Quantum Mechanics
and
the Computational Challenges
for the 21st century

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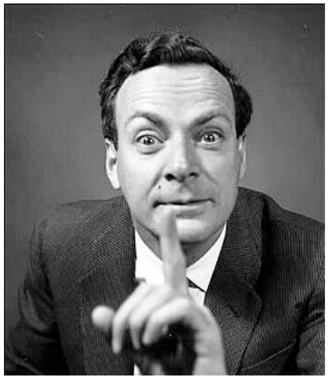
In Quantum Mechanics we usually ....

shut up and calculate!

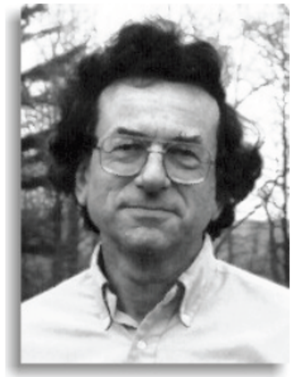
Could Feynman Have Said This?

N. David Mermin
May 2004, page 10

Physics Today



R.P. Feynman



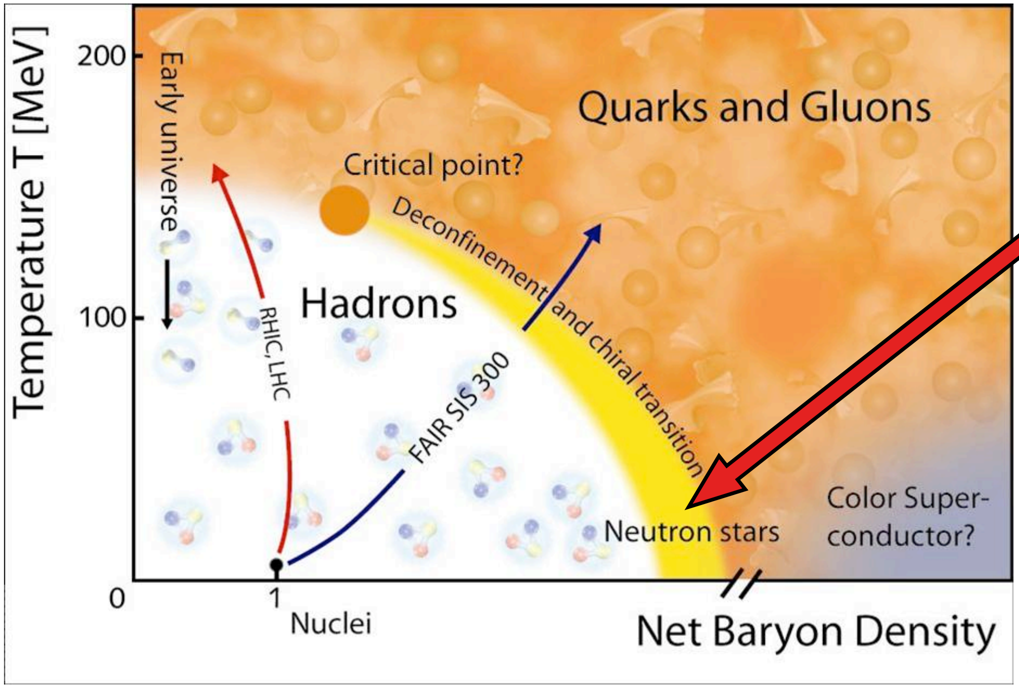
N. David Mermin

What if it is too difficult to calculate?

Many interesting problems fall in this class!

How to calculate in quantum many body physics
<u>without a small parameter</u>
is the challenge for the 21st century!

