World-line approach to Sign Problems

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Outline

- ★ XY model + chemical potential
  - ➡ world-line approach
  - ➡ solving the silver blaze problem!
- ★ Two component bosons + Abelian gauge fields
- ★ Grassmann variables and fermionic worldlines
- ★ Massless Thirring model + chemical potential
  - ➡ world-line approach
  - ➡ solving the silver blaze problem!
  - ➡ more flavors + solving sign problems
- ★ Applications to QCD Physics (static quarks)
- ★ Suggestions for QCD
- ★ Conclusions

The Origin of Sign Problems

We are usually interested in a quantum partition function

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

Always possible to write this as

$$Z = \sum_{([C])} \mathrm{Sign}([C])\,\mathrm{W}([C])$$

+1 or -1 positive definite

Conceptual Question: By a proper choice of [C] can we write

$$Z = \sum_{([C])} \mathrm{W}([C])$$

positive definite

Ofcourse yes!
We can always go to the energy eigenstate basis!

Clearly not guaranteed in local variables,
since we are dealing with quantum mechanics where
complex phases arise naturally and can
lead to interesting physics!

Recent progress seems to suggest that there may
be a natural variables, which are non-local!

Bosons: World-lines

Fermions: Fermion Bags

Gauge Fields: World sheets

Here I will present some examples
which reflect these observations

XY model

Action:

$$S = -\frac{\beta}{2} \sum_{x,\alpha} \left(e^{i\phi_{x+\alpha} - i\phi_x} + e^{i\phi_x - i\phi_{x+\alpha}} \right) \qquad 0 \leq \phi_x < 2\pi$$

Partition function:

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

Can use "cluster algorithms" to solve this simple field theory!

Wolff, (1989)

But, what happens if we add a chemical potential?

Let us add a chemical potential!

Action:

$$S([\phi]) = -\frac{\beta}{2}\sum_{x,\alpha}\left(\mathrm{e}^{i\phi_{x+\alpha}-i\phi_x-\mu\delta_{\alpha,t}} + \mathrm{e}^{i\phi_x-i\phi_{x+\alpha}+\mu\delta_{\alpha,t}}\right)$$

action becomes complex!
just like in QCD!!

A complex action is a generic feature
in the presence of a chemical potential
in the conventional formulation!

Can we solve this sign problem?

World-line approach

(strong coupling expansion to all orders!)

Expand partition function in powers of β to all orders

$$Z = \int [d\phi] \; \mathrm{e}^{\sum_{x,\alpha} \left\{ \frac{\beta}{2} \left(\mathrm{e}^{i\phi_{x+\alpha} - i\phi_x - \mu\delta_{\alpha,t}} \right) + \frac{\beta}{2} \left(\mathrm{e}^{i\phi_x - i\phi_{x+\alpha} + \mu\delta_{\alpha,t}} \right) \right\}}$$

using the identity on each bond

$$\exp\Big\{\beta\cos(\phi)\Big\} = \sum_{k=-\infty}^{\infty} I_k\Big(\beta\Big)\mathrm{e}^{ik\phi},$$

$$Z = \sum_{[k_{x,\alpha}]} \prod_{[x,\alpha]} \mathrm{e}^{\mu\delta_{\alpha,t}k_{x,\alpha}} \; I_{k_{x,\alpha}}(\beta) \; \delta\Big(\sum_{\alpha} [k_{x,\alpha} - k_{x-\alpha,\alpha}] \Big)$$

Called the current loop model!

$$Z = \sum_{[k_{x,\alpha}]} \prod_{[x,\alpha]} e^{\mu \delta_{\alpha,t} k_{x,\alpha}} \, I_{k_{x,\alpha}}(\beta) \, \delta\Big(\sum_{\alpha} [k_{x,\alpha} - k_{x-\alpha,\alpha}] \Big)$$

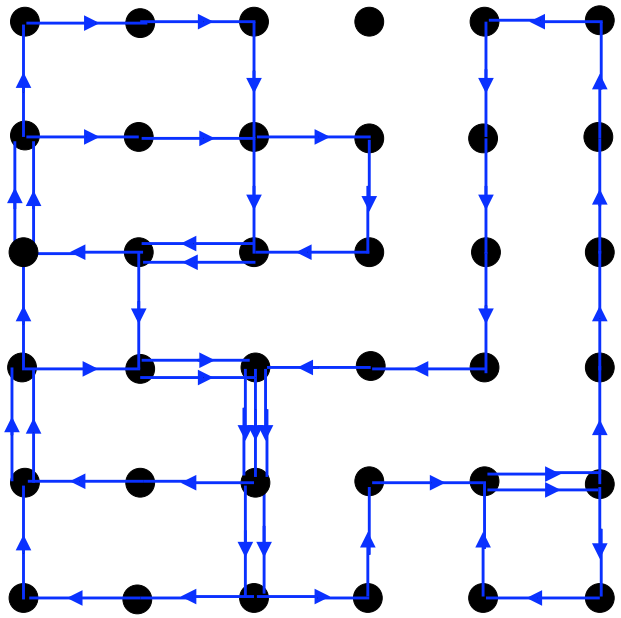
current conservation

no sign problem!

