Fermion Bag Solutions to some Sign Problems

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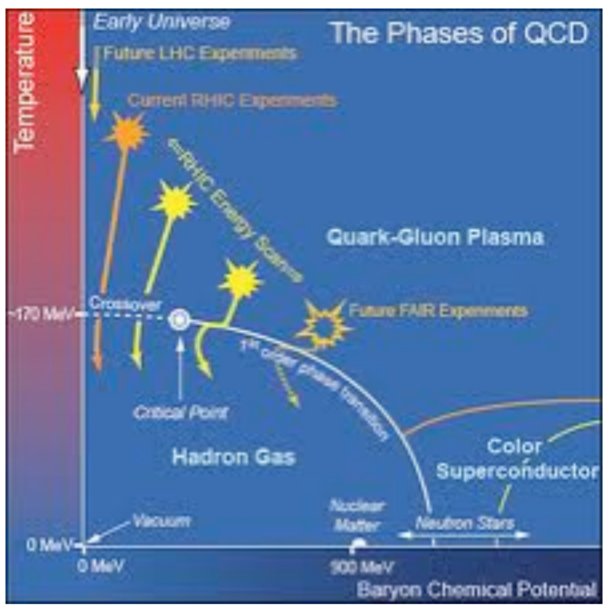
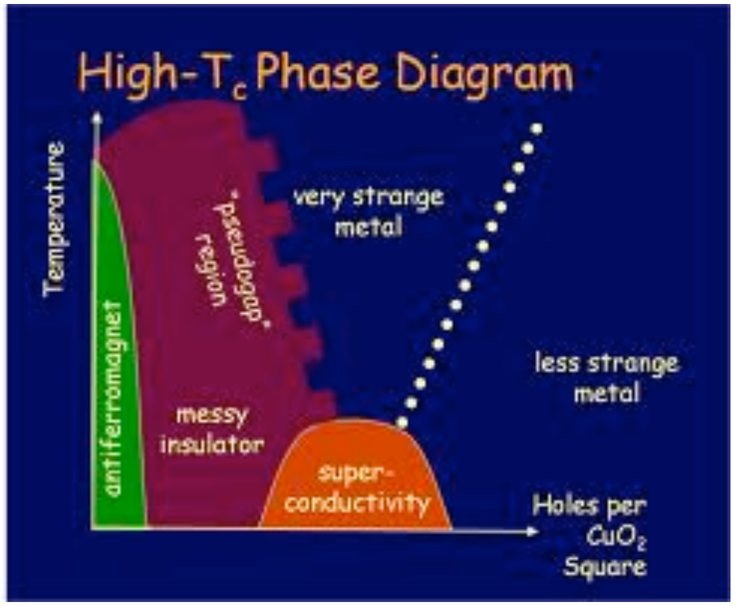
Motivation

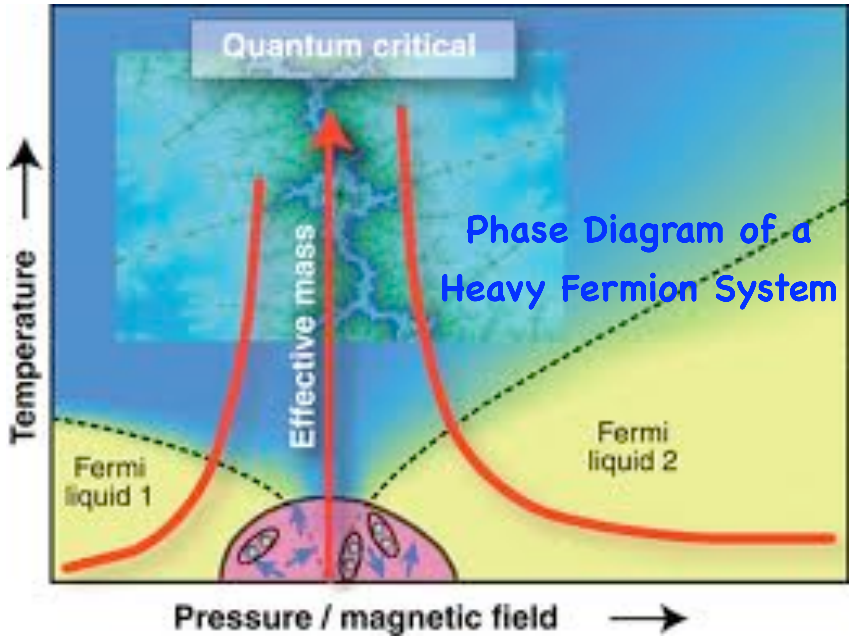
Challenge:
uncover phases of strongly correlated matter