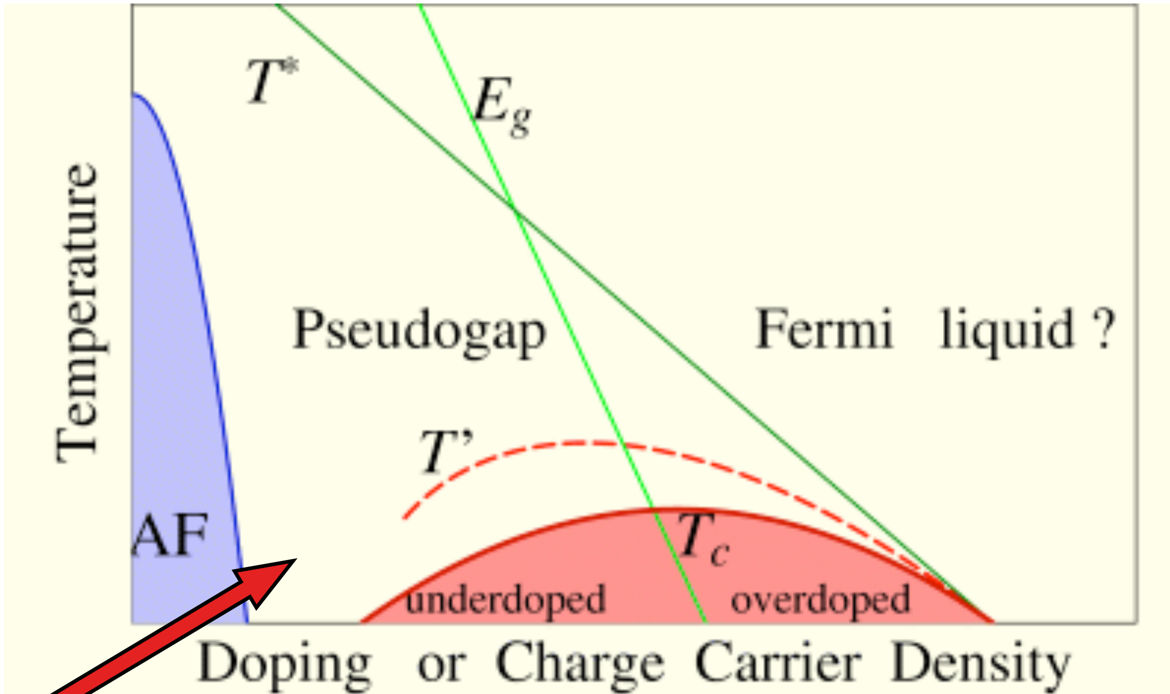
Example 1: The QCD Phase Diagram



Region of competing interactions

A first principles calculation in QCD is still missing!

Example 2: Phase Diagram of a High Tc Material



Region of competing interactions

A first prinicples calculation within a "good" model which reproduces all the features is still missing

- many more examples:
  - metal insulator transitions
  - de-confined quantum critical points
  - conformal phase transitions
  - dynamical supersymmetry breaking
  - ...

All examples have some things in common!

quantum mechanics important
(phases and interference play a role)

Strong interactions
(no small parameter)

competing interactions/orders
(frustrations)

long range forces
(light particle exchange)

Most calculations today involve uncontrolled approximations!

Origin of the Problem

Need to compute expectation values
in quantum statistical mechanics

$$\langle O \rangle = \frac{1}{Z} \mathrm{Tr}\left(\hat{O} \left\{ \frac{\mathrm{e}^{-\frac{\hat{H}}{kT}}}{Z} \right\} \right) \qquad Z = \mathrm{Tr}\left(\mathrm{e}^{-\frac{\hat{H}}{kT}} \right)$$

where Z is the partition function

This calculation is not easy in general without a small parameter!

computational approach is the only alternative

But "two challenges" exist!

First Challenge

Find an expansion such that

$$Z = \sum_C W([C])$$

positive

$$\langle O \rangle = \sum_C O([C]) \left\{ \frac{W([C])}{Z} \right\}$$

Probability distribution

Second Challenge

Develop an "efficient" Monte Carlo method to generate "[C]"

Can we always write Z using the Feynman path integral

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

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

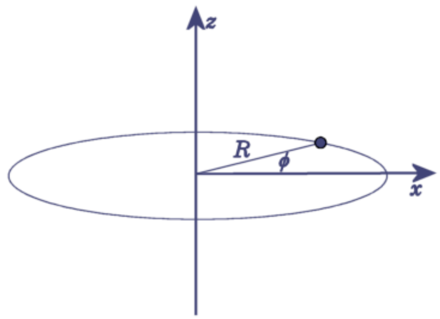
positive?

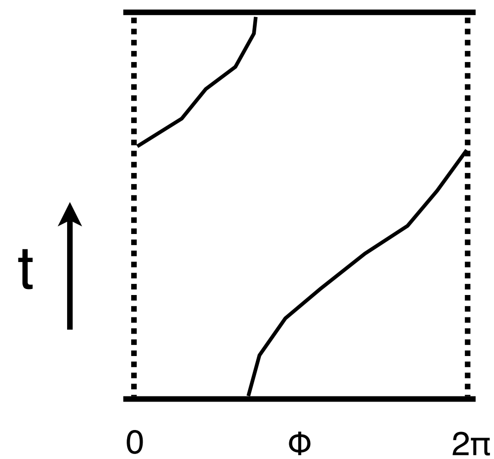
If the action is real
then the first challenge can be overcome!

If the action is real
Quantum Statistical Mechanics ≡ Classical Statistical Mechanics

The second challenge could still remain!

Example: Quantum Particle on a circle





$$S([\phi]) = \frac{mR^2}{2} \int_0^{1/(kT)} dt \quad \left(\frac{d\phi(t)}{dt} \right)^2$$

world line of the particle

For a free particle
the action is indeed real!

