Lattice Quantum Chromodynamic for Mathematicians

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Tutorial in

“ Derivatives, Finite Differences and Geometry”

Comparison of Chemistry & QCD : K. Wilson (1989 Capri):

"lattice gauge theory could also require a <u>10^8 increase in computer</u> power AND <u>spectacular algorithmic</u> advances before useful interactions with experiment ..."

- ab initio Chemistry
  1. 1930+50 = 1980
  2. 0.1 flops → 10 Mflops
  3. Gaussian Basis functions

- ab initio QCD
  1. 1980 + 50 = 2030?*
  2. 10 Mflops → 1000 Tflops
  3. Clever Multi-scale Variable?

"Almost 20 Years ahead of schedule!"

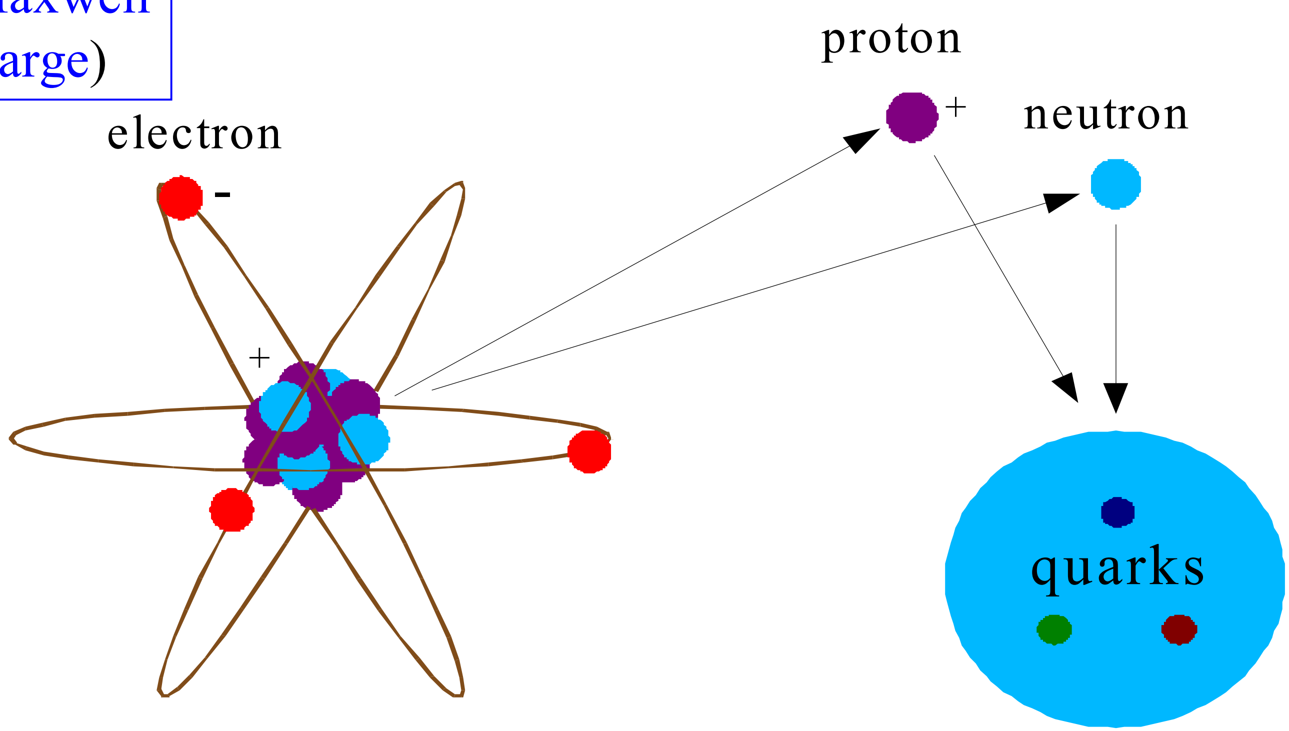
*Fast Computers + Smart Algorithms + Rigorous QCD Theoretical Analysis

= *ab inition predictions*

Forces in Standard Model

Nuclei Weak
N=2 (Isospin)

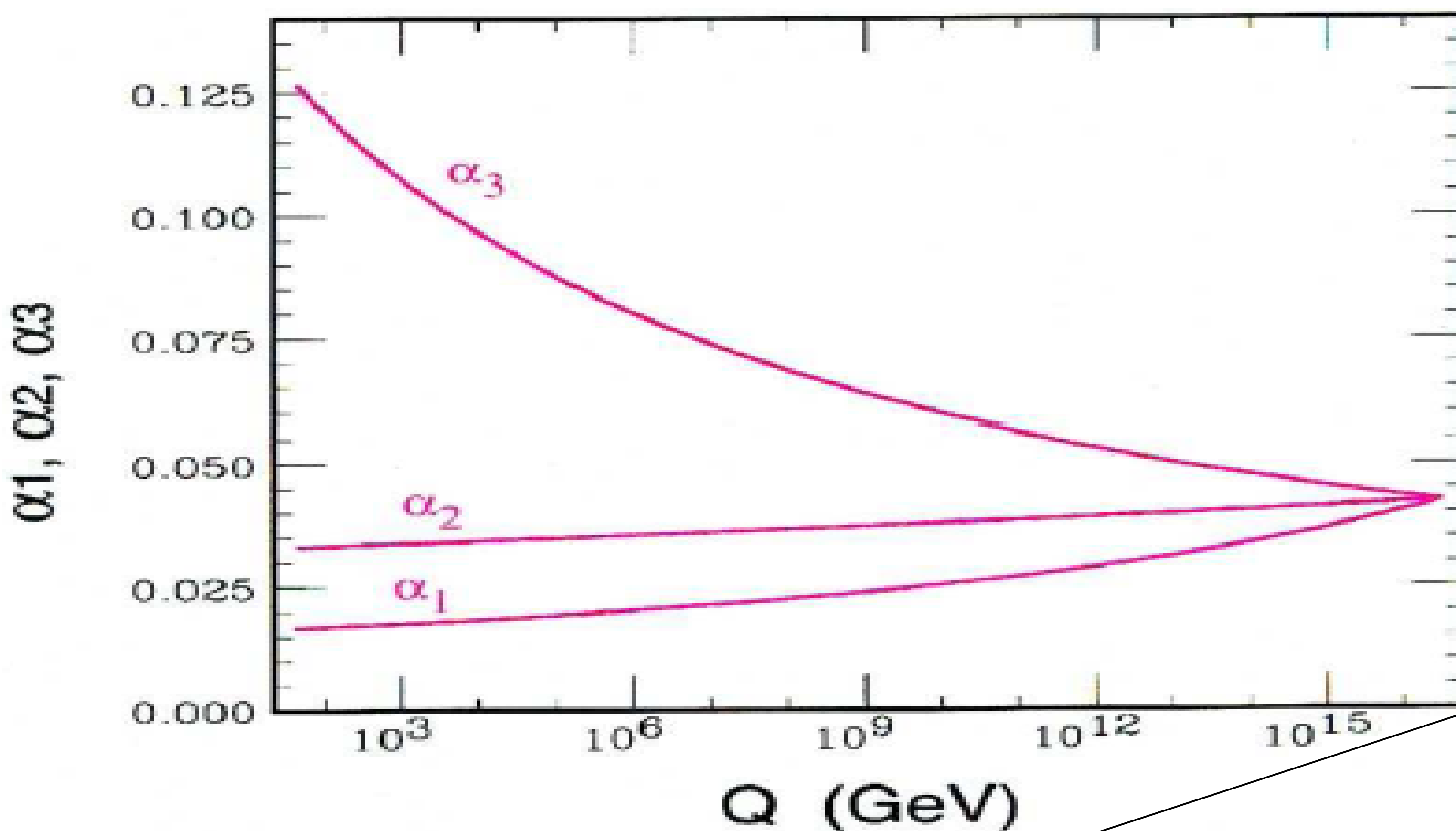
Atoms: Maxwell
N=1(charge)



Sub nuclear: Strong
N=3 (Color)

Standard Model: U(1) £ SU(2) £ SU(3)

Running Coupling Unification

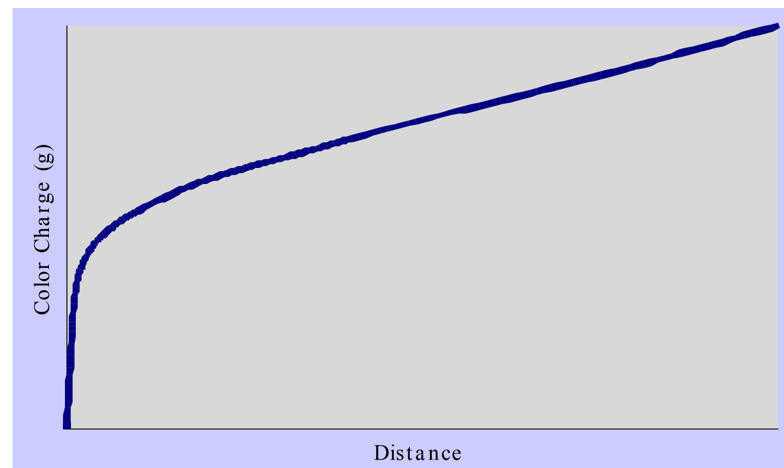


$M_{planck} = 10^{18}$

But QCD has charged Quarks and Gluons

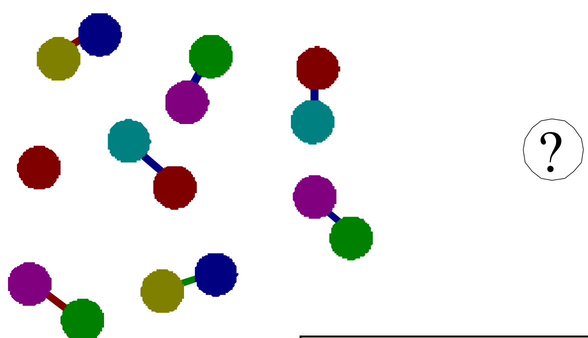
Quark-Antiquarks polarize just like e^+- e^- pairs

"But Gluon Act with Opposite Sign!"