QCD



High Tc



Kondo Lattice

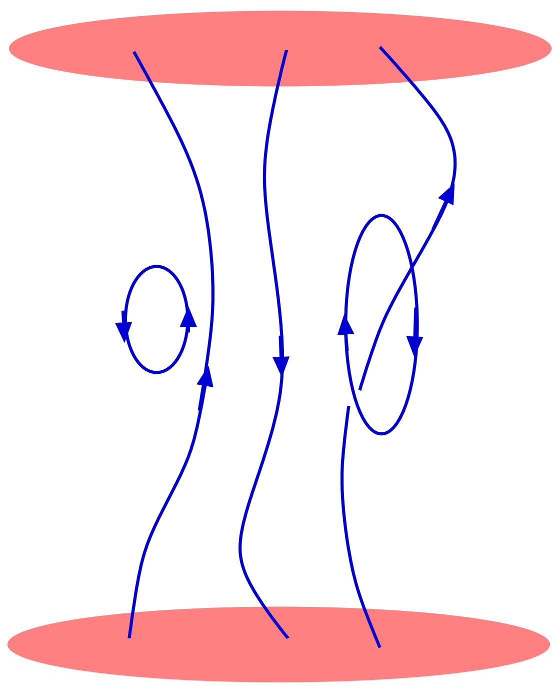
Many more examples:
BSM, Graphene, ...

Require Monte Carlo methods
Contain fermions
Suffer from Sign Problems!

Fermion Path Integrals

Partition function written as a Grassmann integration

$$\mathbf{Z} = \int [\mathbf{d}\psi(\mathbf{r},\mathbf{t})\ \overline{\psi}(\mathbf{r},\mathbf{t})]\ \mathrm{e}^{-\mathbf{S}([\psi(\mathbf{r},\mathbf{t}),\overline{\psi}(\mathbf{r},\mathbf{t})])}$$



Grassmann integrals equivalent to sum over worldline configurations [C]

$$\mathbf{Z} = \sum_{[\mathrm{C}]} \mathrm{Sign}[\mathrm{C}]\ \mathbf{W}[\mathrm{C}]$$

How to rewrite Z such that it is free of Sign Problems?

Conventional Approach

Convert the problem into an interacting fermion-boson problem where

Action :

$$\mathbf{S} \; = \int \mathbf{dr\;dt\;dr'\;dt'}\;\overline{\psi}(\mathbf{r},\mathbf{t})\;\mathbf{M}(\mathbf{r},\mathbf{t};\mathbf{r}',\mathbf{t}';\phi)\;\psi(\mathbf{r}',\mathbf{t}')+\mathbf{S_b}([\phi])$$

Partition function :

$$\mathbf{Z} = \int [\mathbf{d}\phi]\;\mathrm{e}^{-\mathbf{S_b}([\phi])}\;\int [\mathbf{d}\psi(\mathbf{r},\mathbf{t})\mathbf{d}\overline{\psi}(\mathbf{r},\mathbf{t})]\;\mathrm{e}^{-\overline{\psi}(\mathbf{r},\mathbf{t})\mathbf{M}(\mathbf{r},\mathbf{t};\mathbf{r}',\mathbf{t}';\phi)\psi(\mathbf{r}',\mathbf{t}')}$$

Fermions are free except for moving in background potentials generated by bosons

$$\mathbf{Z} = \int [\mathbf{d}\phi]\ \mathrm{e}^{-\mathbf{S_b}([\phi])} \int [\mathbf{d}\psi(\mathbf{r},\mathbf{t})\mathbf{d}\overline{\psi}(\mathbf{r},\mathbf{t})]\ \mathrm{e}^{-\overline{\psi}(\mathbf{r},\mathbf{t})\mathbf{M}(\mathbf{r},\mathbf{t};\mathbf{r}',\mathbf{t}';\phi)\psi(\mathbf{r}',\mathbf{t}')}$$