Can update this system extremely efficiently with the "worm algorithm"

prokof'ev and Svustinov

example of a world line configuration



Each world line configuration is defined by a set of constrained integers on bonds $[k_{x,\alpha}]$

Solution to the Silver Blaze Problem

Chemical potential enters only through world-lines that wrap around the temporal direction.

$$Z = \sum_{q=-\infty}^{\infty} Z_q \; \mathrm{e}^{(q\mu N_t)}$$

$$Z_q = \mathrm{e}^{-F_q N_t}$$

Partition function with temporal winding number q (canonical partition function)

If at μ=0 we are in a "massive phase" then $F_q > F_0$

Configurations with temporal windings are exponentially suppressed in the partition function until μ reaches a critical value

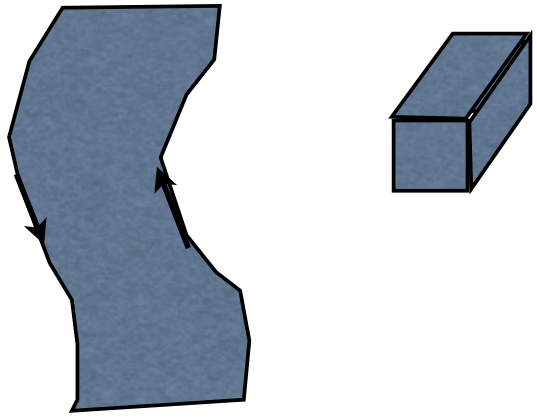
A two component bosons interacting with abelian gauge fields

The action is again complex given by

$$
\begin{aligned}
S \;=\; & -\frac{\kappa}{2}\sum_{x,\alpha}\left(\mathrm{e}^{i\phi_{x+\alpha}-i\phi_x-\mu\delta_{\alpha,t}+iA_{x,\alpha}}+\mathrm{e}^{-i\phi_{x+\alpha}+i\phi_x+\mu\delta_{\alpha,t}-iA_{x,\alpha}}\right)\\
& -\frac{\kappa}{2}\sum_{x,\alpha}\left(\mathrm{e}^{i\theta_{x+\alpha}-i\theta_x+\mu\delta_{\alpha,t}+iA_{x,\alpha}}+\mathrm{e}^{-i\theta_{x+\alpha}+i\theta_x-\mu\delta_{\alpha,t}-iA_{x,\alpha}}\right)\\
& -\beta\sum_{p}\cos(A_p)
\end{aligned}
$$

Again by performing a strong coupling expansion
in both κ and β the sign problem is completely solved.

Configurations now involve
bosonic world lines and
world sheets (due to gauge plaquettes)
which form either closed surfaces or
open surfaces with boson world lines at the edges.



Fermion Worldlines

(directly with Grassmann varibales)

Partition function

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

Here ψ and $\overline{\psi}$ are Grassmann valued fields on a Hypercubic lattice

Grassmann integration

$$\int d\psi = 0 \qquad \int d\psi\, \psi = 1$$

What does the Grassmann path integral (on the lattice) mean?

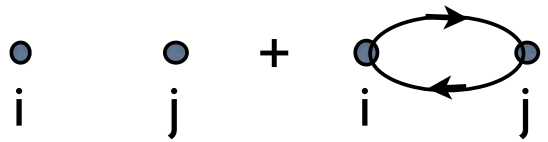
There are statements in the literature which say
"... there is no way to represent Grassmann variables on a computer
so we integrate them away! ... "

Grassmann variables help in generating world lines configurations

The partition function is made of products of terms on each bond .
Each of this term can be one of the following

$$e^{\eta_{ij}\overline{\psi}_i\psi_j} = 1 + \eta_{ij}\overline{\psi}_i\psi_j \quad =$$

$$e^{U\overline{\psi}_i\psi_i\overline{\psi}_j\psi_j} = 1 - U\ \overline{\psi}_i\psi_j\ \overline{\psi}_j\psi_i \quad =$$



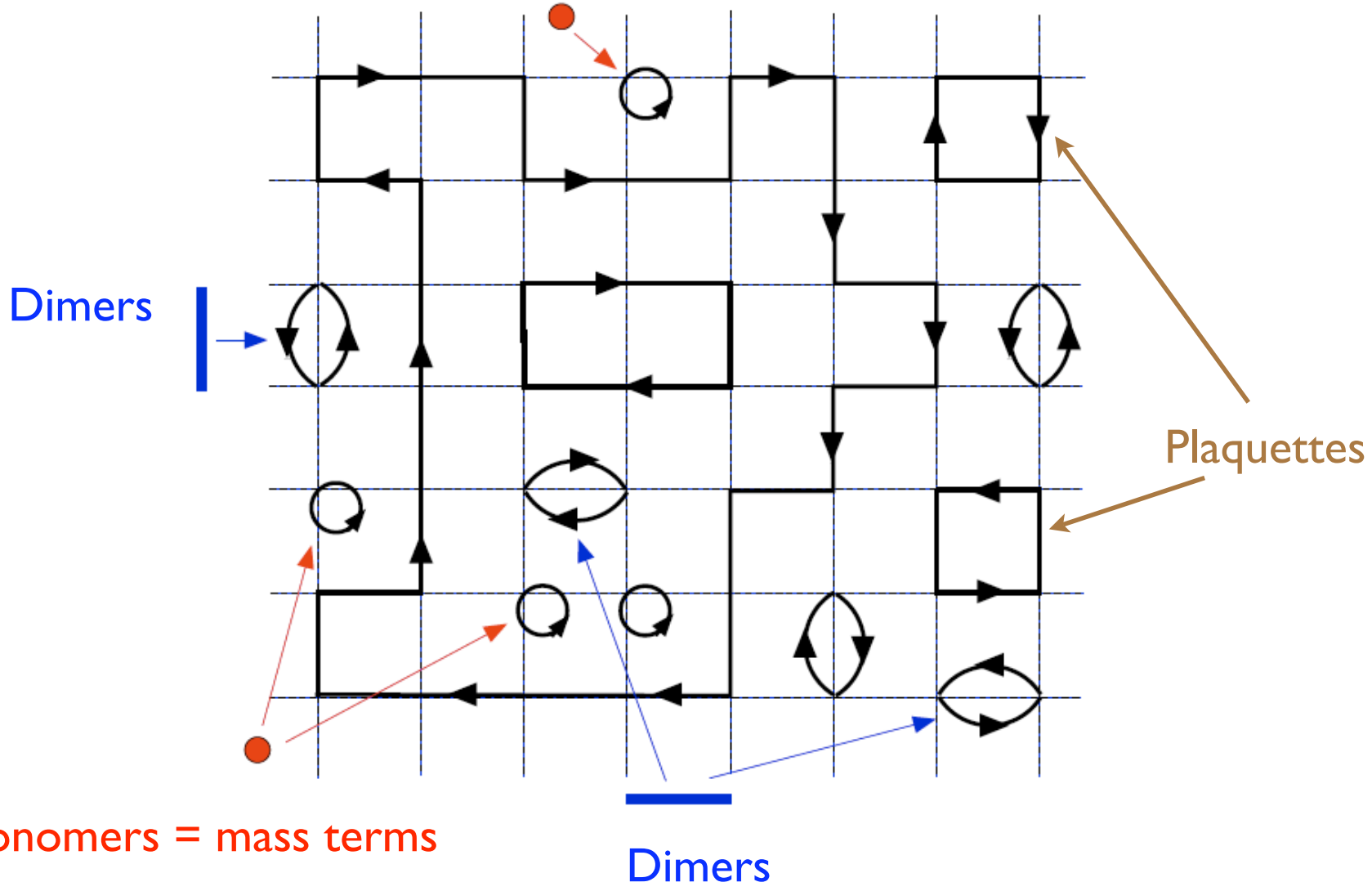
$$e^{-m\overline{\psi}_i\psi_i} = 1 - \overline{\psi}_i\psi_i \quad =$$