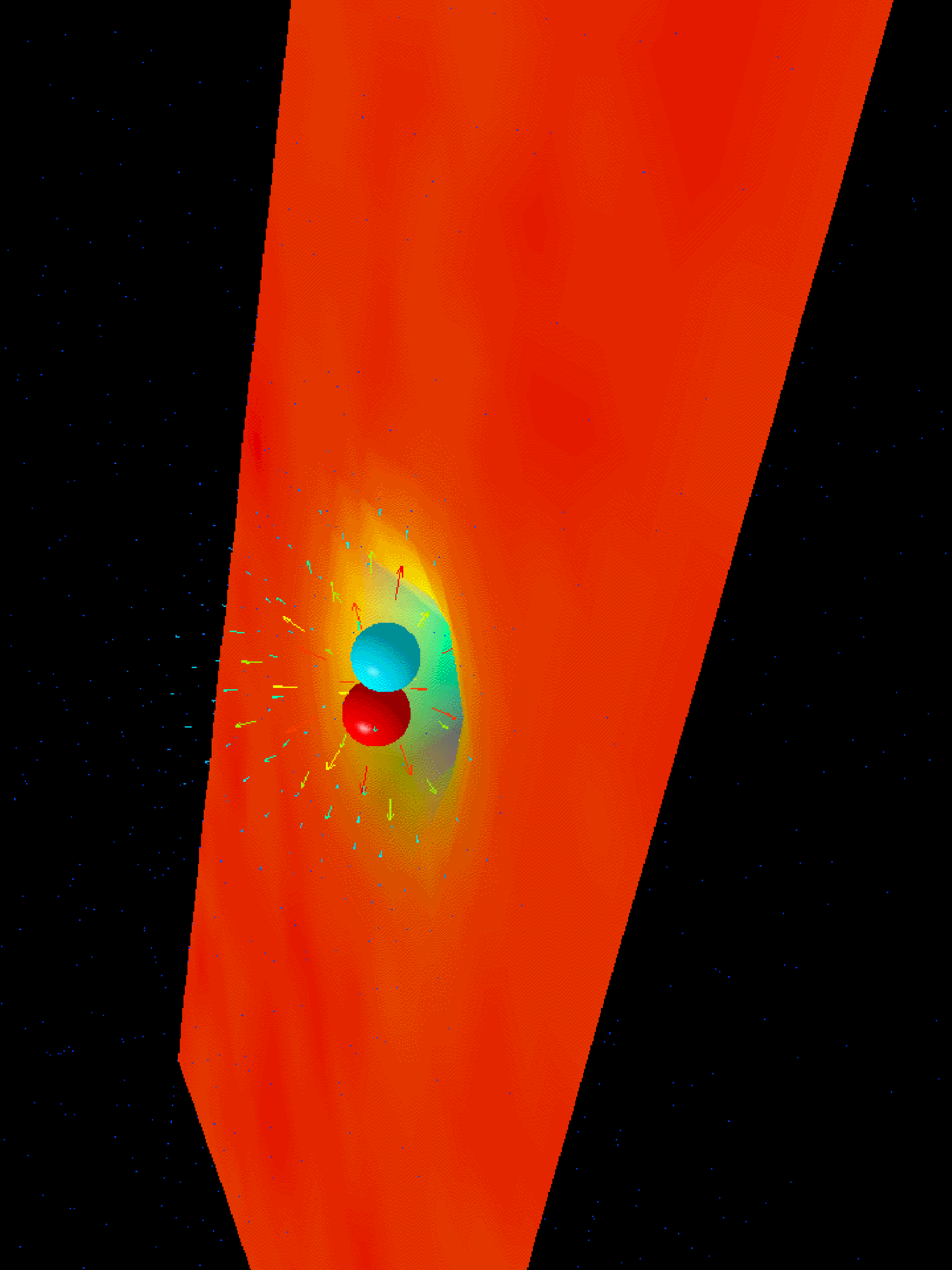


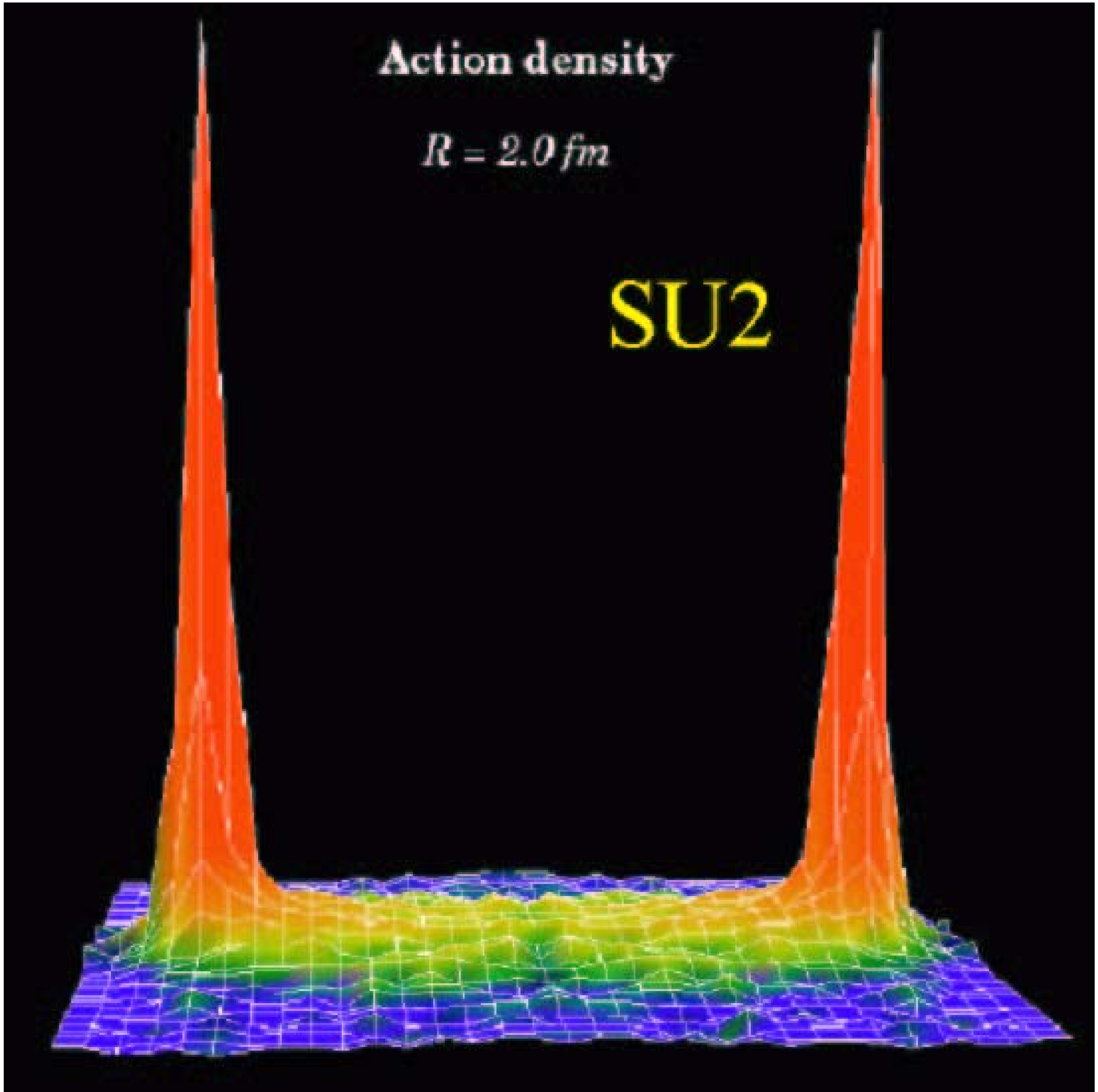
Δ X

QCD (anti-)screening

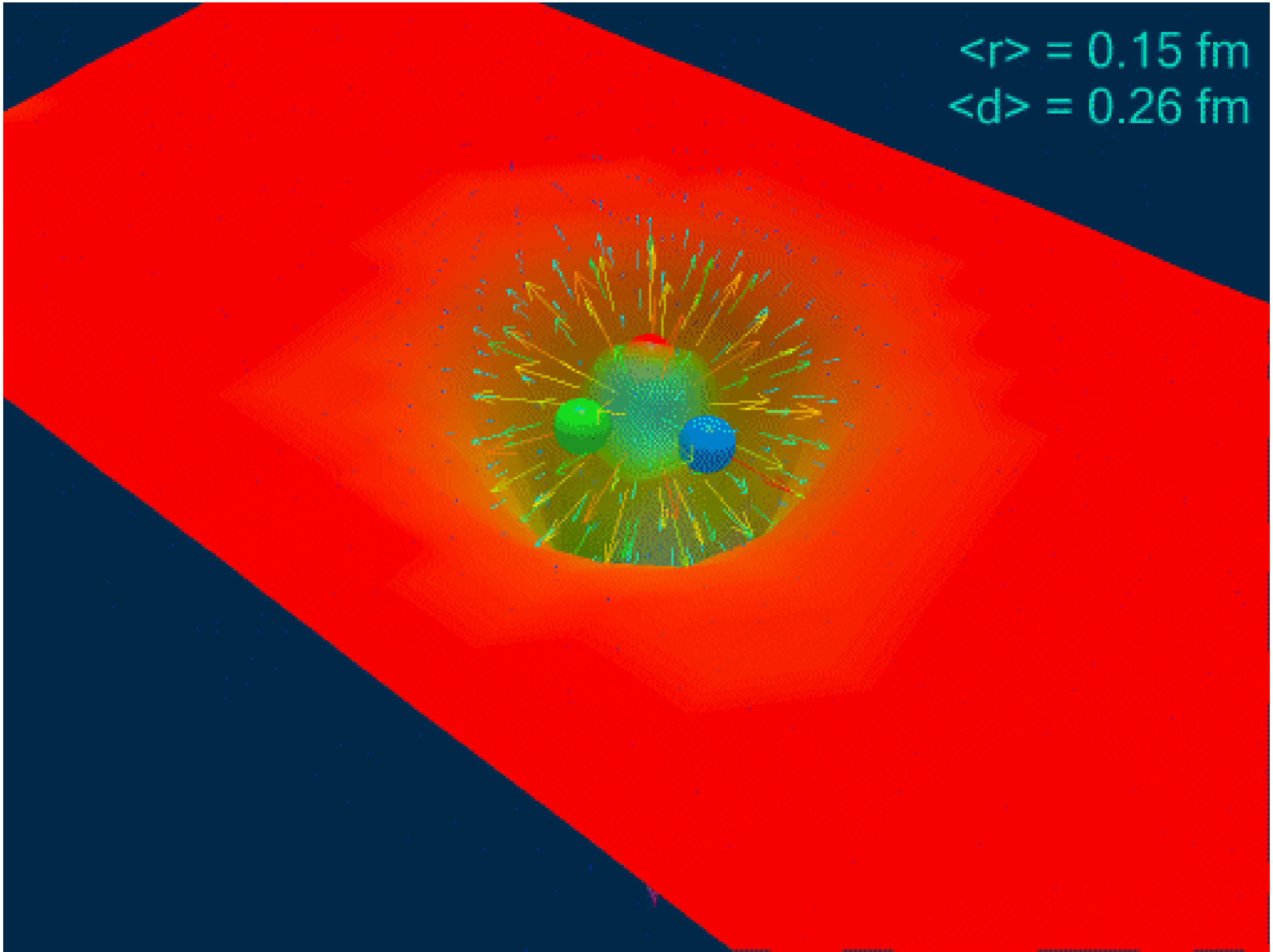


$$\frac{1}{g_{eff}^2} \simeq [\frac{11N}{6} - \frac{n_f}{3}] \times \log(\frac{1}{M \Delta X})$$