It is not always easy find an expansion such that

$$Z = \sum_C W([C]) \qquad \langle O \rangle = \sum_C O([C]) \left\{ \frac{W([C])}{Z} \right\}$$

positive

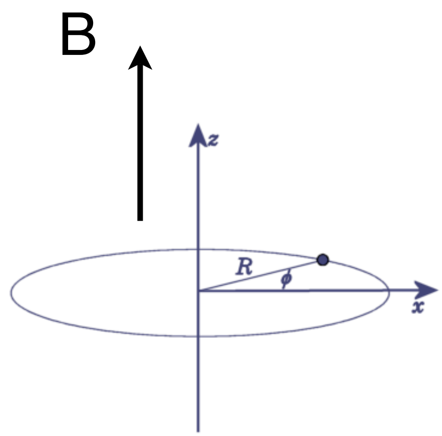
Remember that $Z = \mathrm{Tr}\left(\mathrm{e}^{-\frac{\hat{H}}{kT}} \right)$

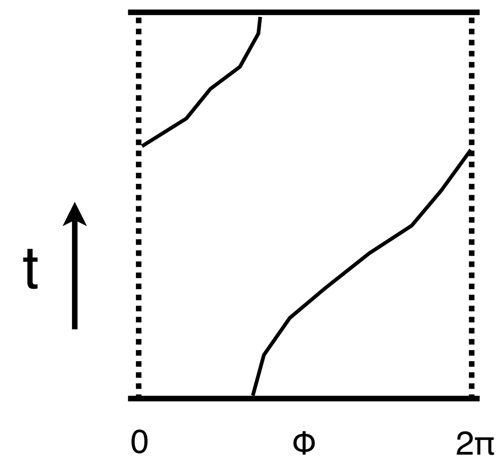
So Z > 0!
but not necessarily W([C])

In quantum mechanics "phases" can and do arise
and usually contain interesting physics!

If the first challenge cannot be overcome
we say
there is a "sign problem"

Particle on a circle in a magnetic field





winding number: $\omega = 1$

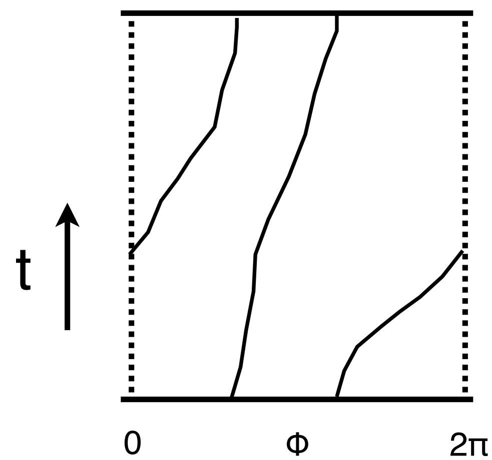
$$S([\phi]) = i\ \omega\ \gamma B + \frac{mR^2}{2} \int_0^{1/(kT)} dt \ \left(\frac{d\phi(t)}{dt} \right)^2$$

action is complex!

Aharanov Bohm phase

Fermions and the Pauli Principle

world-line for two identical fermions



The two world lines cannot touch! (Pauli principle)

ω is the spatial winding

$$S([\phi]) = i\ \omega\ \pi + \frac{mR^2}{2}\int_0^{1/(kT)} dt \left\{ \left(\frac{d\phi_1(t)}{dt}\right)^2 + \left(\frac{d\phi_2(t)}{dt}\right)^2 \right\}$$

complex action!

Origin is the quantum mechanical (Pauli principle)

Important note

The Feynman path integral is not unique
depends on the “basis” used in constructing it!

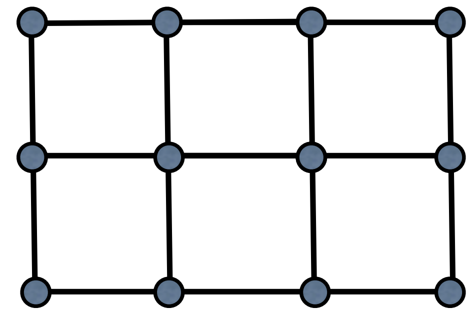
We can write the path integral
in different ways and explore if there is any
description where the “sign problem” is solved!

A solution to the sign problem can be
a conceptually interesting “physics” result

It may show that the under-lying quantum physics
has an “effective classical description”

Complex scalar field theory

Lattice Field: $\mathrm{e}^{i\phi_x}$ $\quad 0 \leq \phi_x < 2\pi$



Lattice Action:

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

Action is real!

Partition function: $\quad Z = \int [d\phi]\ \mathrm{e}^{-S([\phi])}$

(# of particles = # of antiparticles)

But, what happens if we have more particles than antiparticles?

Let us add a chemical potential!
(more particles than antiparticles!)

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!

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

Can we solve this sign problem? (First Challenge!)