Grassmann nature:
Each site can have one incoming and one outgoing line
There are sign factors that come from Grassmann ordering.

Grassmann variables help enumerate “world-lines” which are
self avoiding loops!

Fermion World-line configuration

(hopping parameter expansion to all orders!)



Thus, the fermionic partition function can be written as

$$Z = \sum_{C \in \text{fermion loops}} \text{Sign}([C])\, W([C])$$

This is like a world line representation!

The sign function depends on the loop and the model.

1. Signs factors come from local phases.
2. Every fermion loop has a negative sign.

Can we solve sign problems in this world line representations?

Research over the past decade shows that sign problems can sometimes be solved in novel ways!

Solutions to fermion sign problems always involve
some kind of resummation over a class of world-line configurations
(natural in quantum mechanics, physics of interference)

The determinant approach is clearly one well known solution!

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

Can be positive!

The "meron cluster" approach was another solution which
was discovered in the Hamiltonian formulation

S.C and Wiese, 1999

Lesson!
We must explore resummation techniques over atleast
a class of fermion world-line configurations
Will call this "fermion bags"

Effects of chemical potential

- Very similar to the bosonic world lines
- No "new" sign problems due to a chemical potential.
- Some solutions to sign problems may no longer work!
- chemical potential enters only through temporal winding loops
- if we can argue that temporal winding loops are absent then chemical potential does not enter the dynamics!
- silver blaze problem is always solved in this way!

Massless Thirring Model

Hands, Strouthos, et. al.,

Action

$$S(\psi,\overline{\psi}) = -\sum_{\langle ij\rangle}\left\{\ \eta_{ij}\ (\overline{\psi}_i\psi_j - \overline{\psi}_j\psi_i)\ +\ U\ \overline{\psi}_i\psi_i\ \overline{\psi}_j\psi_j\ \right\}$$

The theory contains a $U_c(1)$ x $U_f(1)$ symmetry

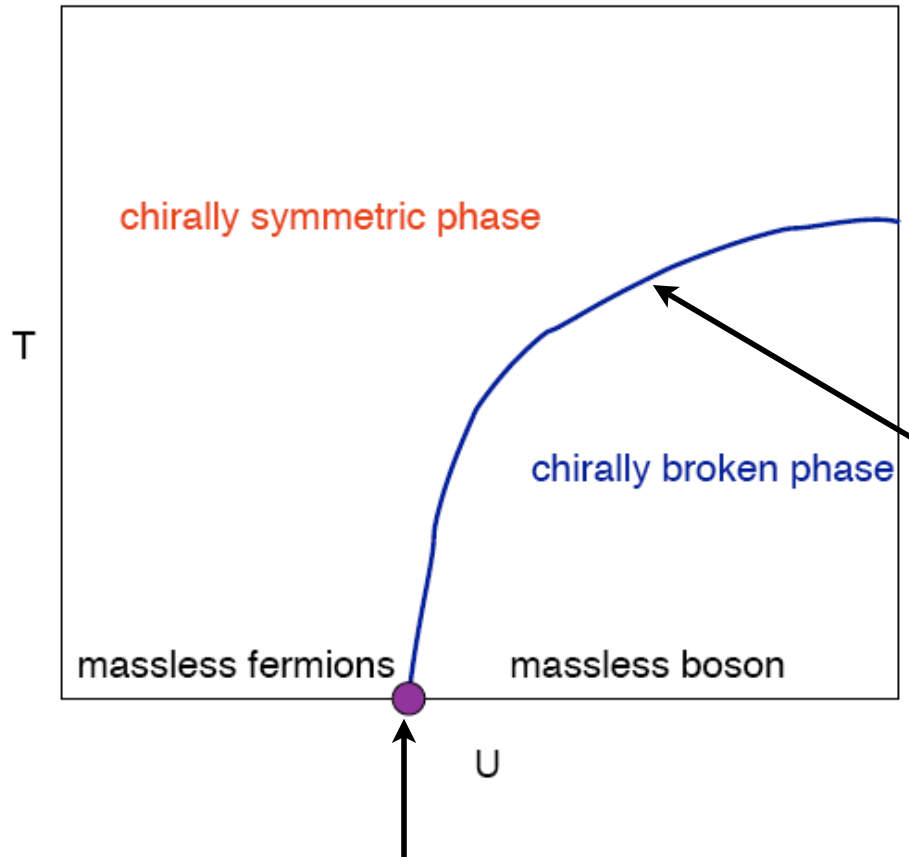
$U_c(1)$ is a "chiral symmetry"