One "integrates out"
free fermions

$$\mathbf{Z}\ =\ \int [\mathbf{d}\phi]\ \mathrm{e}^{-\mathbf{S_b}([\phi])}\ \mathrm{Det}(\mathbf{M}(\mathbf{r},\mathbf{t};\mathbf{r}',\mathbf{t}';\phi))$$

Sign problem is solved if

$$\mathrm{Det}(\mathbf{M}(\mathbf{r},\mathbf{t};\mathbf{r}',\mathbf{t}';\phi)) \geq \mathbf{0}$$

Most calculations in fermion field theories use this approach today.

Very few problems fall in this class!

Fermion Bags

A new technique
which solves "some" sign problems
NOT solvable through the above methods

Basic Idea
Try to find "optimal" fermion degrees
of freedom that need to be
integrated over to solve sign problems

Fermion Bags ≡ Diagrammatic Methods

S.C (2005) — Rubtsov, Savkin, Lichtenstein (2005)

In lattice field theories

Fermion Bag is a more general idea

work at both Weak and Strong Couplings

Weak-Strong Coupling Duality

S.C & Anyi Li PRL108, (2012), 140404

Many new applications!

S.C & Anyi Li PRD85, 091502(R) 2012

S.C arXiv: 1205.0084 accepted in PRD(R)

Lattice Yukawa Model (in 3d)

Action

$$\mathbf{S}(\phi,\overline{\psi},\psi) = \sum_{\mathbf{xy}} \overline{\psi}_{\mathbf{x}} \mathbf{D}^{\mathbf{0}}_{\mathbf{xy}} \psi_{\mathbf{x}} \;-\; \mathbf{g} \sum_{\mathbf{x}} \phi_{\mathbf{x}} \overline{\psi}_{\mathbf{x}} \psi_{\mathbf{x}} - \beta \sum_{\mathbf{x},\alpha} \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}$$

x,y ≡ cubic lattice sites, α=1,2,3 refers to directions

$\psi_{\mathbf{x}}, \overline{\psi}_{\mathbf{x}}$ are two Grassmann fields per lattice site

