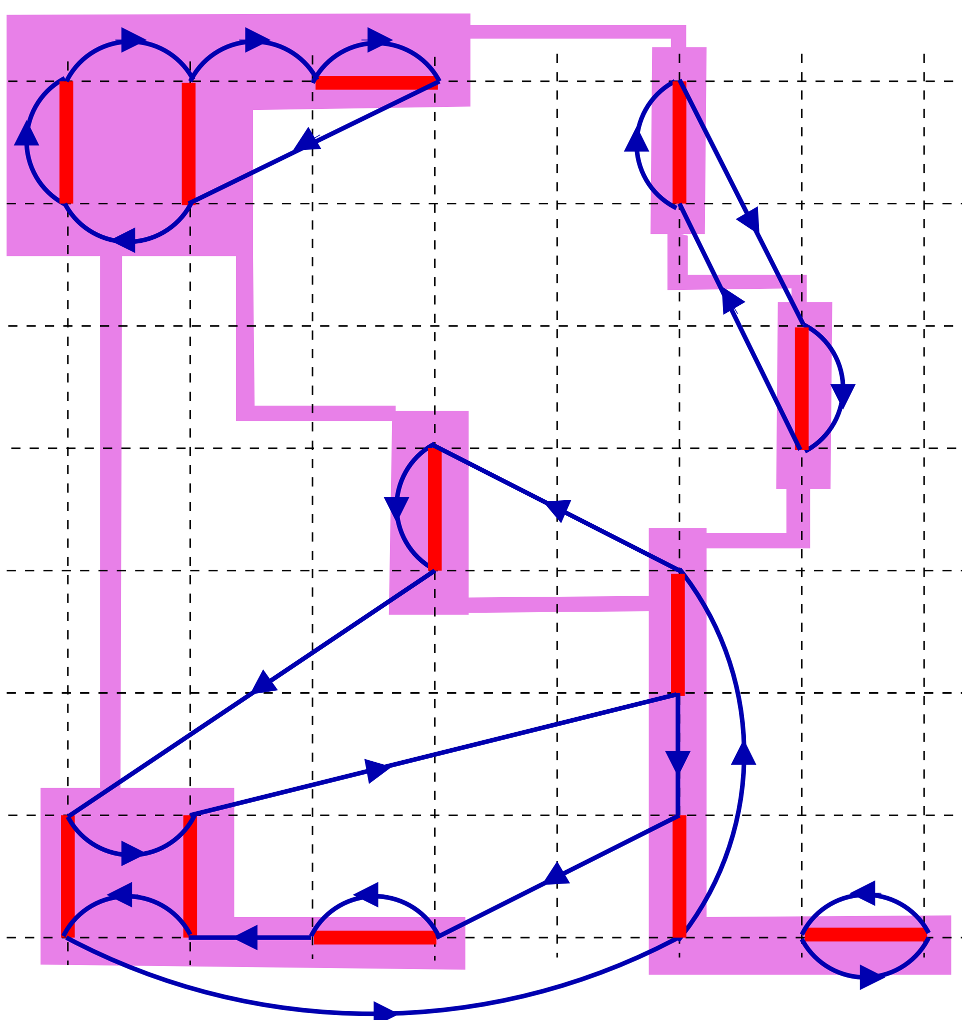
$$Z = \sum_{[d]} U^{N_D}\ \mathrm{Det}(M)\ \mathrm{Det}(G_{\mathrm{prop}})$$