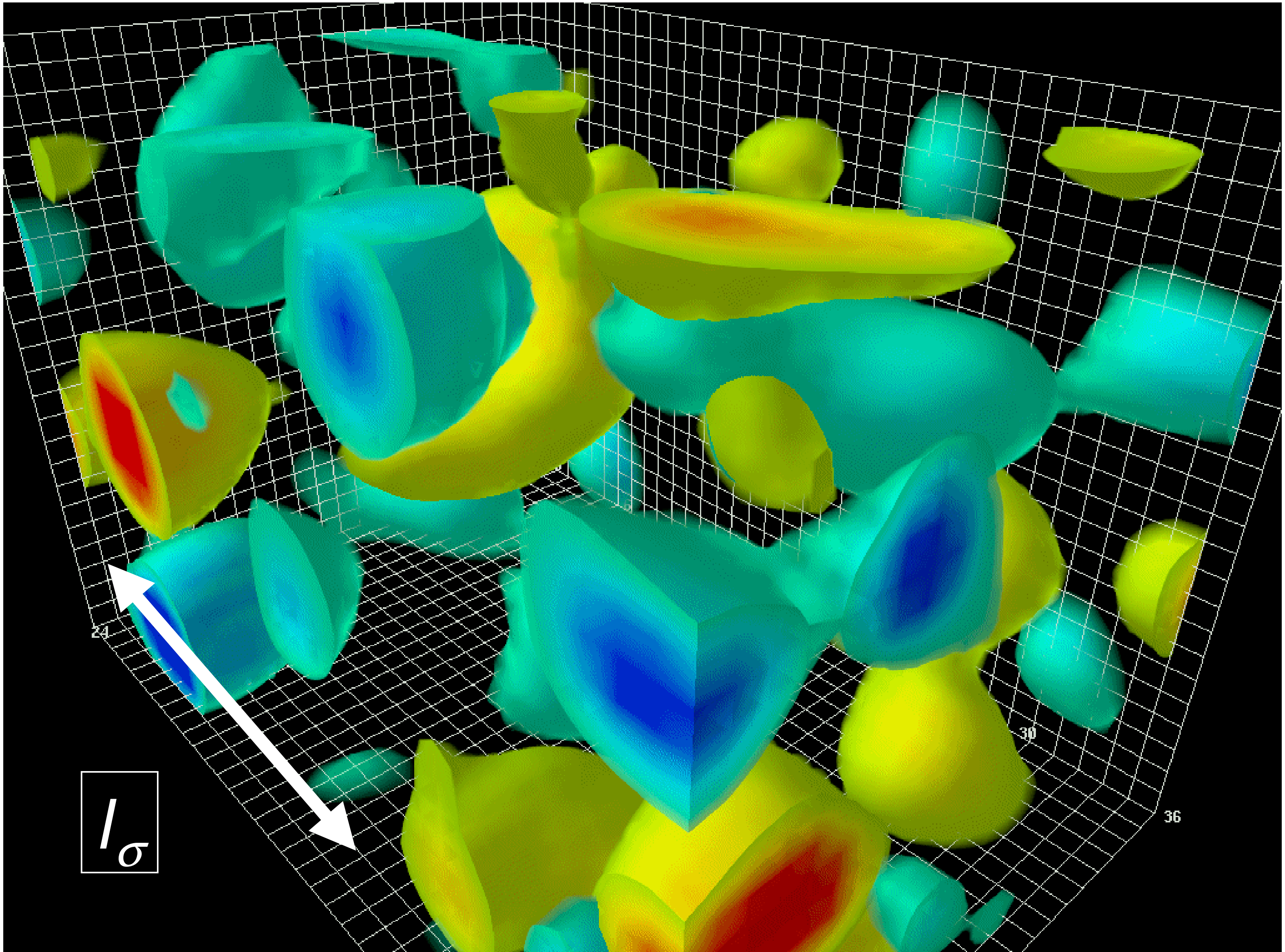



Action density
R = 2.0 fm
SU2

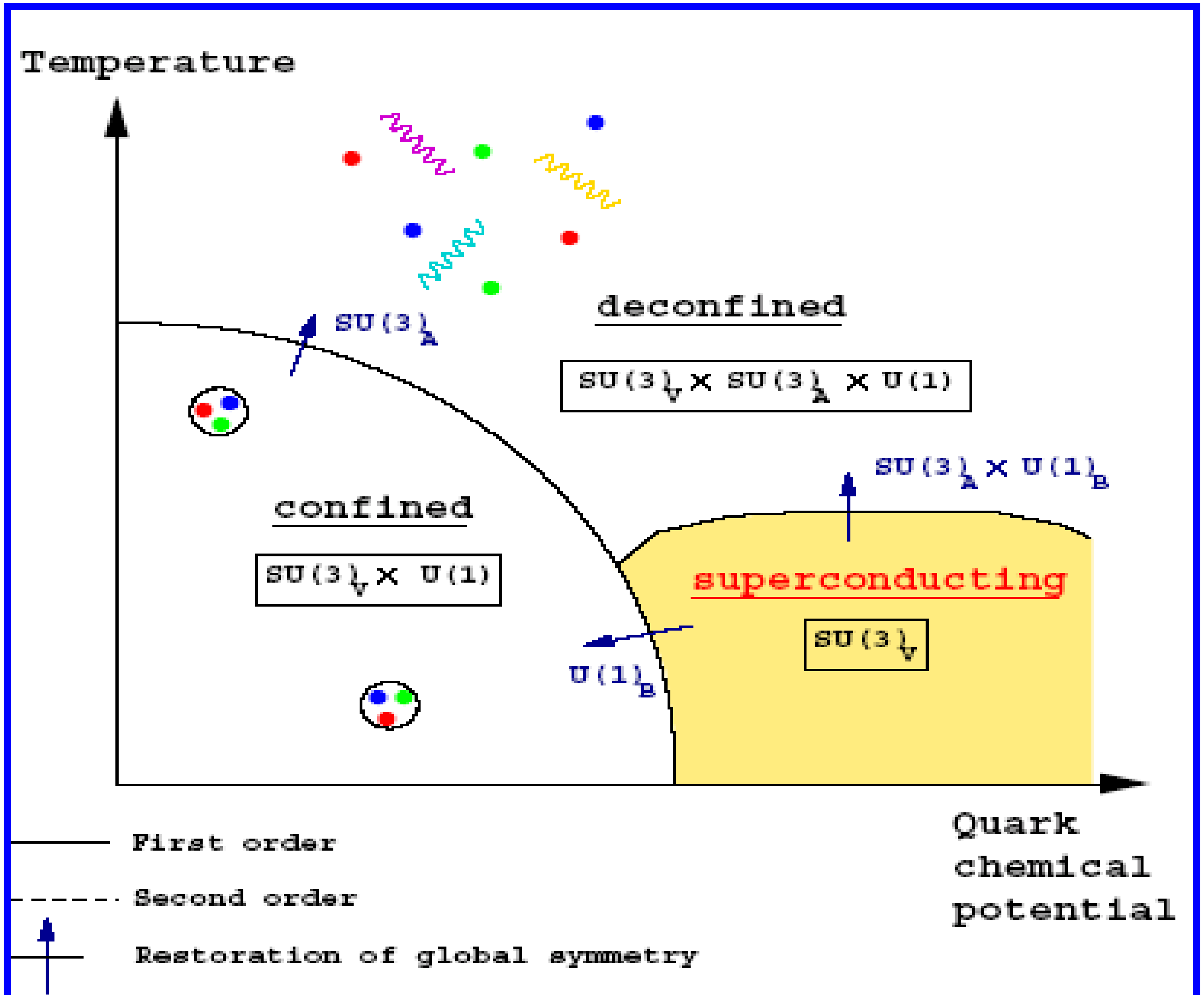
3 Color → 3 quarks in Proton



Instantons, Topological Zero Modes (Atiyah-Singer index) and Confinement length l_σ



QCD Plasma Physics



QCD: Theory of Nuclear Force

Partition function

Anti-quark

quark

Gauge (Glue)

$$= \int d\bar{\Psi}(x) d\Psi(x) dA_\mu(x) \quad \text{[Probability Density]}$$

$$= \int d\bar{\Psi}(x) d\Psi(x) dA_\mu(x) \quad \exp[-\int d^4x \bar{\Psi} D \Psi - \frac{1}{g^2} \int d^4x F^2]$$

$$= \int dA_\mu(x) \quad Det[D] \quad \exp[-\frac{1}{g^2} \int d^4x F^2]$$

Maxwell (Curl)

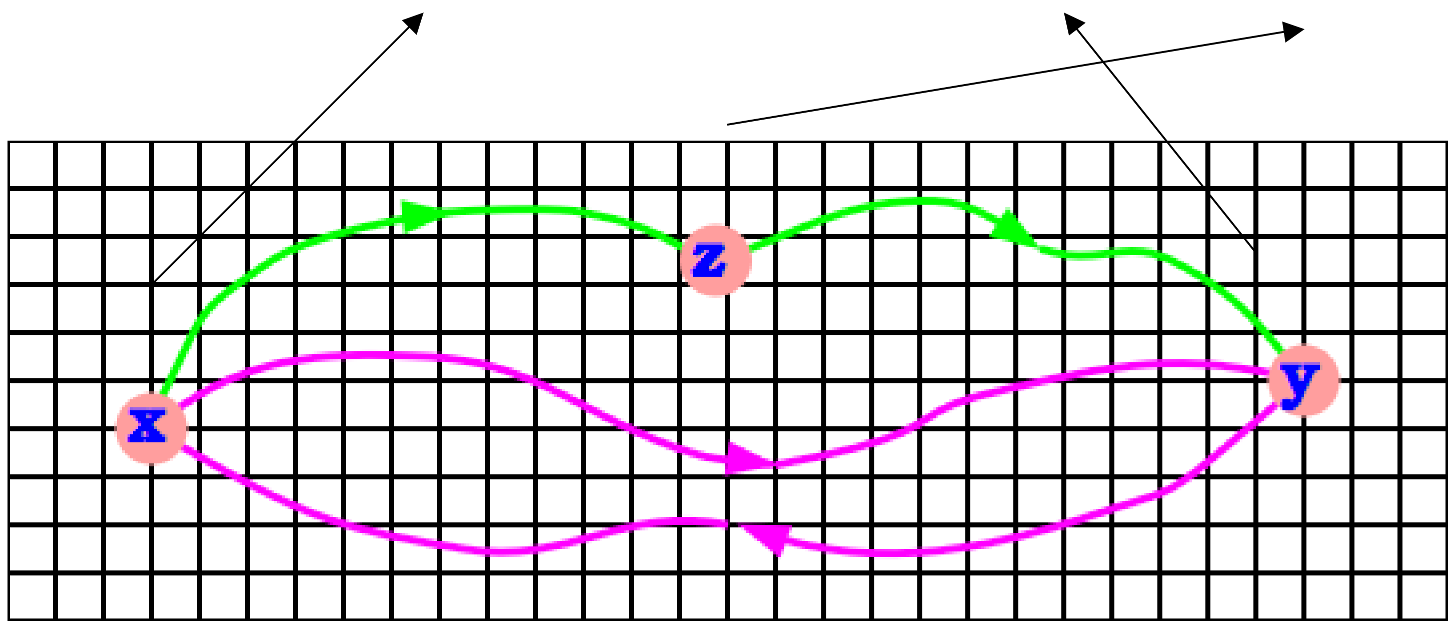
Dirac Operator

QCD Lattice Measurement

$$\int dU_\mu d\bar{\Psi} d\Psi \; [\; \Psi(x)^3 \quad \bar{\Psi}(z)\gamma_\mu \Psi(x) \quad \bar{\Psi}(y)^3 \;] e^{-S} =$$