$\Phi_x = \pm 1$ is an Ising field

D^0 is the massless staggered matrix

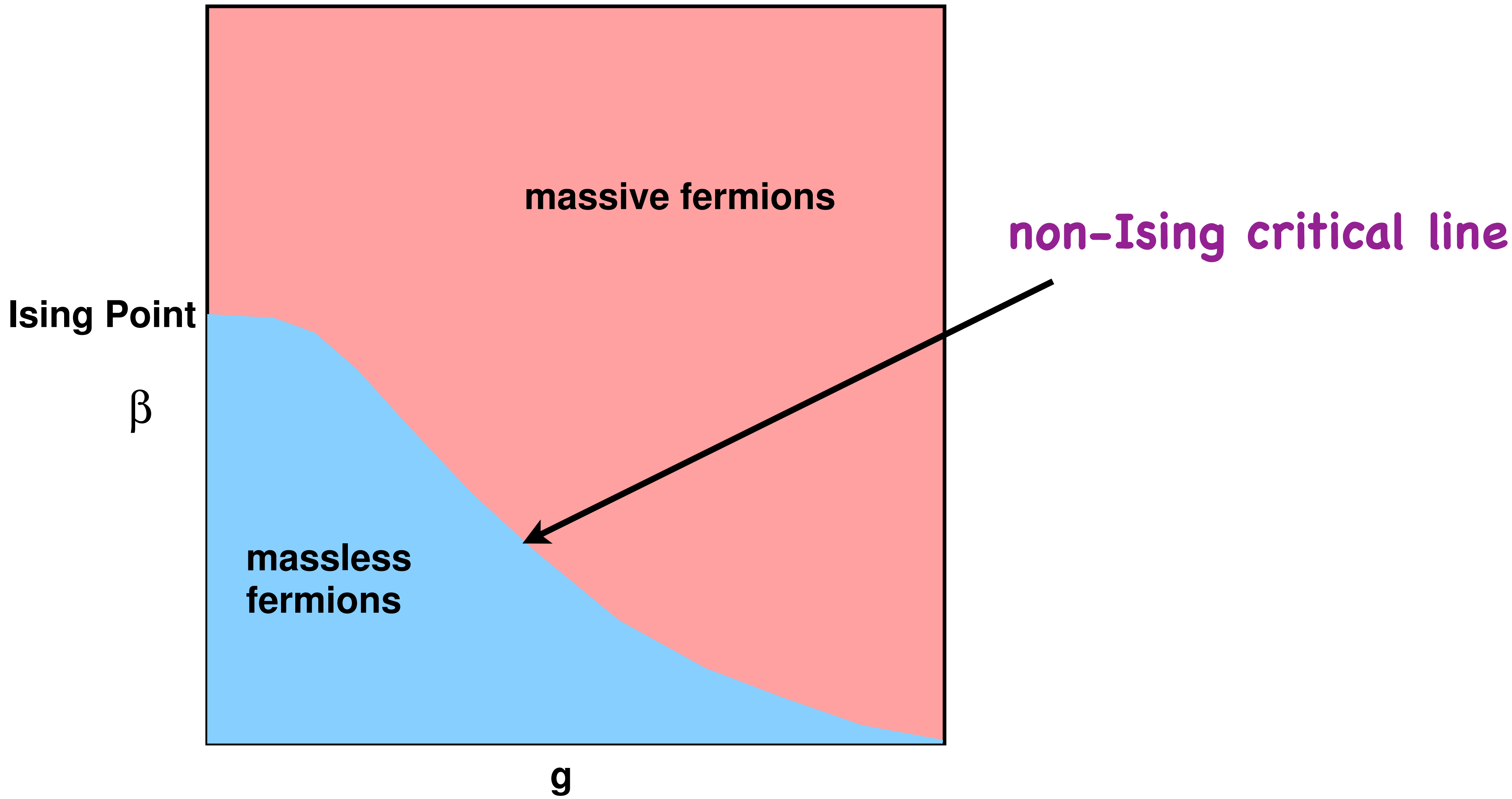
g,β are couplings and

Can rewrite the action

$$\mathbf{S}(\phi,\overline{\psi},\psi) = \sum_{\mathbf{xy}} \overline{\psi}_{\mathbf{x}}\; \mathbf{M}_{\mathbf{xy}}[\phi]\; \psi_{\mathbf{x}} - \beta \sum_{\mathbf{x},\alpha} \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}, \quad \mathbf{M}_{\mathbf{xy}}[\phi] = \mathbf{D}^{\mathbf{0}}_{\mathbf{xy}} - \;\mathbf{g}\; \phi_{\mathbf{x}}\; \delta_{\mathbf{xy}}$$

Zero Temperature (minimal) Phase Diagram

$$\mathbf{S}(\phi, \overline{\psi}, \psi) = \sum_{\mathbf{xy}} \overline{\psi}_{\mathbf{x}} \mathbf{D}^{\mathbf{0}}_{\mathbf{xy}} \psi_{\mathbf{x}} \; - \; \mathbf{g} \sum_{\mathbf{x}} \phi_{\mathbf{x}} \overline{\psi}_{\mathbf{x}} \psi_{\mathbf{x}} - \beta \sum_{\mathbf{x},\alpha} \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}$$



Quantum critical line for g > 0

is interesting but remains unexplored!

Sign Problem!

Partition function

$$\mathbf{Z} = \sum_{[\phi]} \left(\prod_{\mathbf{x},\alpha} \mathrm{e}^{\beta \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}} \right) \int [\mathbf{d}\overline{\psi}\mathbf{d}\psi]\ \mathrm{e}^{-\overline{\psi}\ \mathbf{M}[\phi]\ \psi}$$

$$\mathbf{Z} = \sum_{[\phi]} \left(\prod_{\mathbf{x},\alpha} \mathrm{e}^{\beta \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}} \right) \mathrm{Det}(\mathbf{M}(\phi))$$

$$\mathbf{M}_{\mathbf{xy}}[\phi] = \mathbf{D}^{\mathbf{0}}_{\mathbf{xy}} - \mathbf{g}\ \phi_{\mathbf{x}}\ \delta_{\mathbf{xy}}$$

M(Φ) has the form $\mathbf{M} = \begin{pmatrix} d_1 & A \\ -A^T & d_2 \end{pmatrix}$

Determinant of M(Φ) is not guaranteed to be positive!