World-line approach

One can rewrite the partition function in terms of "currents"

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

Use the Identity $\exp\left\{\beta\cos(\phi)\right\} = \sum_{k=-\infty}^{\infty} I_k\left(\beta\right)\mathrm{e}^{ik\phi},$

to write the partition function in terms of current variables

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

No sign problem!

current conservation

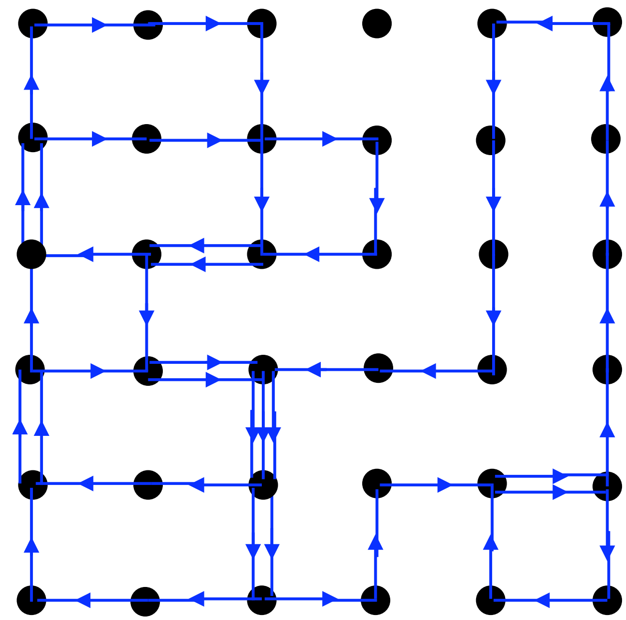
(First challenge overcome!)

Can update this system efficiently with the "worm algorithm"

Prokof'ev & Svistunov, 2000

(Second challenge overcome!)

example of a world line configuration



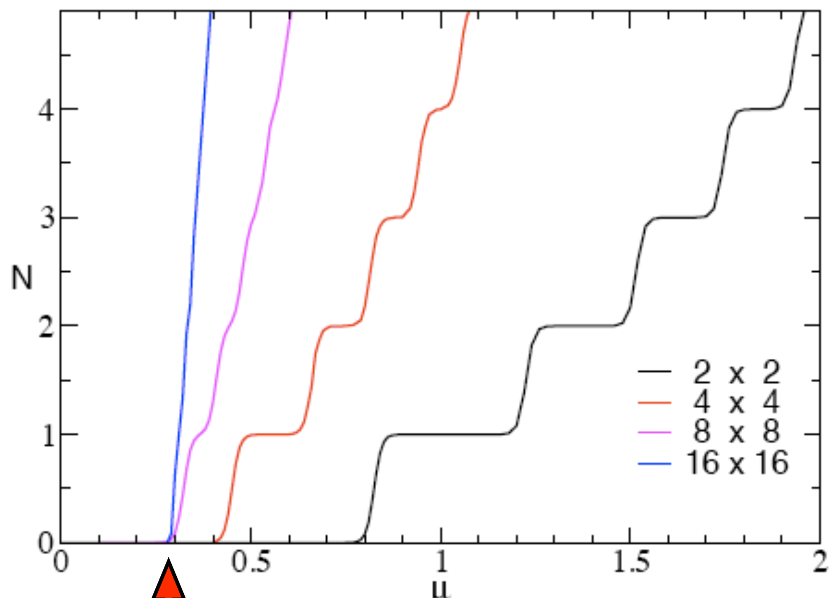
Each world line configuration is defined by a set of constrained integers on bonds [$k_{x,\alpha}$]

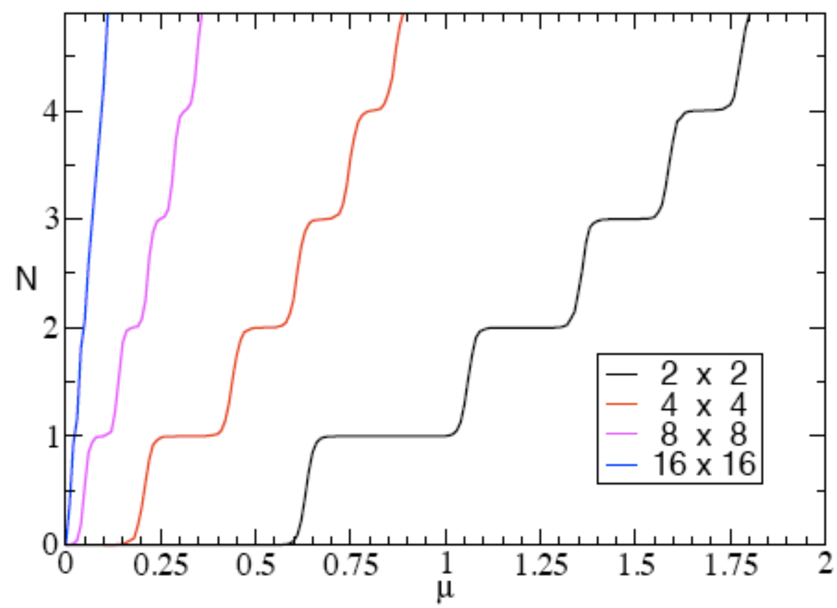
β - μ phase diagram has not yet been computed

At μ=0 there is an order-disorder phase transition at β ≈0.45

ongoing work by TIFR students

Debashish Banerjee, Sayantan Sharma, Jyotirmoy Maiti





μ_c

β=0.43

β=0.5

Fermions

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 lattice.