$$\int dU_\mu \; Det[D] \; [\; D^{-1}(x,y) D^{-1}(x,y) \; D^{-1}(x,z)\gamma_\mu D^{-1}(z,y) \;] e^{-S} +$$

$$\int dU_\mu \; Det[D] \; [\; D^{-1}(x,y) D^{-1}(x,y) D^{-1}(x,y) \; Tr[\gamma_\mu D^{-1}(z,z) \;] e^{-S}$$



Outline

- Maxwell Equations
  1. 2-d, 3-d & 4-d curl -- continuum vs lattice
  2. Moving a charge
  3. Dirac Electron

- Repeat Maxwell 1-2-3 for SU(3) matrices

- Exp[- Action] & Quantum Probabilities in Space-time

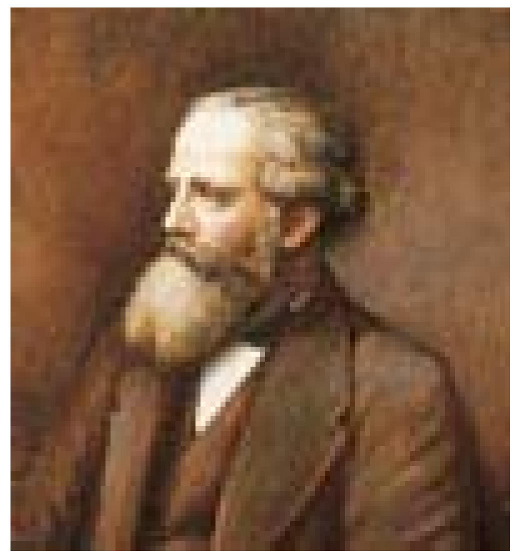
- Topology and the (near) null space

- Linear Algebra Problems
  1. Solve $A x = b$) $x = A^{-1} b$
  2. Find Trace[A^{-1}]
  3. Find Det[A] = exp[Tr log A]

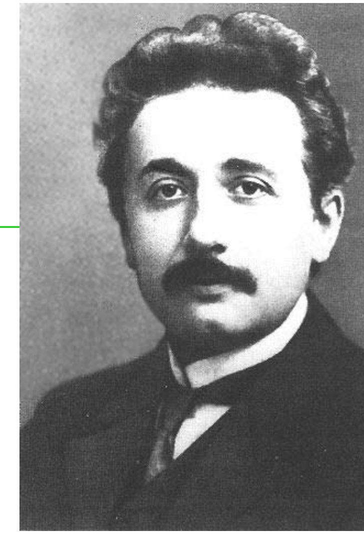
4 Maxwell Equations

Really only One!