The Fermion Bag solution!

Rewrite the partition function as

$$\mathbf{Z} = \sum_{[\phi]} \left(\prod_{\mathbf{x},\alpha} \mathrm{e}^{\beta \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}} \right) \int [\mathbf{d}\overline{\psi}\mathbf{d}\psi]\ \mathrm{e}^{-\overline{\psi}\ \mathbf{D^0}\ \psi} \prod_{\mathbf{x}} \left(\mathrm{e}^{\mathbf{g}\ \phi_{\mathbf{x}}\ \overline{\psi}_{\mathbf{x}} \psi_{\mathbf{x}}} \right)$$

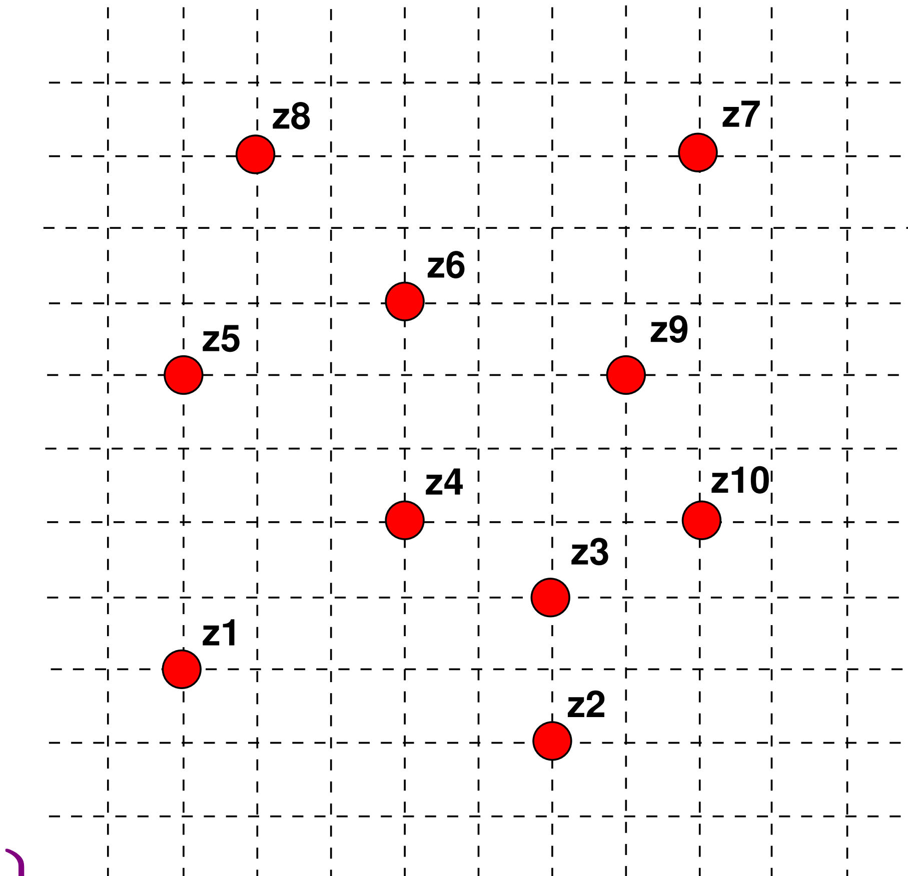
Due to the Grassmann nature

$$\mathrm{e}^{\mathbf{g}\ \phi_{\mathbf{x}}\ \overline{\psi}_{\mathbf{x}} \psi_{\mathbf{x}}} = \mathbf{1} + \mathbf{g}\ \phi_{\mathbf{x}} \overline{\psi}_{\mathbf{x}} \psi_{\mathbf{x}} = \sum_{\mathbf{n_x}=\mathbf{0},\mathbf{1}} \left(\mathbf{g}\ \phi_{\mathbf{x}} \overline{\psi}_{\mathbf{x}} \psi_{\mathbf{x}} \right)^{\mathbf{n_x}}$$