Grassmann Calculus encodes the Pauli principle!

$$\psi_1\psi_2 = -\psi_2\psi_1 \qquad \psi^2 = 0 \qquad \int d\psi = 0 \qquad \int d\psi\, \psi = 1$$

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! ... "

Massless Thirring Model

Action

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

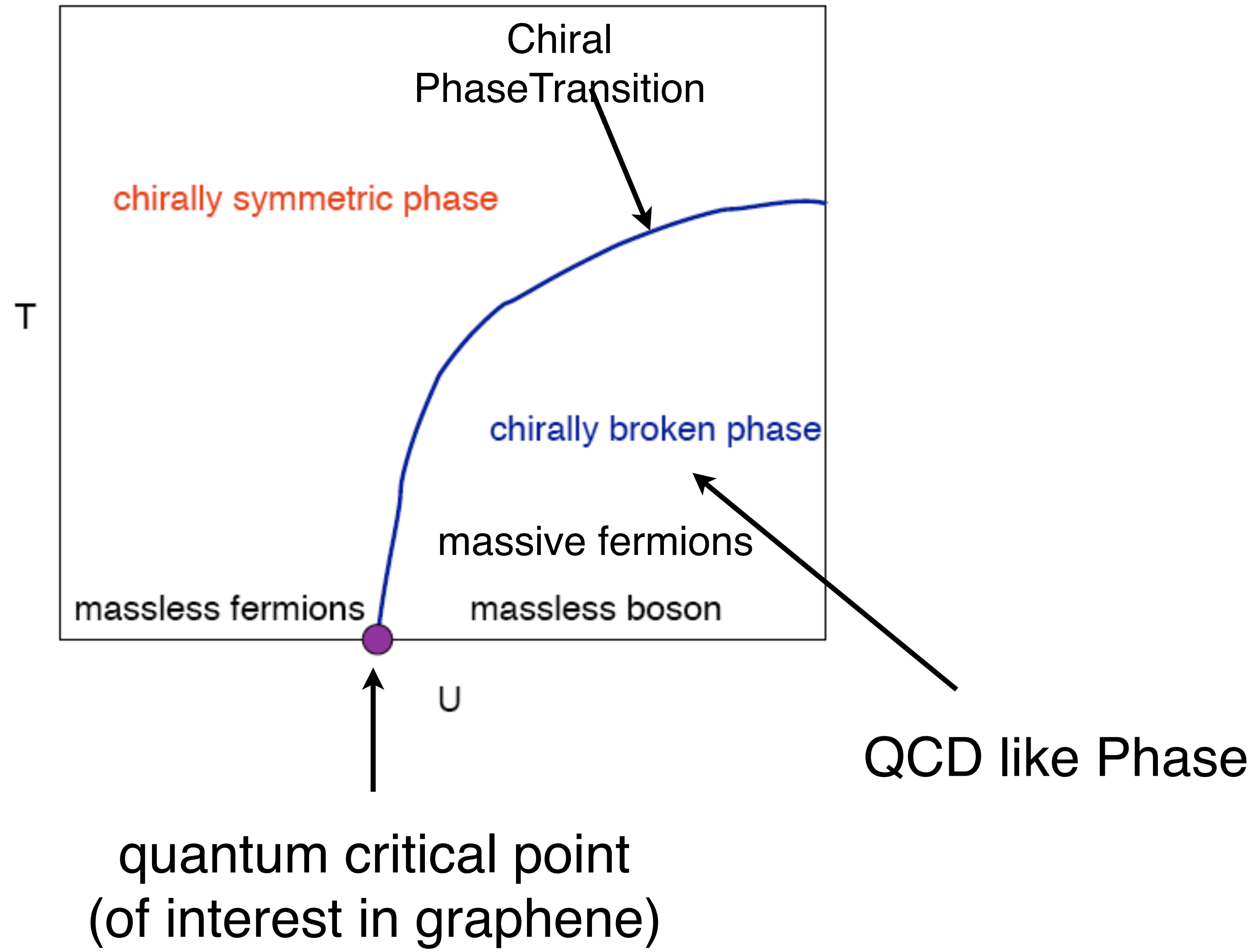
A proper choice of η_{ij} we can
get massless Dirac fermions at U = 0.

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

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

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

Physics of the model



Conventional Approach

Hirsch, Scalapino, Sugar,...(1980's)

Action

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

Using the Hubbard-Stratanovich transformation

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

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

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

Integrating out the fermions we get

$$\int [d\psi\ d\overline{\psi}]\ \mathrm{e}^{\overline{\psi} M[\phi]\psi} = \mathrm{Det}(M[\phi]) \quad \longrightarrow \quad Z = \int [d\phi]\mathrm{Det}(M[\phi])$$

If $\mathrm{Det}(M[\phi]) \geq 0$ then first challenge has been solved!