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

2k x 2k matrix

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

Feynman Diagram Configuration

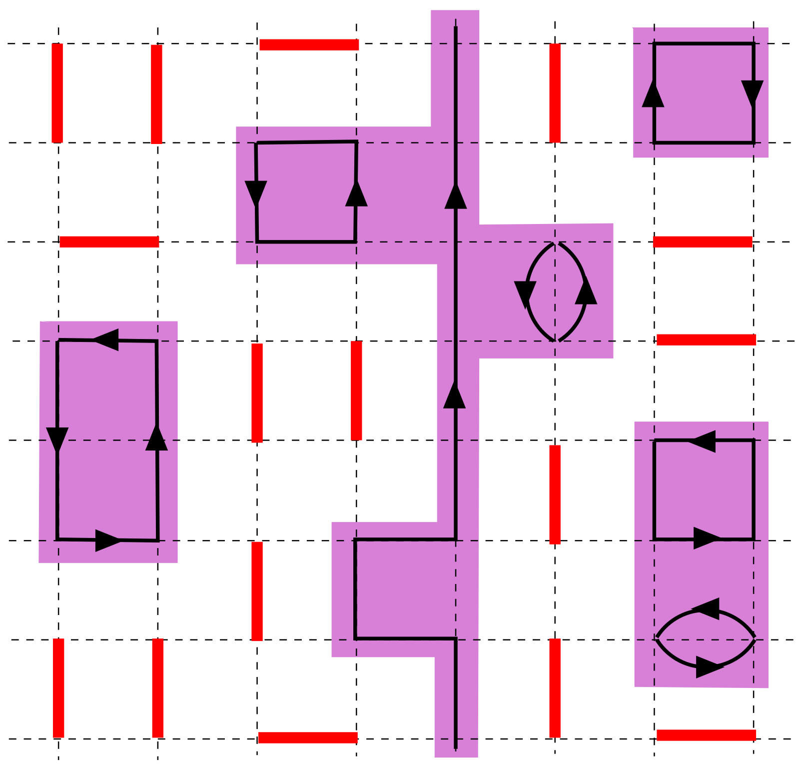


At weak couplings
k will be small

Duality: Weak Coupling versus Strong Coupling

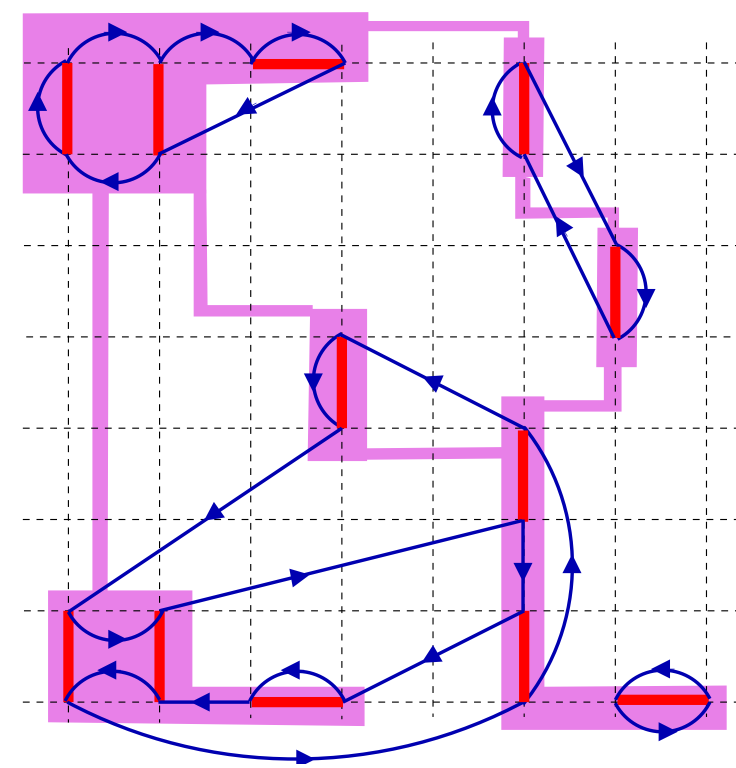
$$Z = \sum_{[d]} U^{N_D} \int [d\overline{\psi}\; d\psi]\; e^{-S_0(\overline{\psi},\psi)}\; (-\overline{\psi}_{x_1}\psi_{y_1}\overline{\psi}_{y_1}\psi_{x_1})\ldots(-\overline{\psi}_{x_k}\psi_{y_k}\overline{\psi}_{y_k}\psi_{x_k})$$

strong coupling



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

weak coupling



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

Signal to noise ratio: conformal dimensions at large charge

Banerjee, SC,Orlando PRL (to appear)