We can then rewrite

$$\mathbf{Z} = \sum_{[\mathbf{n_x}]} \sum_{[\phi]} \left(\prod_{\mathbf{x},\alpha} \mathrm{e}^{\beta \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}} \right) \int [\mathbf{d}\overline{\psi}\mathbf{d}\psi]\ \mathrm{e}^{-\overline{\psi}\ \mathbf{D^0}\ \psi} \prod_{\mathbf{x}} \left(\mathbf{g} \phi_{\mathbf{x}} \overline{\psi}_{\mathbf{x}} \psi_{\mathbf{x}} \right)^{\mathbf{n_x}}$$

example of configuration $[n_x]$ with $k = 10$



For a given configuration [n]

let $z_1\ z_2\ \ldots\ z_k$ be the k sites

where $n_x = 1$

at all other sites $n_x = 0$

$$\mathbf{Z} = \sum_{[\mathbf{n}]} \mathbf{g}^{\mathbf{k}} \left\{ \sum_{[\phi]} \left(\prod_{\mathbf{x},\alpha} e^{\beta \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}} \right) \prod_{\mathbf{x}} (\phi_{\mathbf{x}})^{\mathbf{n}_{\mathbf{x}}} \right\}$$

$$\left\{ \int [\mathbf{d}\overline{\psi}\mathbf{d}\psi]\ e^{-\overline{\psi}\ \mathbf{D^0}\ \psi}\ \overline{\psi}_{\mathbf{z_1}} \psi_{\mathbf{z_1}} \ldots \overline{\psi}_{\mathbf{z_k}} \psi_{\mathbf{z_k}} \right\}$$

Bosonic integral

Fermionic integral

Fermion Bag Approach

Fermion Integral is a k-point correlation function

$$\left\{ \int [\mathbf{d}\overline{\psi}\mathbf{d}\psi]\ \mathrm{e}^{-\overline{\psi}\ \mathbf{D^0}\ \psi}\ \ \overline{\psi}_{\mathbf{z_1}}\psi_{\mathbf{z_1}}\ldots\overline{\psi}_{\mathbf{z_k}}\psi_{\mathbf{z_k}} \right\}$$

$$= \ \mathrm{Det}(W^0) \geq \ 0$$

W^0 is a (V-k) x (V-k) matrix

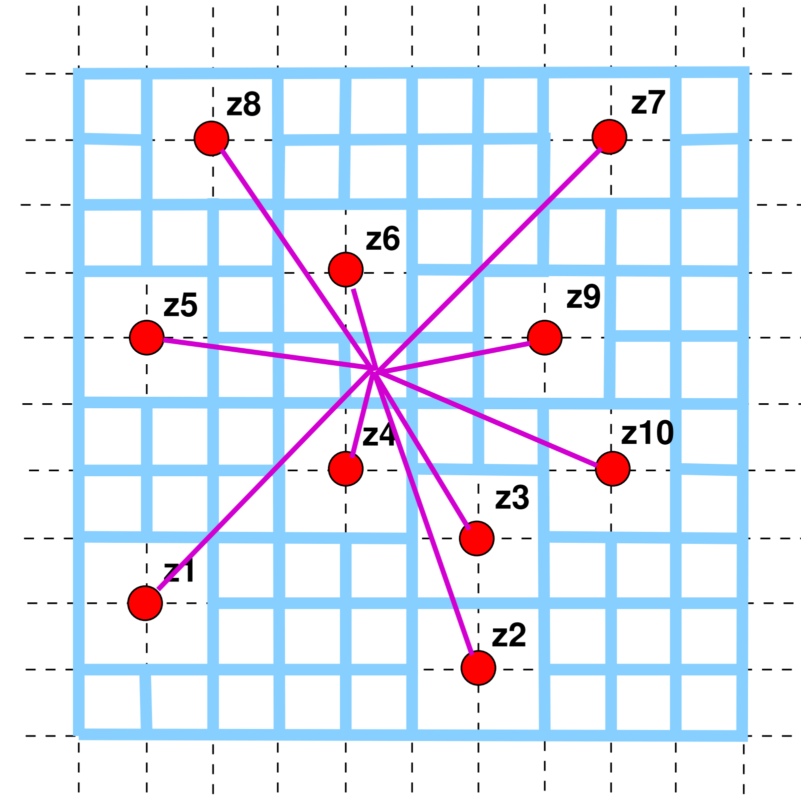
obtained by dropping sites z_1 ... z_k in D^0