$$\psi_x \to \mathrm{e}^{i(-1)^x\theta}\ \psi_x, \quad \overline{\psi}_x \to \overline{\psi}_x\ \mathrm{e}^{i(-1)^x\theta}$$

By a proper choice of the η_{ij} we can
get massless Dirac fermions.

In the lattice QCD literature these are called staggered fermions.

Physics of the model



Classical XY
critical behavior

quantum critical point

One such quantum critical point is of interest
in the physics of Graphene

Conventional Approach

Action

$$S(\psi,\overline{\psi}) = -\sum_{\langle ij\rangle}\left\{\ \eta_{ij}\ (\overline{\psi}_i\psi_j - \overline{\psi}_j\psi_i)\ +\ U\ \overline{\psi}_i\psi_i\ \overline{\psi}_j\psi_j\ \right\}$$

Using the Hubbard Stratanovich transformation

$$\mathrm{e}^{U\ \overline{\psi}_i\psi_i\ \overline{\psi}_j\psi_j}\ =\ \int\ \frac{d\phi}{2\pi}\ \mathrm{e}^{\sqrt{U}\left[\eta_{ij}(\mathrm{e}^{i\phi}\overline{\psi}_i\psi_j\ -\ \mathrm{e}^{-i\phi}\overline{\psi}_j\psi_i)\ \right]}$$

we can then write $$Z = \int\ [d\psi d\overline{\psi} d\phi]\ \mathrm{e}^{-S(\overline{\psi},\psi,\phi)}$$

$$S(\psi,\overline{\psi}) = -\sum_{\langle ij\rangle}\left\{\ \eta_{ij}(1+\sqrt{U}\mathrm{e}^{i\phi_{ij}})\overline{\psi}_i\psi_j - \eta_{ij}(1+\sqrt{U}\mathrm{e}^{-i\phi_{ij}})\overline{\psi}_j\psi_i)\ \right\}$$

Thus we have written the action as fermion bilinear

$$S(\psi, \overline{\psi}, \phi) = -\overline{\psi}_i M([\phi])_{ij} \psi_j$$

So we can now write

$$Z = \int [d\phi] \, \mathrm{Det}\big(M([\phi])\big)$$

Positive determinant: sign problem solved!

But at the cost of the following:

The problem has become completely non-local!

For large U, the matrix M has a large number of small eigenvalues.

Monte Carlo Algorithms become inefficient!

Adding chemical potential

Action

$$S = -\sum_{\langle ij \rangle} \left(\left\{ \eta_{ij} (\overline{\psi}_i \psi_j \mathrm{e}^{\mu_{ij}} - \overline{\psi}_j \psi_i \mathrm{e}^{-\mu_{ij}}) \right\} \quad + \quad U \ (\overline{\psi}_i \psi_i \overline{\psi}_j \psi_j) \right)$$

$$\mu_{ij} = \mu \text{ for temporal bonds}, \quad \mu_{ij} = 0 \text{ for spatial bonds}$$

Conventional Approach

$$S = -\sum_{\langle ij \rangle} \left(\left\{ \eta_{ij} \mathrm{e}^{\mu_{ij}} (1 + \sqrt{U} \mathrm{e}^{i\phi_{ij}}) \overline{\psi}_i \psi_j - \eta_{ij} \mathrm{e}^{-\mu_{ij}} (1 + \sqrt{U} \mathrm{e}^{-i\phi_{ij}}) \overline{\psi}_j \psi_i) \right\} \right)$$

leads to a complex determinant and no solution to the sign problem for all values of U!

In particular no solution to the silver blaze problem too!

The worldline approach suggests other methods!

Instead of the Hubbard Stratanovich, consider writing

$$Z = \int [d\overline{\psi} d\psi] \mathrm{e}^{-S_0(\psi,\overline{\psi})} \prod_{\langle ij \rangle} \left(1 + U\, \overline{\psi}_i \psi_i\, \overline{\psi}_j \psi_j\right)$$

free fermions

$$Z = \sum_{[b]} \left(\prod_{ij} U^{b_{ij}} \right) \Big\{ {\sum_{\text{free fermions}}}' \mathrm{Sign}([C,b])\; W([C,b]) \Big\}$$