In our model this is true
But in many problems sign problems remain unsolved!

Second challenge still remains!

The problem has become completely non-local and unintuitive!

For large U, the matrix M has a large number of small eigenvalues and algorithms become inefficient

Many fermionic field theories including QCD fall in this class

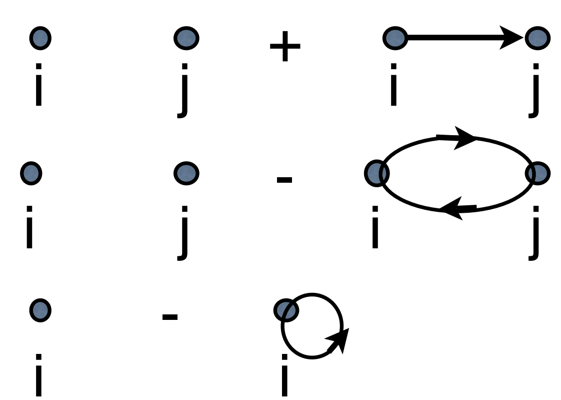
Fresh Ideas:
World-line Approach to fermions

Grassmann variables help in
generating world lines configurations

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

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

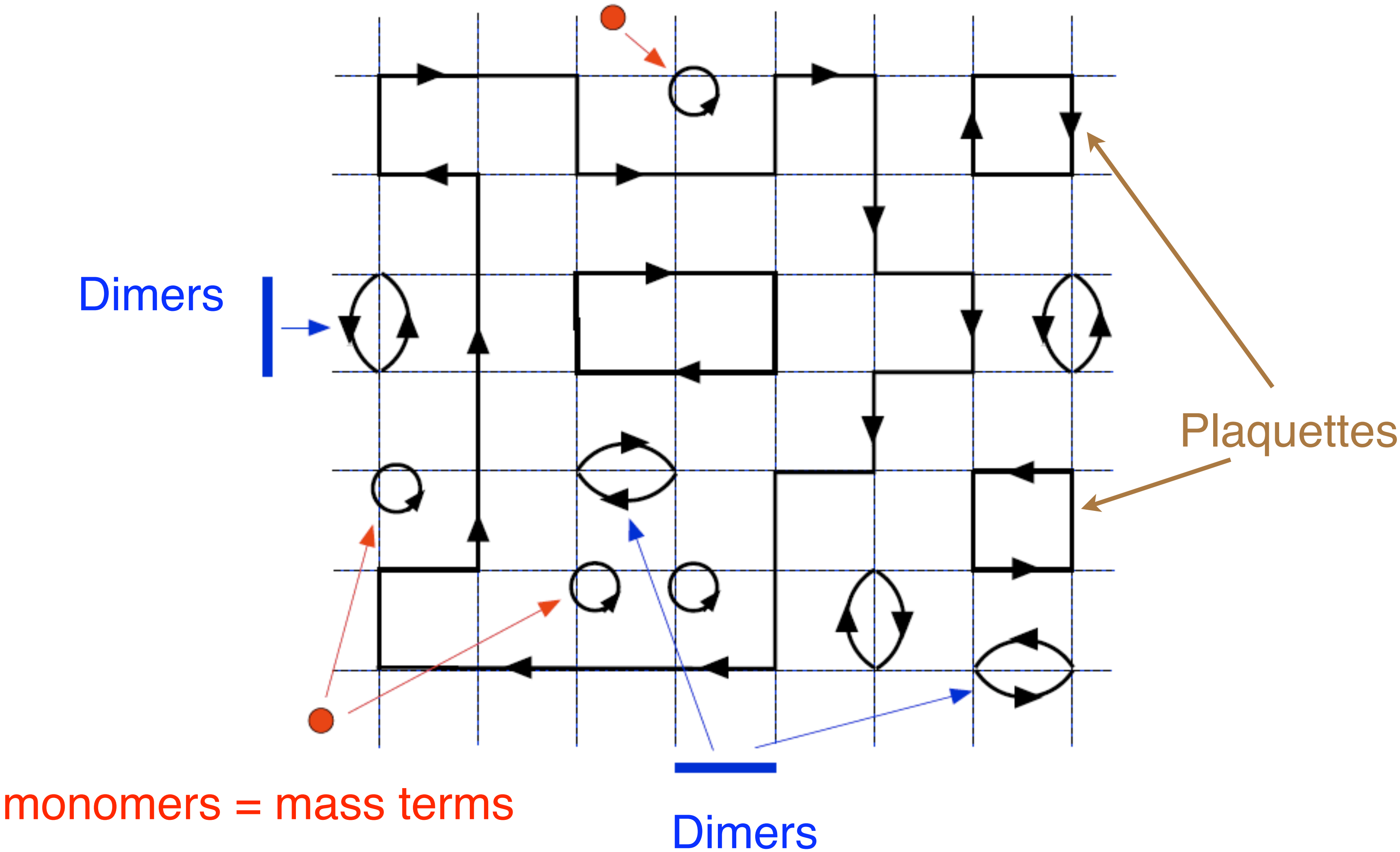
$$e^{-m\overline{\psi}_i\psi_i} = 1 - \overline{\psi}_i\psi_i =$$



Each site can have one incoming and one outgoing line
Every loop is associated with a negative sign.