Maxwell's Equ: $\partial_\mu F_{\mu\nu} = J_\nu$



100 Years Ago



- Maxwell (E&M)

  r ¢ E = ρ, r ¢B= 0,

  r £ E = J, r £ B = 0

- Relativity + Quantum Mechanics

Set c = ~ =1 so one unite left m=E=p=1/x=1/t

No scale x ! λ x

- Potential: E = - e^2/r e^2/4 ¼ ' 1/137

3-d Maxwell: $B(x_1, x_2, x_3)$

$$\text{Replace} \quad \vec{\nabla} \cdot \vec{B} = 0 \quad \text{and} \quad \vec{\nabla} \times \vec{B} = \vec{J}$$

$$\vec{B} = \vec{\nabla} \times \vec{A} \quad \text{and} \quad -\vec{\nabla}^2 \vec{A} + \vec{\nabla}(\vec{\nabla} \cdot \vec{A}) = \vec{J}$$

Should use anti-symmetric tensor:

Note: d(d-1)/2 = d for d =3

$$F_{ij} \equiv \begin{bmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{bmatrix} = \frac{\partial}{\partial x_i} A_j(x_1, x_2, x_3) - \frac{\partial}{\partial x_j} A_i(x_1, x_2, x_3)$$

Only case where anti-sym d£d matrices looks like a (pseudo) vector

4-d Maxwell[y]: $E(x_0, x_1, x_2, x_4)$ & $B(x_0, x_1, x_2, x_3)$

$$F_{\mu\nu} = \begin{bmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & B_3 & -B_2 \\ -E_2 & -B_3 & 0 & B_1 \\ -E_3 & B_2 & -B_1 & 0 \end{bmatrix} = \frac{\partial}{\partial x_\mu} A_\nu(x) - \frac{\partial}{\partial x_\nu} A_\mu(x)$$

$$\text{or} \quad F_{\mu\nu} = i\left[\frac{\partial}{\partial x_\mu} - iA_\mu(x) \, , \, \frac{\partial}{\partial x_\nu} - iA_\nu(x) \right]$$

Lagrangian Density:

$$\frac{1}{4}\sum_{\mu,\nu} F_{\mu\nu}F^{\mu\nu} = \frac{1}{2}(\vec{E}^2 - \vec{B}^2) = \frac{1}{2}\partial_\mu \vec{A} \cdot \partial_\mu \vec{A} - \frac{1}{2}(\vec{\nabla} \times \vec{A})^2$$

[y] Now d(d-1)/2 = 4*3/2 = 6 elements!

Quiz: What is F in 2-d?

$$F_{ij} \equiv \begin{bmatrix} 0 & B_3 \\ -B_3 & 0 \end{bmatrix} = \frac{\partial}{\partial x_i} A_j(x_1, x_2) - \frac{\partial}{\partial x_j} A_i(x_1, x_2)$$

Relativistic Notation: $\mu, \nu = 0, 1, 2, 3$

$x = x_\mu = (x_0, x_1, x_2, x_3)$ $x_0 =$ "time"; ususally imaginary time!

$\partial_\mu A_\nu(x) = \frac{\partial}{\partial x_\mu} A_\nu(x)$, etc.

General expression uses differential form:

$A = A_1\, dx^1$ $F = dA = F_{1o}\, dx^1$ Æ dx^o

) $dF = 0$ & $d^*F = J$

Covariant Derivative, Gauge invariance and all that!

$$\frac{\partial}{\partial x_\mu}\phi(x) \to [\frac{\partial}{\partial x_\mu} - iA_\mu(x)]\phi(x)$$

Now derivative commutes with phase rotation:

$$\phi(x) \to e^{i\theta(X)}\phi(x) \qquad A_\mu(x) \to A_\mu^{\theta(x)}(x) + \partial_\mu\theta(x)$$

implies

$$[\frac{\partial}{\partial x_\mu} - iA_\mu(x)]\phi(x) \to e^{i\theta(x)}[\frac{\partial}{\partial x_\mu} - iA_\mu(x)]\phi(x)$$

Lagrangian is invariant

$$\mathcal{L} = \frac{1}{4e^2}\sum_{\mu,\nu} F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}([\partial_\mu - iA_\mu]\phi(x))^*[\partial_\mu - iA_\mu]\phi(x) + \frac{1}{2}m^2\phi^*(x)\phi(x)$$

Finite difference for a lattice

x ——→ x+ a[1] = x_1

Finite difference: $$\frac{\partial \phi(x)}{\partial x_\mu} \rightarrow \Delta_\mu \phi(x) = \frac{\phi(x+a\mu) - \phi(x)}{a}$$

With Gauge field replace: $$\Delta_\mu \phi(x) = \frac{e^{i\int_{x+a\mu}^{x} A_\mu dx_\mu}\phi(x+a\mu) - \phi(x)}{a}$$

The new factor is covariant constant.

$$\left[\frac{\partial}{\partial x_\mu} - iA_\mu(x)\right] e^{i\int_{x_1}^{x} A_\mu dx_\mu} = 0$$

This is the Lattice Guage link: $U(x, x+a\mu) = e^{iaA_\mu(x)}$

The Dirac PDE (for Quarks)

$$\sum_{\mu=1}^{4} \gamma_\mu^{ij}[\frac{\partial}{\partial x_\mu} - iA_\mu^{ab}(x)]\psi_{jb}(x) + m\psi_{ia}(x) = b_{ia}(x)$$

4x4 sparse spin matrices: 4 non-zero entries 1,-1, i, -i

3x3 color gauge matrices

$x_\mu = (x_1,x_2,x_3,x_4)$ (space,time)

On a Hypercubic Lattice (**x_μ = integer, a = lattice spacing**):

$$\sum_{\pm\mu} \frac{\pm\gamma_\mu - 1}{2} U(x, x\pm\mu)\psi(x\pm\mu) + (am+4)\psi(x) = b(x)$$

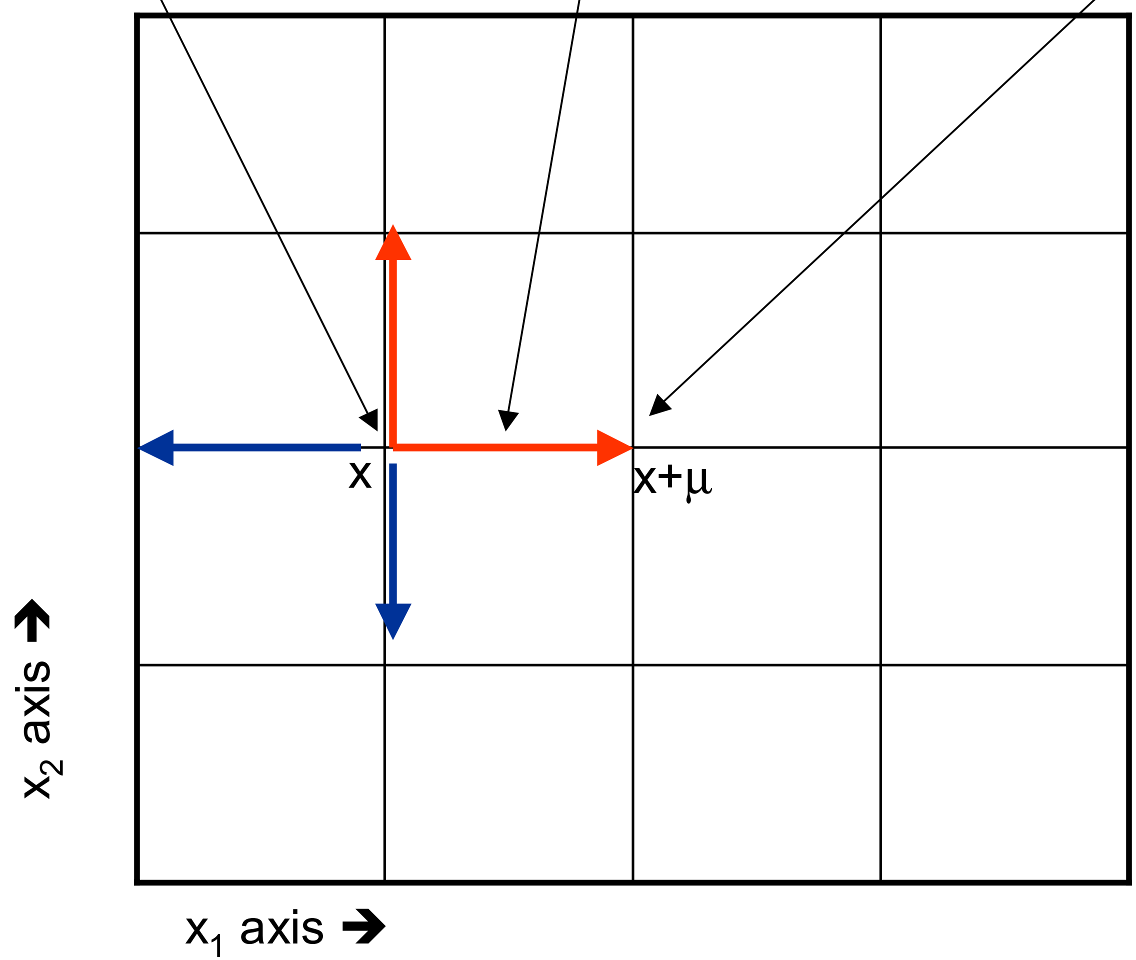
3x3 Unitary : $U(x,x+\mu) = \exp[i\, a\, A_\mu(x)]$ and $U(x,x-\mu) = U^y(x-\mu,x)$

