

# Algorithmic Issues for Lattice Gauge Theory

Michael Creutz

Brookhaven National Laboratory

## Mathematical formulation

- Gauge fields  $A$ , quark fields  $\psi$ , observable  $O$
- $\langle O \rangle = \frac{1}{Z} \int (dA)(d\psi d\bar{\psi}) O e^{-S}$
- $Z = \int (dA)(d\psi d\bar{\psi}) e^{-S}$
- $S = S_G + S_F = \int d^4x \left( \frac{1}{4} F_{\mu\nu} F_{\mu\nu} + \bar{\psi} M(A) \psi \right)$

$Z$  is formally a partition function in Statistical Mechanics

- 4-dimensional path integral makes problem classical
- spins  $\longrightarrow$  unitary 3 by 3 matrices
- many degrees of freedom; ripe for Monte Carlo simulation

## Euclidian space

- $e^{-iH} \rightarrow e^{-H}$
- excited states, scattering hard to extract

## Gauge fields alone

- Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller algorithm
- excellent convergence
- supercomputing not necessary

## Quarks in the valence/quenched approximation

- pure gauge simulation gives background gauge fields
- calculate quark propagators  $M^{-1}$  in these backgrounds
- use conjugate gradient algorithm
- combine propagators into hadrons
- measure spectra, matrix elements, etc.

## Dynamical simulations

- $\psi$  and  $\bar{\psi}$  are Grassman variables; action is not a number
- analytically integrate fermionic quadratic form
- $\int (d\psi d\bar{\psi}) e^{-\bar{\psi} M(A) \psi} = |M(A)|$
- classical statistical mechanics with a non-local interaction

$$Z = \int (dA) |M(A)| e^{-S_G(A)}$$

## Introduce pseudofermionic fields

$$Z \propto \int (dA)(d\phi d\bar{\phi}) e^{-S_G - \bar{\phi} M^{-1} \phi}$$

- evolve with hybrid of molecular dynamics and Monte Carlo
- 100 times more computer time than valence approximation
- current state of the art

## Issues

Conjugate gradient convergence poor as quarks become light

- use chiral extrapolations in quark mass
- need actions with good chiral properties

Need  $|M| \geq 0$

- OK for even number of degenerate “flavors”
- odd flavors not rigorous; i.e. two light and one intermediate ( $u, d, s$ )
- simulate with 4 flavors; insert  $n_f/4$  into force term
- probably ok for heavy quarks

Chemical potential and the sign problem

- with a background baryon density, sign of  $|M|$  fluctuates
- exponential slowing of Monte Carlo methods
- mathematically equivalent to doped Hubbard model
- exact diagonalization methods?

## Fermion actions and chiral symmetry

Extra symmetry as  $m_q \rightarrow 0$

- pion mass driven to zero
- helps extrapolate to physical quark masses

Chiral symmetry not natural on the lattice

- known anomalies must be incorporated

Considerable recent theoretical progress

- domain wall fermions: surface modes on 5 dimensional lattice
- overlap fermions: extract essential degrees of freedom from DWF

Ginsparg-Wilson relation

- continuum  $\gamma_5 M = -M \gamma_5$  replaced with  $\gamma_5 M = -M \hat{\gamma}_5$
- $\hat{\gamma}_5$  non-local,  $\hat{\gamma}_5^2 = 1$
- topology:  $\text{Tr} \hat{\gamma}_5 = 2\nu$  defines a winding number

## Computational issues

- domain wall fermions need larger fermionic matrices
- factor of about 10; depends on details of gauge action
- overlap requires extra conjugate gradient inversion
- both actively being investigated; gains justify extra computation

## Chiral gauge theories

- neutrinos are left handed
- no known lattice formulation without mirror right handed neutrinos
- lattice essential to defining the theory
- not a practical problem since weak interactions are perturbative

## Summary

Working algorithms exist for even number of massive quark flavors

Conjugate-gradient sparse-matrix inversions dominate computer time

Several unresolved issues:

- sign problem with chemical potential
- chiral gauge theories
- odd number of light quarks