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

A Fermion World-line configuration



Thus, the fermionic partition function can be written as

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

The sign of a configuration 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 the sign problems?

Research over the past decade shows that sign problems can indeed be solved in many ways!

Solutions to "fermion sign problems" always involve some kind of summation over a class of configurations (natural in quantum mechanics, physics of interference)

The determinant approach is one well known solution!

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

depending on "M" can be positive!

The "meron cluster" approach where the system is subdivided into clusters and configurations inside a cluster are summed

S.C and Wiese, 1999

More recently I have realized that the meron cluster approach is more general and the regions take the form of "fermion bags"

The Fermion-Bag approach to the Thirring model!

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

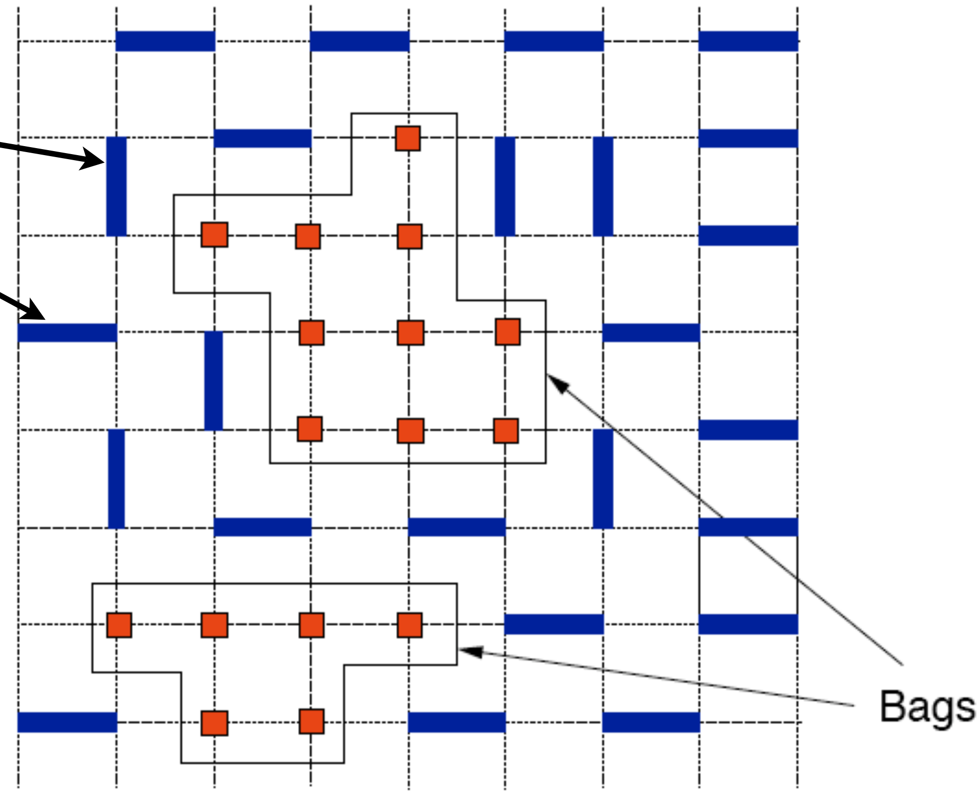
$$Z = \sum_{[b]} \left(\prod_{ij} U^{b_{ij}}\right) \left\{ \sum_{\text{free fermions}}' \mathrm{Sign}([C,b])\, W([C,b]) \right\}$$

Here free fermions hopp
on a lattice not touched by= $\mathrm{Det}\big(Q([b])\big)$
b=1 bonds.

positive definite

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

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



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"