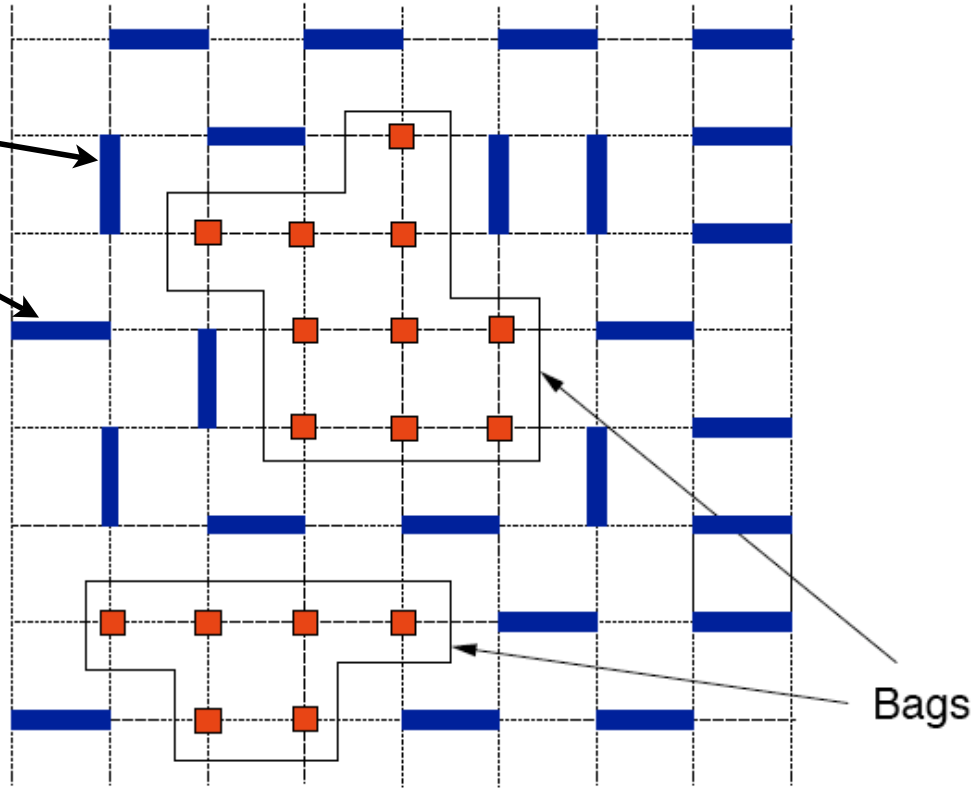
Here free fermions hopp on a lattice not touched by b=1 bonds.

$= \mathrm{Det}\big(Q([b])\big)$

positive definite

$$Z = \sum_{[b]} \left(\prod_{ij} U^{b_{ij}} \right) \mathrm{Det}\big(Q([b])\big)$$

$$(U\overline{\psi}_{x+\hat{\alpha}}\psi_{x+\hat{\alpha}}\overline{\psi}_x\psi_x)$$



fermions are free inside certain regions
"Bag Model"

At large U the "bags" are small, so fermions are confined in small regions.

For small U fermions become "free"

The effort to compute the determinant is "optimal"

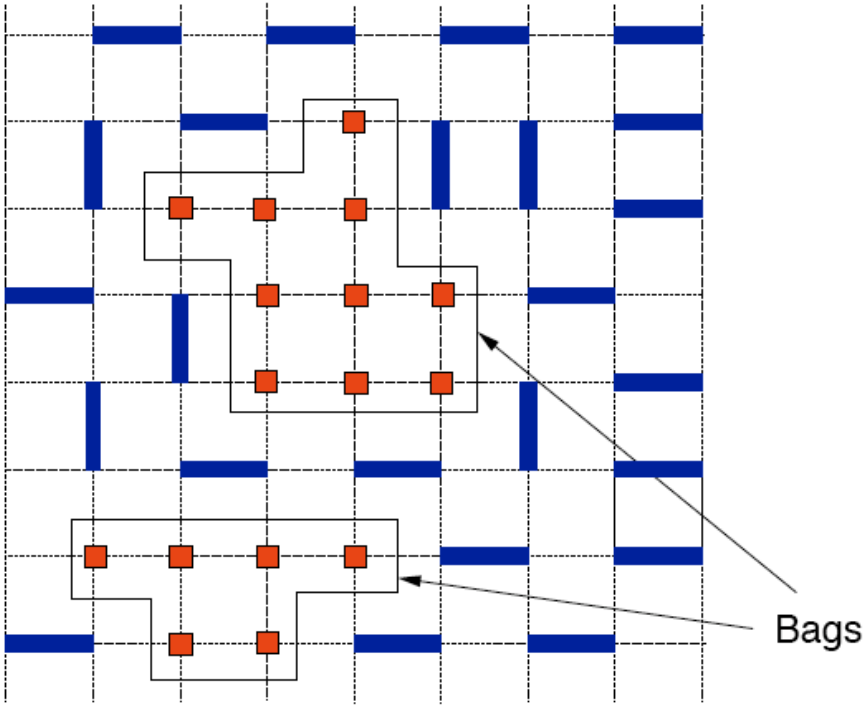
Solution to the silver blaze problem

$$Z = \sum_{[b]} \left(\prod_{ij} U^{b_{ij}} \right) \mathrm{Det}(Q([b]))$$

↑

can be negative in the presence of a chemical potential

But chemical potential only enters if the bags wind in a temporal direction!



Due to the presence of a fermion mass the bags will NOT wind for $U > U_c$ at zero temperature thus solving the silver blaze problem!

Extentions to more flavors

Action

$$S = -\sum_{\langle ij \rangle} \left(\sum_{\alpha=1}^{N_f} \left\{ \eta_{ij} (\overline{\psi}_{i,\alpha} \psi_{j,\alpha} e^{\mu_{ij}} - \overline{\psi}_{j,\alpha} \psi_{i,\alpha} e^{-\mu_{ij}}) \right\} + U \prod_{\alpha-1}^{N_f} (\overline{\psi}_{i,\alpha} \psi_{i,\alpha} \overline{\psi}_{j,\alpha} \psi_{j,\alpha}) \right)$$

Include also a fermion chemical potential

$4N_f$ fermion coupling!

