LECTURE 12:

SIMULATING PURE GAUGE THY

REMINDER: METROPOLIS (from lecture 4)

Φ some field/spin config.

① choose a config. Φ' w. prior prob. $T_0(\Phi' \leftarrow \Phi)$

② accept it with probability

$$T_A(\Phi' \leftarrow \Phi) = \min\left\{1, \frac{T_0(\Phi \leftarrow \Phi')\, e^{-S[\Phi']}}{T_0(\Phi' \leftarrow \Phi)\, e^{-S[\Phi]}}\right\}$$

③ goto 1

special case: $T_0(\Phi \leftarrow \Phi') = T_0(\Phi' \leftarrow \Phi)$

$$\Rightarrow T_A = \min\left\{1, e^{-\Delta S}\right\}$$

$$\Delta S = S(\Phi') - S(\Phi)$$

another special case:

- proposed change is local
- action is local

$\Rightarrow$ calculation of ΔS only involves local terms

$\rightsquigarrow \mathcal{O}(V^0)$ work

cheap

can be satisfied for

e.g. pure gauge $S = S_{plaquette}$

not by QCD

$$S_{eff} = S_{gauge} - \underbrace{\ln\det M[U]}_{\text{non-local}}$$

A COMMON (AND SUBTLE) MISTAKE IN UPDATE ALGORITHMS

The detailed balance condition is correctly written as
NOT ALWAYS

$$\frac{P(\Phi'\leftarrow\Phi)}{P(\Phi\leftarrow\Phi')} = \frac{P_{eq}(\Phi')}{P_{eq}(\Phi)} = \frac{e^{-S[\Phi']}}{e^{-S[\Phi]}}$$

always correct

$P_{eq}(\Phi) \propto e^{-S[\Phi]}$

we assumed ← not always true

$$P(\Phi'\leftarrow\Phi) = T_A(\Phi'\leftarrow\Phi)\, T_0(\Phi'\leftarrow\Phi)$$

e.g. consider $p(x,y) \propto e^{-c(x^2+y^2)}$ and suppose we use polar coordinates

$$p(x,y)\,dx\,dy = p(x,y)\,r\,dr\,d\theta = p(r,\theta)\,dr\,d\theta \Rightarrow p(r,\theta) \propto r e^{-cr^2}$$

so if we make an update $r \to r' = r + \delta r$ e.g. $\delta r \in [-\varepsilon, \varepsilon]$ uniform

then the acceptance probability should be

$$T_A(r'\leftarrow r) = \min\left\{1, \underbrace{\boxed{\frac{r'}{r}}}_{\text{Jacobian factor / measure factor}} \frac{e^{-cr'^2}}{e^{-cr^2}}\right\}$$

{ for our algorithms for pure gauge thy no such Jacobian factor will appear, as they will involve mult. w. SU(N) matrices ⇒ can use props of Haar measure to show }

METROPOLIS FOR PURE SU(N) GAUGE THY (4D)

(plaquette action)

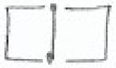
make a local proposal $U_{x\mu} \rightarrow U'_{x\mu}$

$$S[U'_{x\mu}]_{local} = \frac{\beta}{N} \sum_{i=1}^{6} \mathrm{ReTr}(\mathbb{1} - U'_{x\mu} P_i) = \frac{\beta}{N} \mathrm{ReTr}(6\mathbb{1} - U'_{x\mu} A)$$

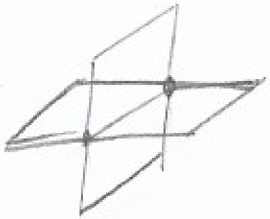
a single link is in 6 plaquettes

$2(d-1)$ (2 in each orthogonal direction)