S.C (2005)

$$= \ \mathrm{Det}\ D^0\ \mathrm{Det}\ G_{[n]} \ \geq \ 0$$

where $G_{[n]}$ is a (k x k) matrix of propagators

Rubtsov, Savkin, Lichtenstein (2005)



fermion bag configurations

Duality Relation : $\mathrm{Det}\ W^0 = \mathrm{Det}\ D^0\ \mathrm{Det}\ G_{[n]}$

strong coupling fermion bag

weak coupling fermion Bag

Worldline Approach

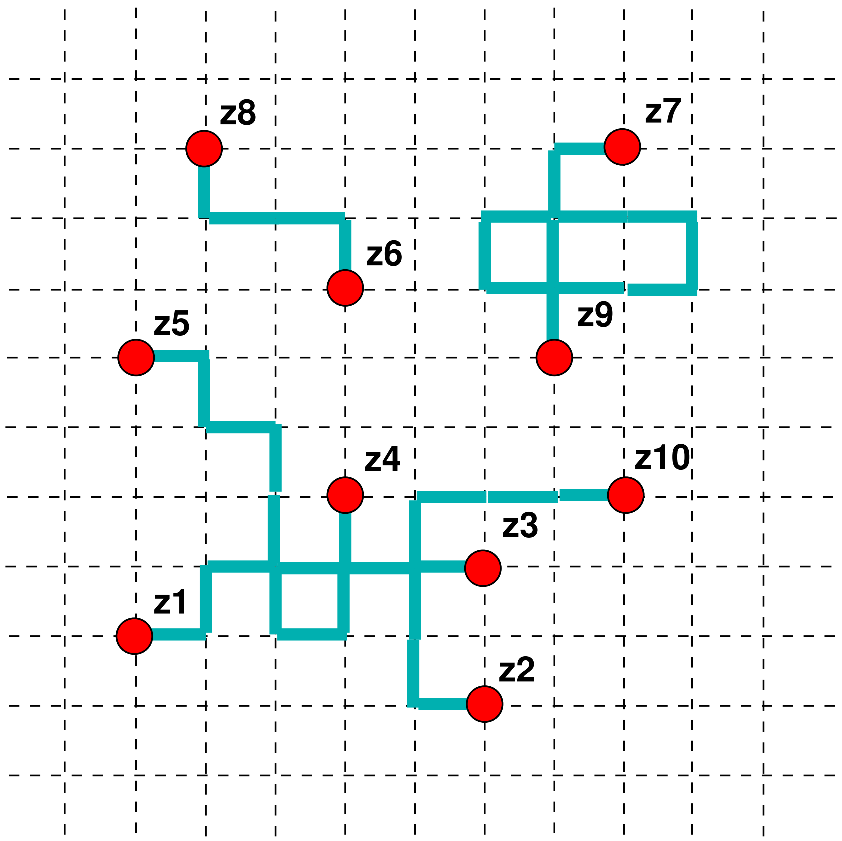
Boson Integral is also a k-point correlation function

$$\sum_{[\phi]} \left(\prod_{\mathbf{x},\alpha} e^{\beta \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}} \right) \prod_{\mathbf{x}} (\phi_{\mathbf{x}})^{\mathbf{n_x}}$$

$$e^{\beta \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}} = \cosh(\beta) + \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha} \sinh(\beta)$$

$$= \mathbf{\Omega_0} + \mathbf{\Omega_1}\ \phi_{\mathbf{x}}\ \phi_{\mathbf{x}+\alpha}$$