A nightmare for Hubbard-Stratanovich approach

Trivial for the world-line approach!

In particular no sign problems for $\mu \neq 0$ when $N_f = 2,4,...$!

What happens at $U = \infty$?

Action reduces to $S(\psi, \overline{\psi}) = -\sum_{\langle ij \rangle} \overline{\psi}_i \psi_i \, \overline{\psi}_j \psi_j$

This leads to the partition function

$$Z = \sum_{C \in \text{closed packed dimers}} 1$$

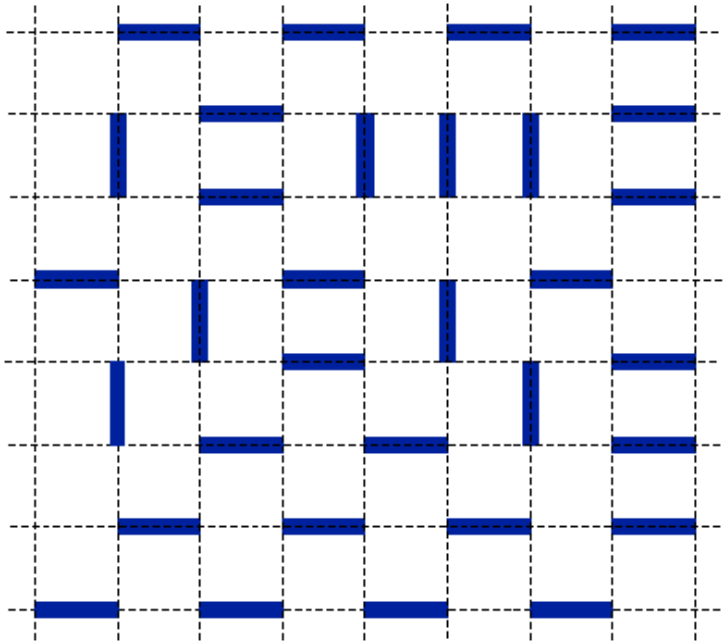
No sign problem!

Fermions are confined into bosons!

What is the long distance physics?

↑

Physics of the XY model!



A typical closed packed dimer configuration!

Bosonic Worldlines with Composite Fermions

XY Model in d-dimensions

$$S = -\sum_{x,i=1,2..,d} \overline{\psi}_x \psi_x \overline{\psi}_{x+i} \psi_{x+i} - T \sum_x \overline{\psi}_x \psi_x \overline{\psi}_{x+t} \psi_{x+t}$$

exact global U(1) symmetry:

$\psi_x \to e^{i\sigma_x \theta} \psi_x$ and $\overline{\psi}_x \to e^{i\sigma_x \theta} \overline{\psi}_x$ where σ_x is $+1$ on even sites and -1 on odd sites

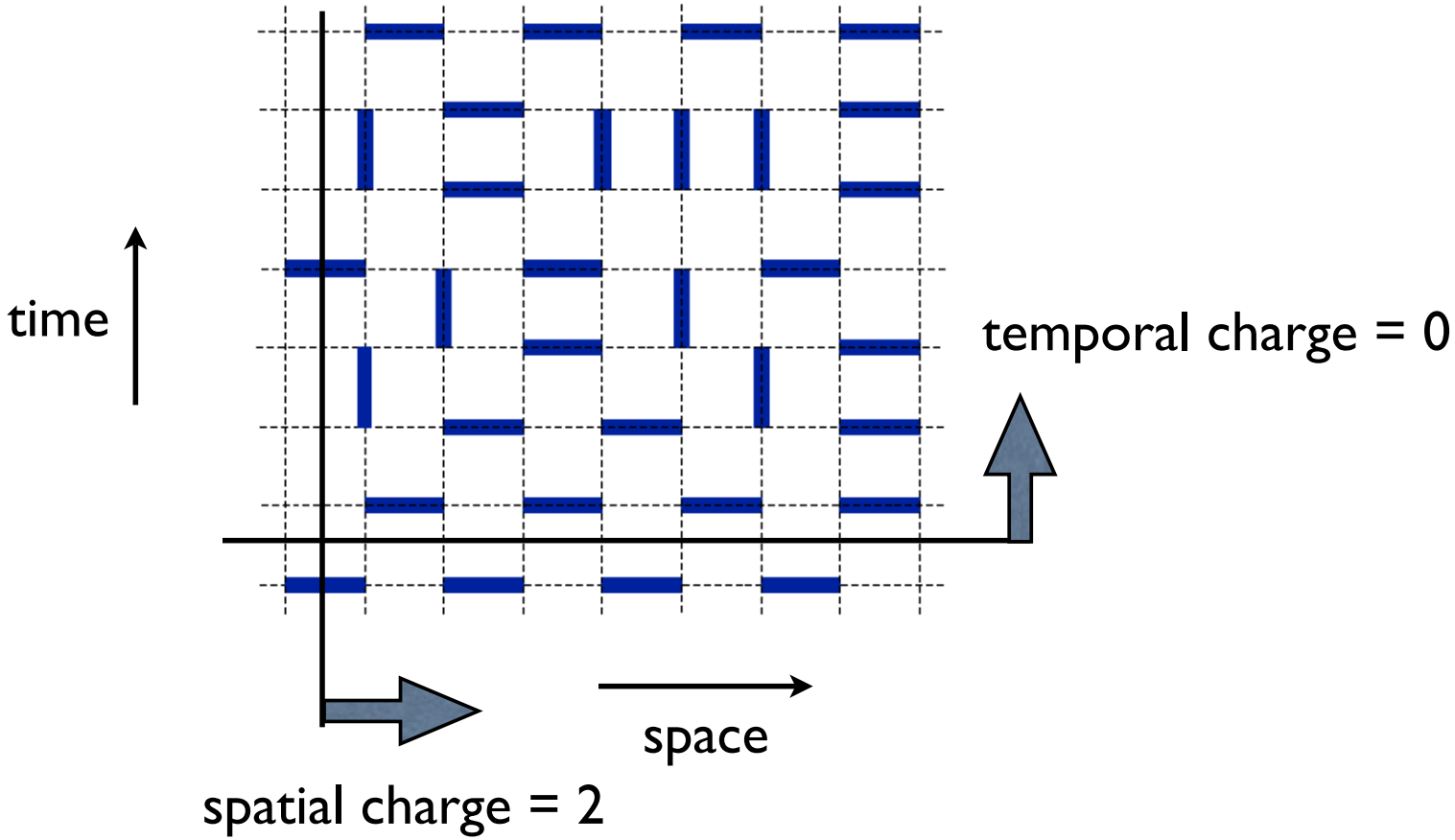
four-fermion terms
make the problem easy!