Put Dirac PDE on hypercubic Lattice

Projection Op

$$\bar{\Psi}_{ia}(x) \quad \frac{1-\gamma_\mu^{ij}}{2} \quad U_\mu^{ab}(x) \quad \Psi_{jb}(x+\mu)$$

Dimension:
μ=1,2,…,d



Color
a = 1,2,3

Spin
i = 1,2,3,4

Symmetries of Dirac Equ: $D\,\psi = b$

$$\frac{1}{2}\sum_{\pm\mu}[\pm\gamma_\mu - 1]U(x, x\pm\mu)\psi(x\pm\mu) + (am+4)\psi(x) = b(x)$$

- **Hermiticity:** $\gamma_5\, D\, \gamma_5 = D^{y}$
  $\gamma_5^2 = 1$ and $\gamma_5 = \gamma_1\, \gamma_2\, \gamma_3\, \gamma_4$

- **Gauge :** $U(x,x+\mu) \rightarrow \Omega_x\, U(x,x+\mu)\, \Omega^{y}_{x+\mu}$
  are unitary transformations of A

- **Chiral:** $D = \exp[i\, \gamma_5\, \theta]\, D\, \exp[\, i\, \gamma_5\, \theta]$ at $m=0$
  (On Lattice use New Operator: $D = 1 + \gamma_5\, sign[\gamma_5\, D]$)

- **Scale:** Only quantum fluctuations break scaling at m=0.
  The breaking is "confinement length" $l_\sigma(\beta)$

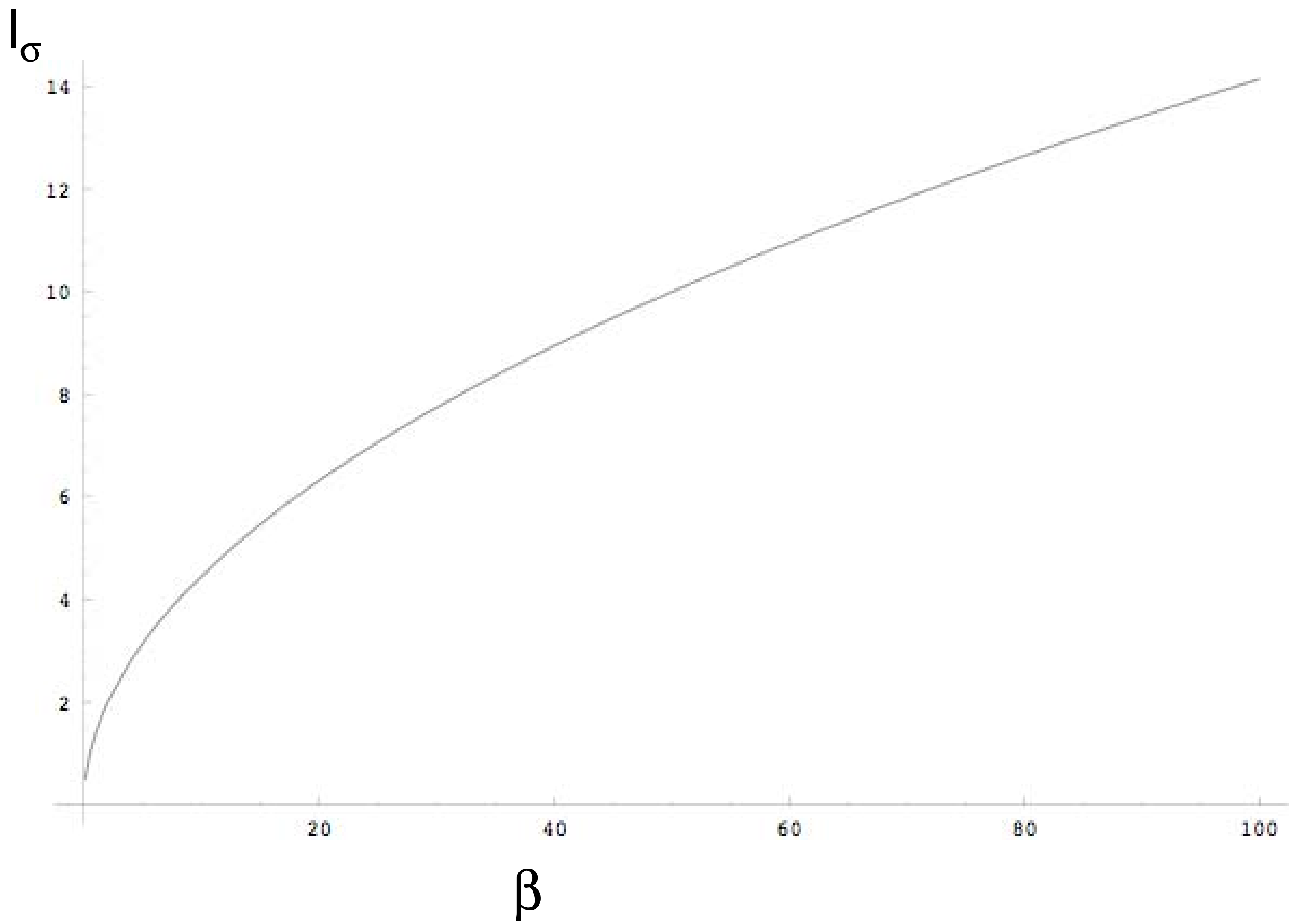
Solve $D^a = b$

2-d Toy Problem: Schwinger Model

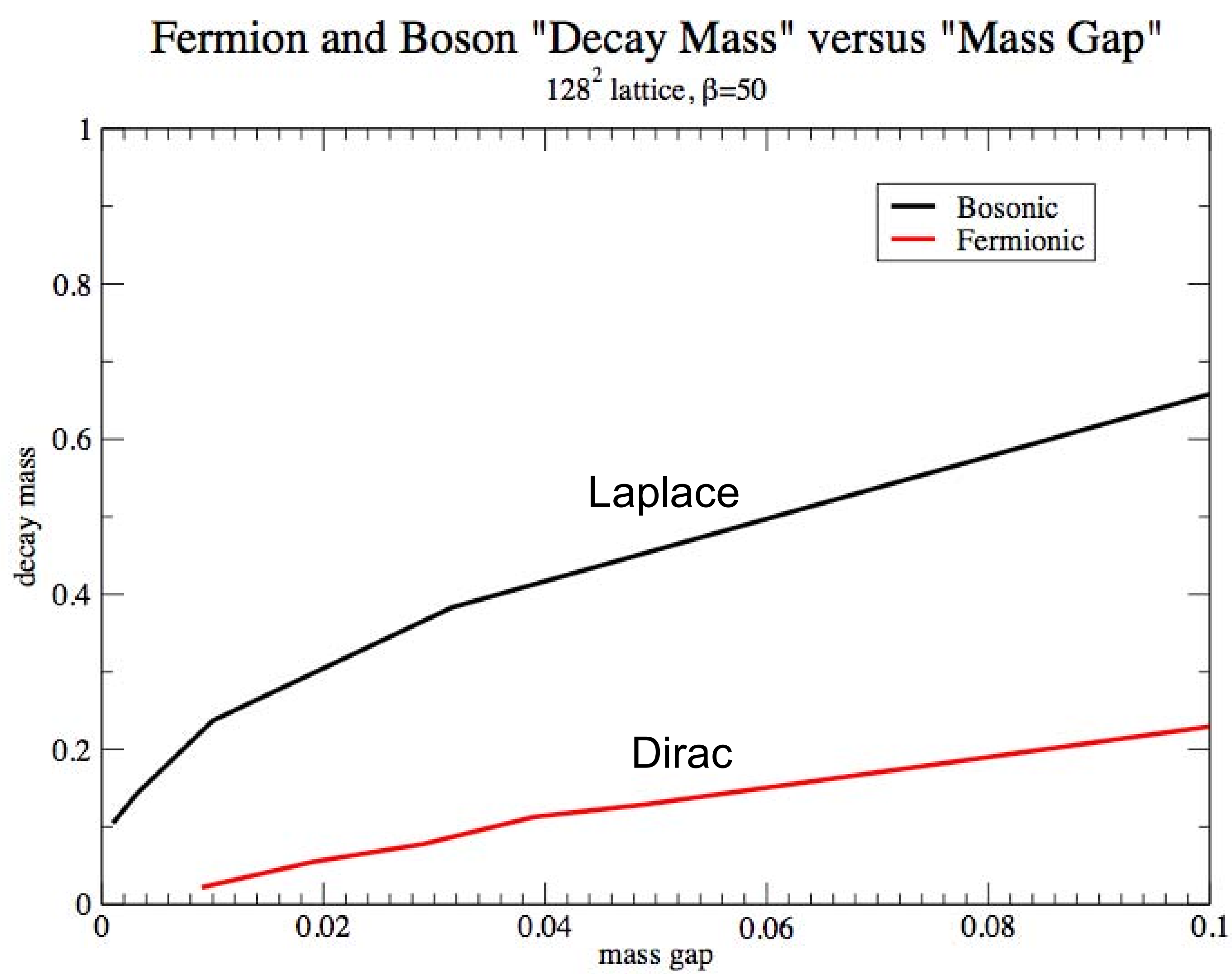
- Space time is 2-d
- Gauge links are E&M
  - $U(x, x+\mu) = \exp[i\, e\, A_\mu(x)]$
  - Instanton) vortex
- Dirac fields has 2 spins (not 4)
- Operator is quaternionic (Pauli) matrix σ_1, σ_2

$$\sum_{\mu=\pm 1,\pm 2} \frac{\pm\sigma_\mu - 1}{2} U(x, x\pm\mu)\psi(x\pm\mu) + (am+2)\psi(x) = b(x)$$