XY model in 3d

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

At the critical point $\kappa_c \approx 0.227082$ the lattice theory describes the Wilson-Fisher fixed point in the IR

At large distances we expect

$$C_Q(|x-y|) \; = \; \langle \mathrm{e}^{iQ\theta_x} \; \mathrm{e}^{-iQ\theta_y} \rangle \sim |x-y|^{-2D(Q)}$$

There are predictions

Hellerman, Orlando, Reffert, and Watanabe JEHP (2015)

$$D(Q) \; = \; \sqrt{\frac{Q^3}{4\pi}} \left(c_{3/2} + c_{1/2} \left(\frac{4\pi}{Q} \right) + \ldots \right) + c_0$$

Challenge is to extract the coefficients, which are universal!

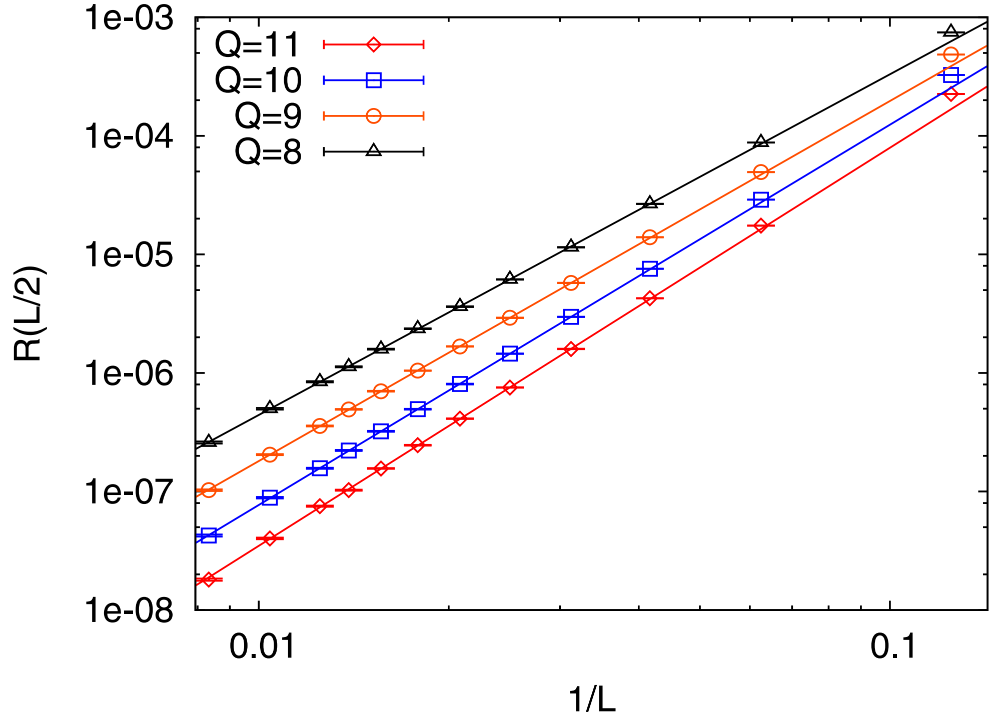
$$C_Q(|x-y|) \;=\; \langle e^{iQ\theta_x}\; e^{-iQ\theta_y}\rangle \sim |x-y|^{-2D(Q)}$$