Kosterlitz-Thouless Transitions
&
XY critical behavior
have been demonstrated!

SC, Strouthos, 2003

Where is the conserved U(1) charge?

$Q = (-1)^i$ dimer number



Thus, we have found new way to formulate
the "XY" model using a purely four-fermion lattice field theory!

Pions with composite fermions

SC, Cecile, (2008)

A $SU(2) \times SU(2) \times U(1)$ model of composite fermions

Action

$$S = -\sum_{x,i=1,2..,d} \mathrm{Tr}[\Sigma_x\, \Sigma_{x+i}] - T\sum_x \mathrm{Tr}[\Sigma_x\, \Sigma_{x+t}] - c\sum_x \det\Sigma_x$$

c≠0
Anomaly

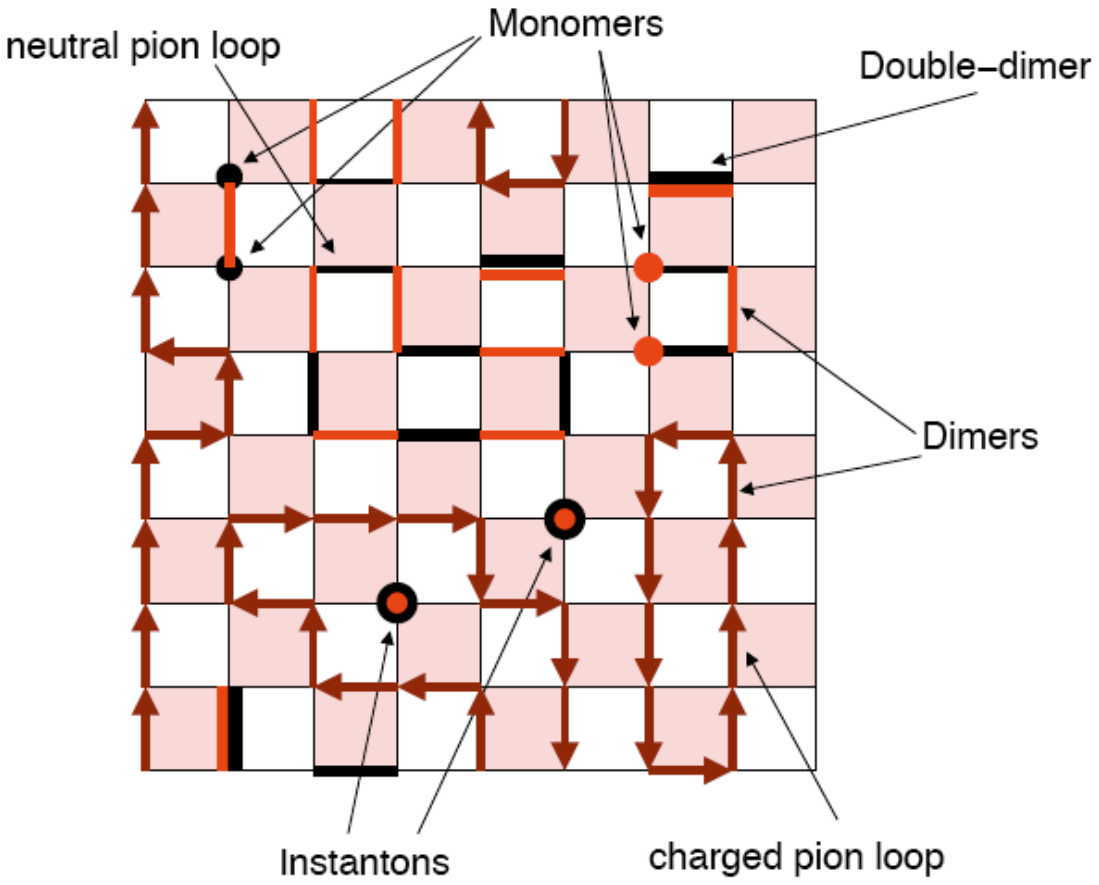
$$\Sigma_x \equiv \begin{pmatrix} u_x \\ d_x \end{pmatrix} \begin{pmatrix} \overline{u}_x & \overline{d}_x \end{pmatrix} = \begin{pmatrix} u_x\overline{u}_x & u_x\overline{d}_x \\ d_x\overline{u}_x & d_x\overline{d}_x \end{pmatrix}$$

Symmetry c = 0

$\Sigma_x \to L\Sigma_x R^\dagger e^{i\phi}$ for x even

$\Sigma_x \to R\Sigma_x L^\dagger e^{-i\phi}$ for x odd

Configurations of the model



It is trivial to add an isospin
chemical potential without a sign problem!