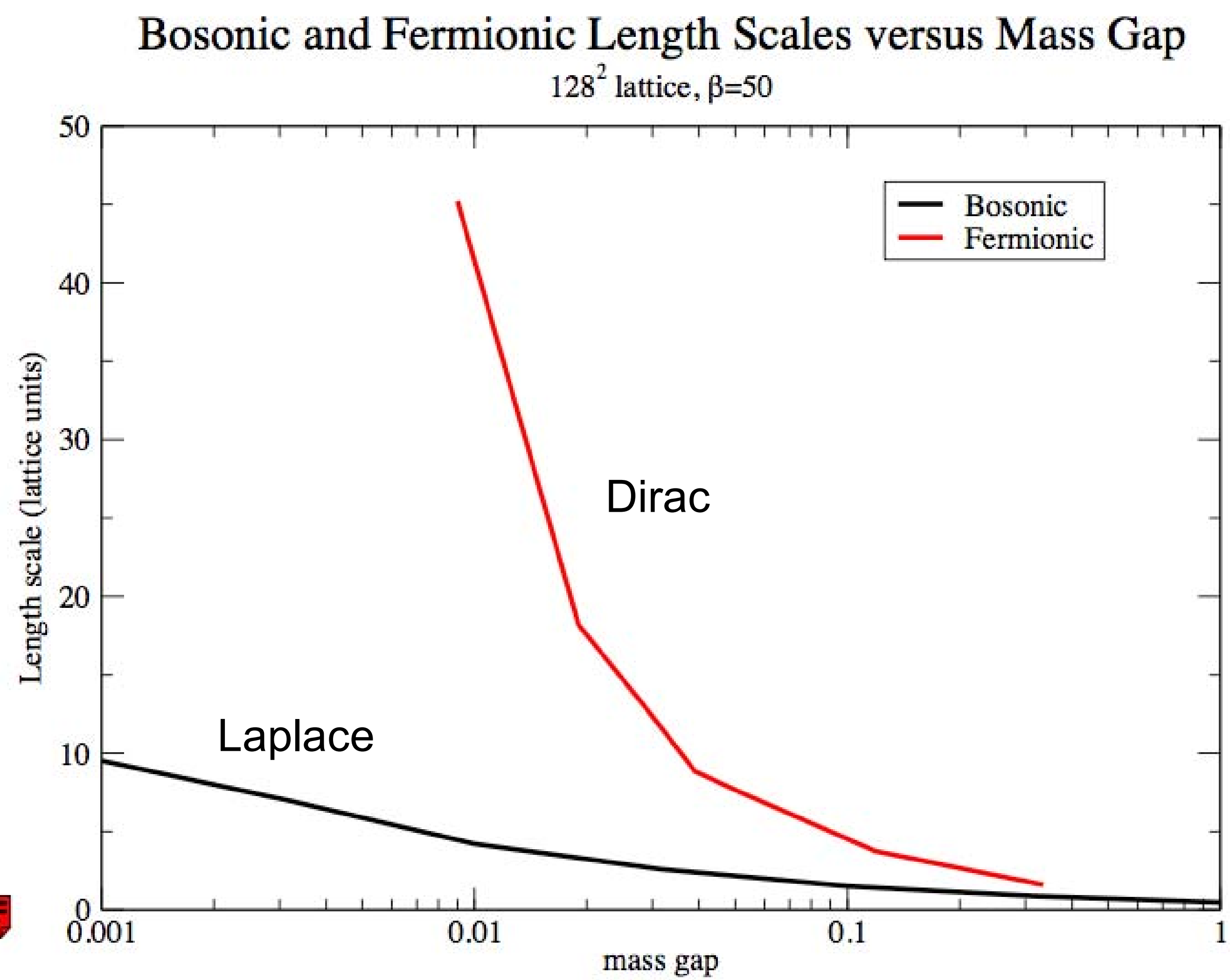
U(1) Gauge length scale



Correlation Mass vs Mass Gap (e.v)



Correlation Length vs Mass Gap (e.v)



Gauge Invariant Projective Multigrid[y]

- Multigrid Scaling (a ➔ 2 a) ---- aka "renormalization group" in QCD
- Map should (must?) preserve long distance spectrum and symmetries.
- Operators $P(x_C,x_F)$ & $Q(x_F,x_C)$ should be "square" in spin / color space!
- Use Projective MG (aka Spectral AMG !)

- Galerkin Example

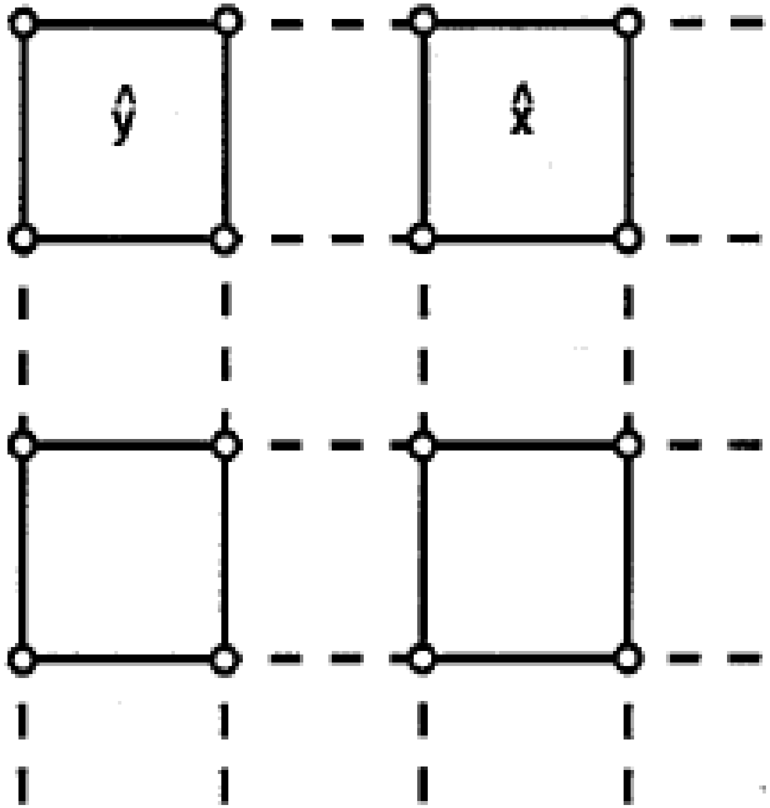
$$A_{CC} = P\, A_{FF}\, Q \;\rightarrow\; A_{x_C,y_C} = P(x_C, x_F)\, A_{x_C,y_C}\, Q(y_C, y_F)$$

$\gamma 5$ Hermitcity constraint: $\gamma 5\, Q\, \gamma 5 = P^y$

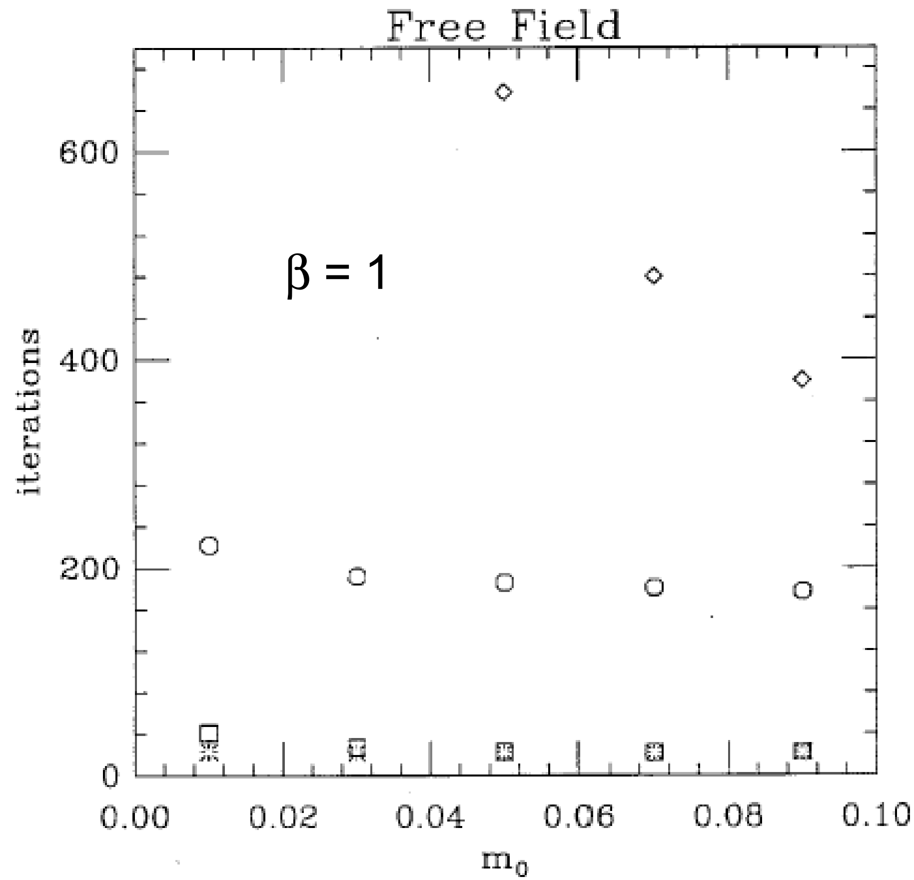
BOTTOM LINE: I can design "covariant" BLACK BOX minimization methods that automatically preserve all (Hermitian,gauge,chiral,scale) symmetries.