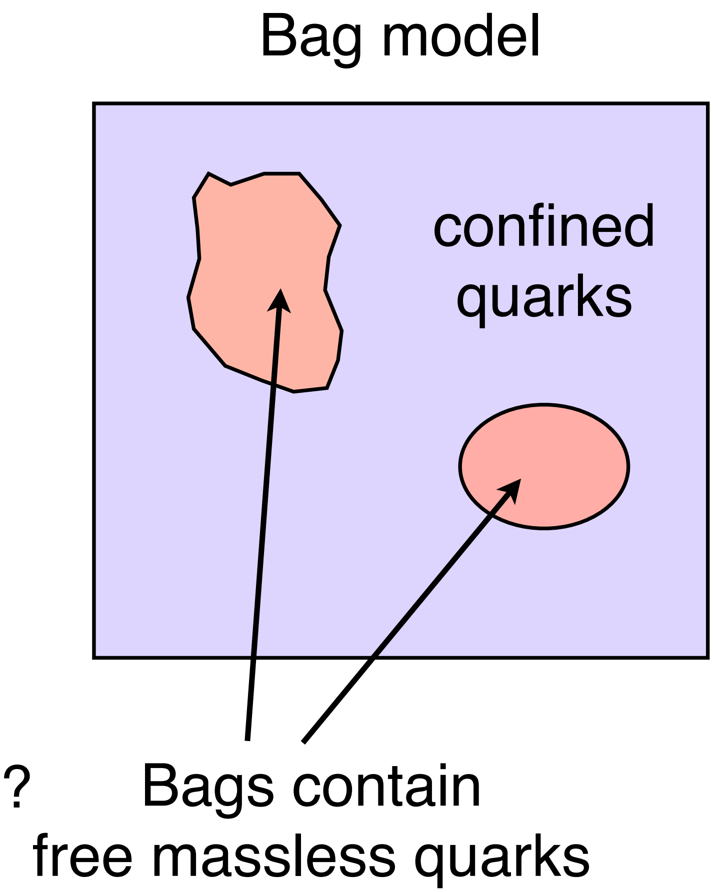
The effort to compute the determinant is "optimal"

Dynamical fermion mass generation

In QCD quarks acquire a mass through dynamics!

How?

The “MIT Bag” model provides a very intuitive way to understand it



Can this picture emerge starting from a QCD partition function?

Challenge for the future!

Chemical Potential and Flavors

Action

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

Include a
fermion chemical potential

$4N_f$ fermion coupling!

A nightmare in the Hubbard-Stratanovich approach

Trivial in the fermion-bag approach!

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

Interactions with gauge fields

The action is again complex in the conventional approach
especially in the presence of matter.

(**First challenge remains unsolved in many cases!**)

With bosons and electromagnetism
the partition function can some times be rewritten
in terms of “world lines” and “world sheets” without a sign problem.

No good algorithms yet to solve these problems efficiently!
(**Second challenge remains**)

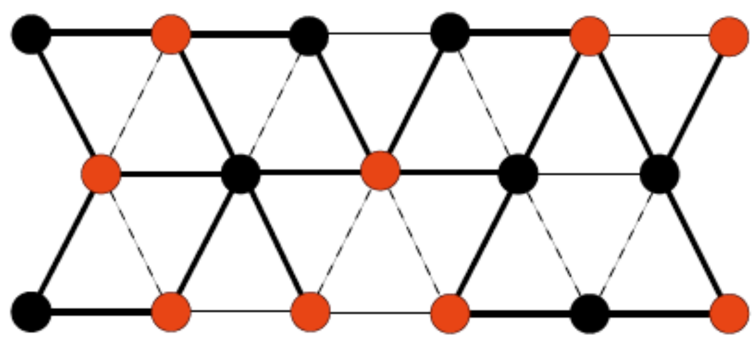
Solving these challenges could help us
a variety of physics of interest
in particle and condensed matter physics

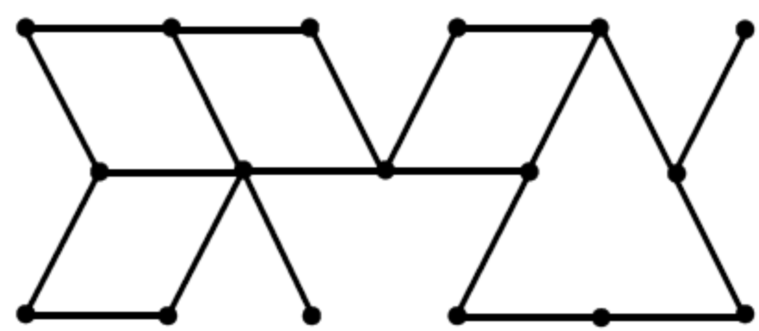
Frustrations

Often sign problems can be traded for frustrations

Problems can often be transformed
into questions in graph theory

Triangular Antiferromagnet





Ground State Partition Function = All graphs with no odd cycles but with maximal number of bonds

Computation and Complexity

- A lot of work going on in computer science on algorithms and complexity.
- complexity class of P versus NP problems are considered
- A sign problem can be thought of as an NP problem
- Once the sign problem is solved the problem becomes a P problem. But we still need to solve it efficiently.
- There are approximation algorithms being developed.

I wonder if something similar can be developed in physics?

Conclusions

- Sign Problems are at the heart of quantum many body physics. Attempts to solve them remains an important challenge for the future. Questions in real time remain even more difficult!
- World-line methods have been developed only over the last decade and appear to be very useful.
- A new "bag" approach for fermions is emerging.

Effective classical description of quantum problems often involve "non-local" objects.

- "Approximation algorithms" may need to be developed.

Quantum Mechanics may force us to develop a new computational paradigm for a host of problems