Applications to QCD physics?

The effective static quark model with Potts interaction

$$Z = \sum_{[z]} \prod_x \left(C_0 + C_1 \mathrm{e}^{-(m-\mu)/T} z_x + C_{-1} \mathrm{e}^{-(m+\mu)/T} z_x^* \right) \prod_{<xy>} \mathrm{e}^{\beta \{z_x \; z_y^* + z_y \; z_x^*\}}$$

sign problem can be solved (similar to xy model!)

old meron cluster solution: Alford,et.al., 2000

$$Z = \sum_{[z]} \prod_{x \in space} \left(C_0 + C_1 \mathrm{e}^{-(m-\mu)/T} z_x + C_{-1} \mathrm{e}^{-(m+\mu)/T} z_x^* \right) \prod_p \mathrm{e}^{\beta \; cos(z_p)}$$

sign problem can be solved (similar to scalar gauge model!)

These examples show that a partial averaging over the "local" Z3 degrees of freedom on "all" the links may reduce the sign problem

Luscher and Weisz

Applications to the static quark limit with SU(3) fields would interesting

One can solve the sign problem completely in strongly coupled QCD with one flavor of staggered fermions in the presence of a baryon chemical potential for all even N_c

extension of Karsch and Mutter, 1991

Is there a simplification at weaker coupling at even N_c ?

One can solve the sign problem completely in strongly coupled QED with one flavor of Wilson fermions in three dimensions!

Wenger, 2009

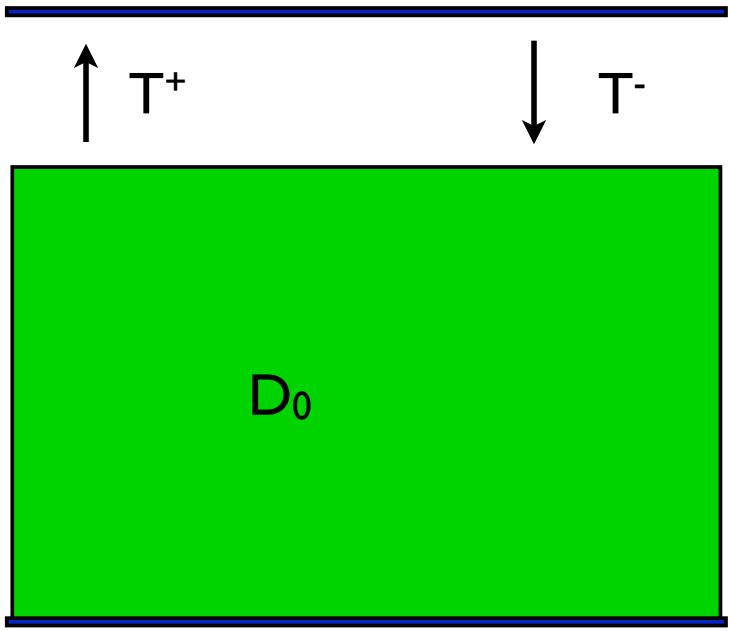
Silver Blaze problem in QCD

QCD partition function

$$Z = \int [DU]\, \mathrm{e}^{-S_g}\, \mathrm{Det}(D)$$

We could split D as follows

$$D = D_0 + \mathrm{e}^{\mu L} T^+ + \mathrm{e}^{-\mu L} T^-$$



$$\mathrm{Det}(D) = \mathrm{Det}(D_0)\mathrm{Det}(1 + \mathrm{e}^{\mu L} T^+ D_0^{-1} + \mathrm{e}^{-\mu L} T^- D_0^{-1})$$

↑

3d matrix!

Danzer and Gattringer, 2008

$$\mathrm{Det}(D) = \mathrm{Det}(D_0)\Big(\sum_q w_q \mathrm{e}^{q\mu L}\Big)$$

w_q will be in general complex!

After Z_3 avergaing partition function can be written as

$$Z \;=\; \int [DU]\; \mathrm{e}^{-S_g}\; \mathrm{Det}(D_0)\Big(\sum_q w_{3q} \mathrm{e}^{3q\mu L}\Big)$$

We expect that at large L (zero T)

$$Z_{3q} \;=\; \int [DU]\; \mathrm{e}^{-S_g}\; \mathrm{Det}(D_0)\; w_{3q} \;\sim\; \mathrm{e}^{-F_{3q} L}$$

canonical ensemble!

For $\mu < \mu_c$ Z is independent of μ

Thus it seems natural to write

$$Z = \int [DU]\, \mathrm{e}^{-S_g}\, \mathrm{Det}(D_0) w_0 \left(\sum_q \frac{w_{3q}}{w_0} \mathrm{e}^{3q\mu L} \right)$$

Positive weight to generate gauge fields

observable

We should find $\left\langle \sum_q \frac{w_{3q}}{w_0} \mathrm{e}^{3q\mu L} \right\rangle \sim 1$

for all μ less than the critical value

Questions:
How much does the quantity fluctuate?
Can averaging over polyakov loop degrees of freedom on every spatial site reduce these fluctuations quickly?

Conclusions

- World line formulations offer an alternative and powerful approach to lattice field theories
- Many bosonic sign problems with and without gauge fields due to a chemical potential can be solved exactly
- Fermionic sign problems remain difficult to solve in the presence of a chemical potential.
- But new insights and solutions emerge for some sign problems.
- In certain cases new "optimal" solutions arise which may yield better algorithm.
- Leads to new ideas to tackle the silver blaze problem in QCD