[y] **R. C. Brower, R. Edwards, C.Rebbi,and E. Vicari, "Projective multigrid forWilson fermions", Nucl. Phys.B366 (1991) 689**

2x2 Blocks for U(1) Dirac

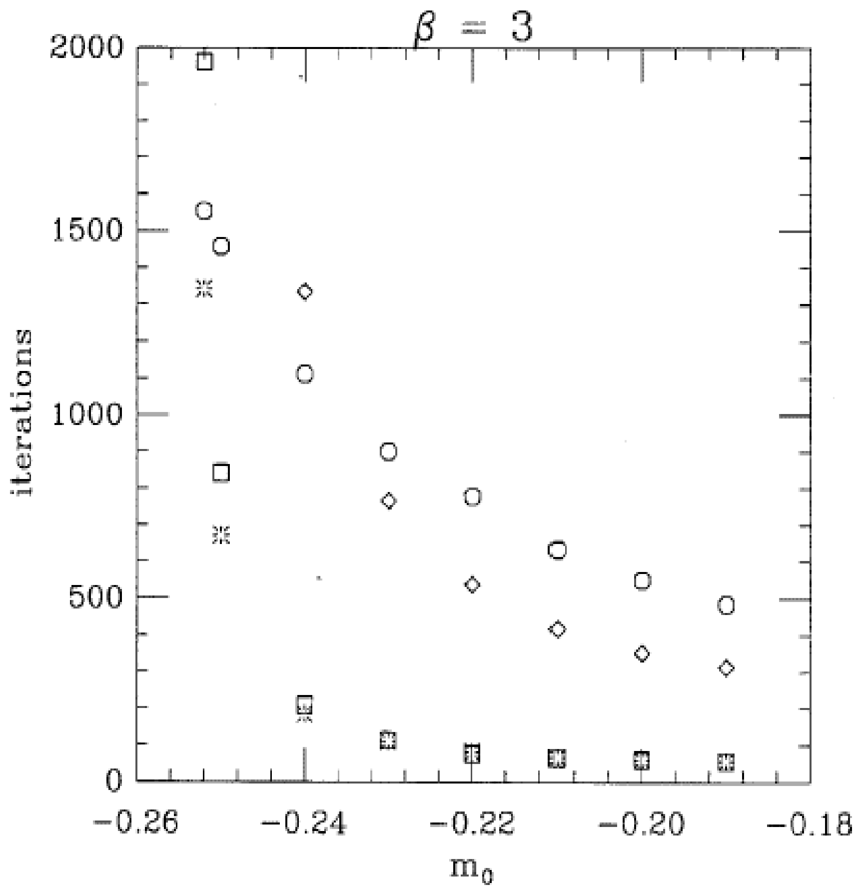


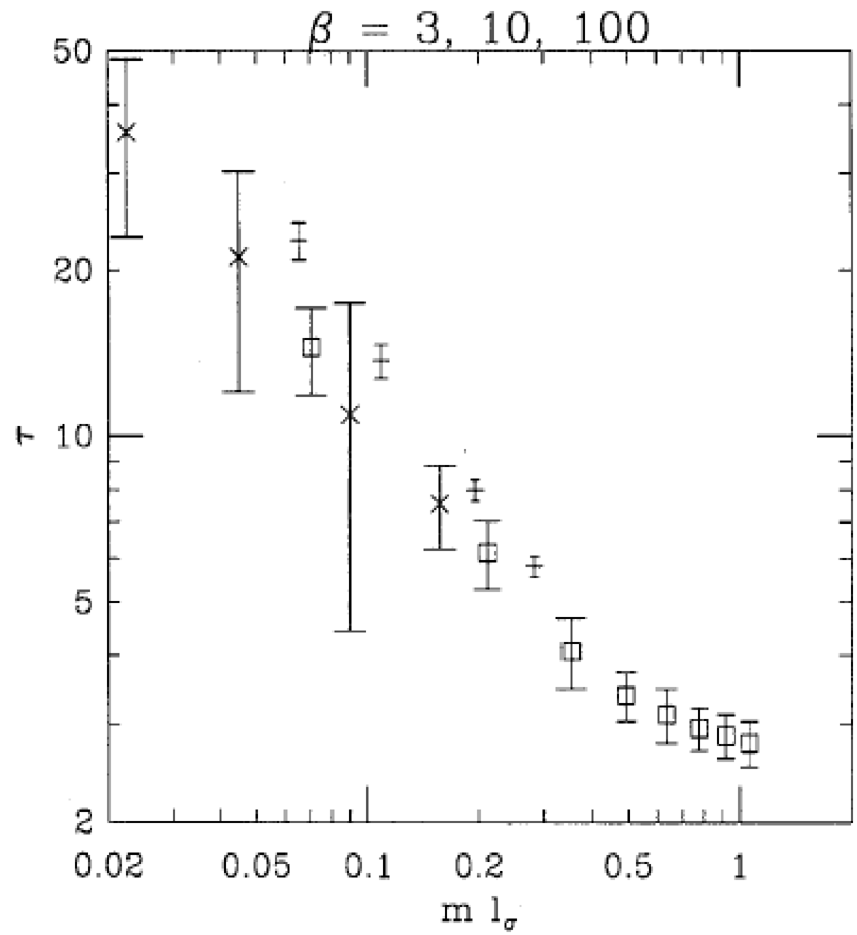
2-d Lattice,
$U_\mu(x)$ on links $\Psi(x)$ on sites



Gauss-Jacobi (Diamond), CG (circle),
V cycle (square), W cycle (star)

Universal Autocorrelation: $\tau = F(m\, l_\sigma)$





Gauss-Jacobi (Diamond), CG(circle), 3 level (square & star)

β = 3 (cross) 10(plus) 100(square)

Trace[(sparse) D^{-1}]

Q: How to take a Trace?
A: Pseudo Fermion Monte Carlo

$$Tr[\mathcal{O}D^{-1}] \sim \int d\phi \quad [D^\dagger \mathcal{O}]_{xy}\phi_y\phi_x^* \quad e^{-\phi_x^*[D^\dagger D]_{xy}\phi_y}$$

- *Can do "standard" Monte Carlo with low eigenvalue subtraction on $H = \gamma_5 D$*
- *Or "perfect" Monte Carlo – Gaussian η_x*

choose $\eta_x \in Prob[\eta] \sim e^{-\eta_x^*\eta_x}$ solve $\phi = D^{-1}\eta$

Standard Deviation

$$\mathcal{A}(\eta) = \eta_x^* A_{xy} \eta_y \Rightarrow Tr[A] \simeq \overline{\mathcal{A}} \pm \frac{\sigma}{\sqrt{N_{sample}}}$$

where $\langle \mathcal{A}(\eta) \rangle_\eta = \overline{\mathcal{A}}$

Gaussian Noise: $\sigma^2_{Gaussian} = \overline{\mathcal{A}^2} - \overline{\mathcal{A}}^2 = \sum_{xy} A^*_{xy} A_{xy}$

Z_2 Noise: $\sigma^2_{Z_2} = \sum_{x \neq y} A^*_{xy} A_{xy}$

(with $\eta_x = (\pm 1 \pm i)/\sqrt{2} \rightarrow \eta_x^* \eta_x = 1$)

Multi-grid Trace Project

Brannick, Brower, Clark, Fleming, Osborn, Rebbi

Everything can work together

BUT it is not Simple to design pre-conditioner and code efficiently!

- MG Speed up Inverse
- Amortize Pre-conditioner with multiple RHS.
- MG variance reduction at long distances.
- Unbiased subtraction at short distance.
- Low eigenvalue projection.
- Dilution.

$$\mathrm{Det}[D] = e^{\mathrm{Tr}[\mathrm{Log}(D)]}$$

Conclusions

- Dirac Operator:
  - Symmetries (gauge, chiral and scale) and topology constrain the spectral properties.
  - Intrinsic quantum length scale l_σ independent of the gap m
  - Generalize to lattice Chiral : 5-d solutions to

$$D = m + 1 + \gamma 5 \, sign[\gamma 5 \, A]$$

- Positive feedback: *The better algorithms allow finer lattice with better multiscale performance!*
- The future for multiscale algorithms in QCD is very bright.