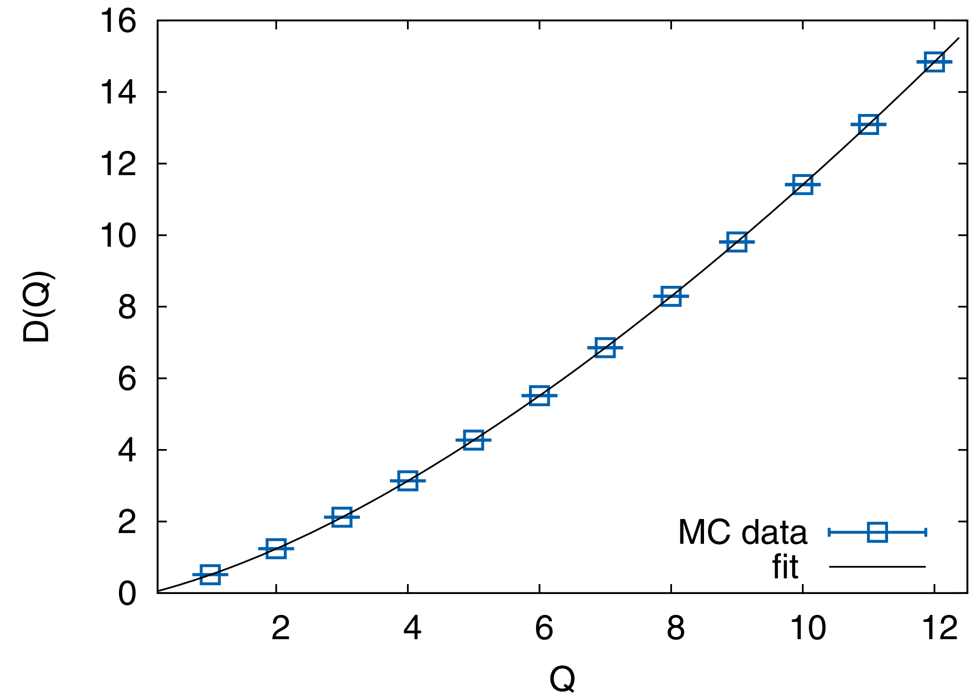
At large Q the it is difficult to compute the correlation functions

Monte Carlo suffers from signal to noise ratio problems!

We can solve this problem using world line formulations and “worm algorithms”

$$R(L/2) = \frac{C_Q(r=L/2)}{C_{Q-1}(r=L/2)}$$





$$c_{3/2} \;=\; 1.195(10),\;\; c_{1/2} \;=\; 0.075(10),\;\;\; c_0 \;=\; -0.094$$

New Ideas with Hamiltonian Lattice Field Theories

Can we construct and study theories of strongly interacting massless Dirac fermions in the Hamiltonian formulation?

Brower, Rebbi, Schaich (2011)

Ulybeshev et. al., (2017), Berkowitz et. al., (2017)

…. (lots more in CM community!)

Advantage: Staggered fermions with less fermion doubling and more symmetries!

Whole new set of models recently discovered recently without sign problems!

Huffman and SC (2014)

Li, Jiang and Yao (2015)

Wei, Wu, Li, Zhang and Xiang (2016)

Consider

$$H = \sum_{\langle ij \rangle} t_{ij} \left(c_i^\dagger c_j + c_j^\dagger c_i \right) + V_{ij} \left(n_i - \frac{1}{2} \right) \left(n_j - \frac{1}{2} \right)$$

In the traditional approach one usually introduces

$$c_i |\psi_i\rangle = \psi_i \, |\psi_i\rangle, \quad \langle \overline{\psi}_i | \, c_i^\dagger = \langle \overline{\psi}_i | \, \overline{\psi}_i$$

This approach breaks particle hole symmetry and leads to sign problems!

New Insight: Introduce Majorana operators

$$\xi_i = (c_i + c_i^\dagger), \quad \overline{\xi}_i = i(c_i - c_i^\dagger)$$

and use them to construct the partition function!

Conclusions

A. Solution to Sign Problems is an exciting new area of research, at the cross roads of mathematical and computational physics.

B. Sign problems usually have a physical origin and its solution usually requires us to “think” about new variables.

C. Understanding the physics has helped us solve many sign (signal-noise-ratio) problems that were thought to be difficult before.

D. Many other complementary ideas are being approached.

E. Non-trivial solutions to sign problem may emerge from thinking carefully about how they emerge within local space-time regions.