$$\sum_{\phi=+1,-1} (\phi)^{\mathbf{k}} = \mathbf{2}\ \delta_{\mathbf{k,mod2}}$$

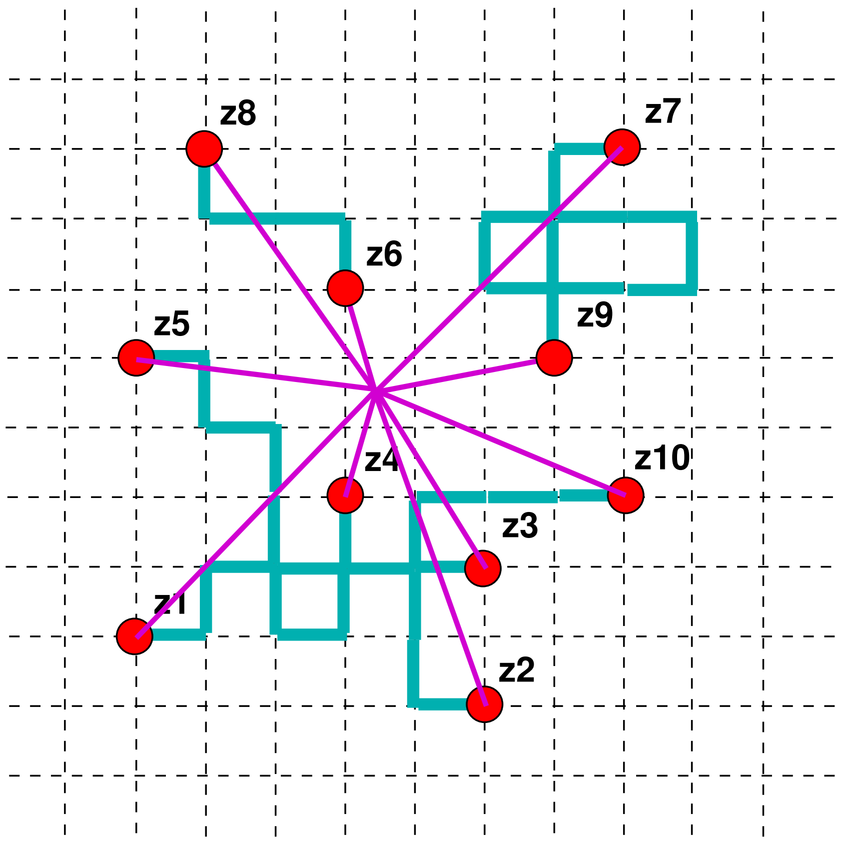


example of a [b] configuration consistent with [n]

$$\sum_{[\phi]} \left(\prod_{\mathbf{x},\alpha} e^{\beta \phi_{\mathbf{x}} \phi_{\mathbf{x}+\alpha}} \right) \prod_{\mathbf{x}} (\phi_{\mathbf{x}})^{\mathbf{n_x}} = \mathbf{2^V} \sum_{[\mathbf{b}]} \prod_{\mathbf{b_{x,\alpha}}} \mathbf{\Omega_{b_{x,\alpha}}} \prod_{\mathbf{x}} \delta_{\mathbf{n_x} + \sum_\alpha (\mathbf{b_{x,\alpha}} + \mathbf{b_{x-\alpha,\alpha}}), \mathbf{mod2}}$$

Thus, the final partition function is given by

$$Z = \mathcal{N} \sum_{[n,b]} \mathrm{Det}(G_{[n]}) \prod_x (g)^{n_x} \prod_{x,\alpha} (\tanh(\beta))^{b_{x,\alpha}}$$
$$\times \prod_x \delta_{n_x + \sum_\alpha (b_{x,\alpha} + b_{x-\alpha,\alpha}),\mathrm{mod}2}$$



There is no sign problem!

[n,b] configurations

What can we solve now?

The new solutions are applicable to many (not ALL!) standard models!

A solvable model with Wilson fermions can be found in

S.C arXiv: 1205:0084

(See Anyi Li's talk for an SU(2) NJL model!)

Models contain

Z_2, U(1), SU(2) symmetries

Many fermionic QCP's are within reach!

Efficient algorithms can also be designed close to QCP!

first calculations of fermionic critical behavior

S.C & Anyi Li PRL108, (2012), 140404

Conclusions

- Solutions to sign problem may require an entire reformulation of the problem both in bosonic and fermionic sectors.
- Some unsolved sign problems are now solvable! How much can we extend?
- New strongly correlated fermion models with QCP are now within reach with efficient algorithms.