$\boxed{2D}$

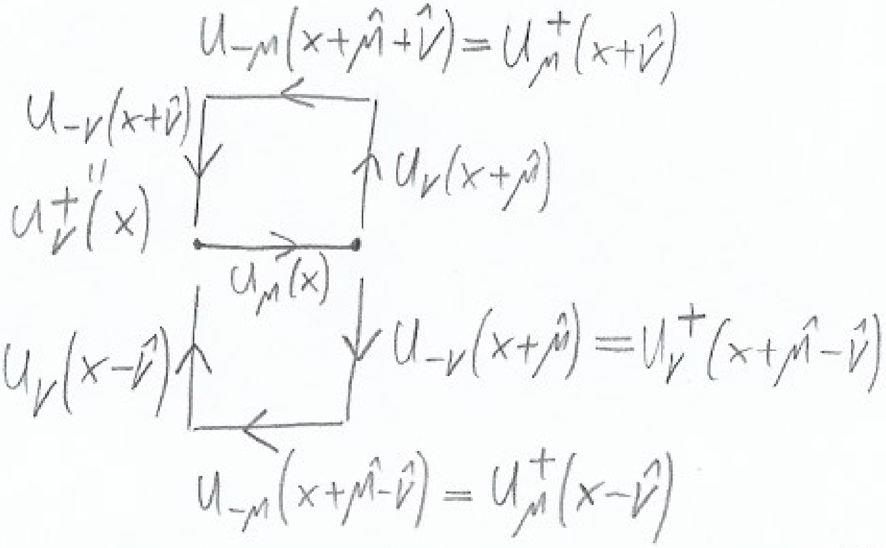


$\boxed{3D}$



$A = \sum_i P_i$ sum of <u>staples</u>

$$A = \sum_{\nu \neq \mu} \Big(U_\nu(x+\hat{\mu}) U^+_\mu(x+\hat{\nu}) U^+_\nu(x) + U^+_\nu(x+\hat{\mu}-\hat{\nu}) U^+_\mu(x-\hat{\nu}) U_\nu(x-\hat{\nu}) \Big)$$



$$\Delta S = S[U'_{x\mu}]_{loc} - S[U_{x\mu}]_{loc} = \frac{\beta}{N} \mathrm{ReTr}\left[(U_{x\mu} - U'_{x\mu}) A\right]$$

HOW TO MAKE THE PROPOSAL?

- $U'_{x,\mu}$ should be close to $U_{x,\mu}$ otherwise acceptance rate is too small
- a typical procedure $U'_{x,\mu} = X U_{x,\mu}$ where $X \in SU(N)$ and close to 1
- $T_0(U_{x,\mu} \to U'_{x,\mu}) = T_0(U'_{x,\mu} \to U_{x,\mu}) \Longleftrightarrow T_0(X) = T_0(X^{-1})$

with this the <u>Metropolis steps</u> are

1. choose a link $U_{x,\mu}$, pick a random X and propose $U'_{x,\mu} = X U_{x,\mu} \leftarrow T_0(X)$
2. calculate the staple sum $A \Rightarrow \Delta S$ and pick an $r \in [0,1]$ uniformly, <u>accept</u> $U'_{x,\mu}$ if $r \leq e^{-\Delta S}$
3. goto 1

one possible choice of picking X $\boxed{SU(2)}$

pick $\underbrace{r_1, r_2, r_3}_{\vec{r}}, r_4 \in \left(-\frac{1}{2}, \frac{1}{2}\right)$ uniform, indep

$$x_i = \varepsilon\, r_i / |\vec{r}| \qquad i = 1,2,3 \qquad x_4 = \operatorname{sign}(r_4) \sqrt{1-\varepsilon^2}$$

$$\Rightarrow x_4^2 + x_1^2 + x_2^2 + x_3^2 = 1 \Rightarrow X = x_4 \mathbb{1} + i\, \vec{x}\vec{\sigma} \in SU(2)$$

ε: free parameter, guarantees that X remains close to $\mathbb{1}$

$\boxed{SU(3)}$ use 3 $SU(2)$ subgroups $R = \begin{pmatrix} * & * & 0 \\ * & * & 0 \\ 0 & 0 & 1 \end{pmatrix}$ $S = \begin{pmatrix} * & 0 & * \\ 0 & 1 & 0 \\ * & 0 & * \end{pmatrix}$ $T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & * & * \\ 0 & * & * \end{pmatrix}$

$$X = RST \in SU(3) \qquad R, S, T \text{ close to } \mathbb{1} \Rightarrow \text{so is } X$$

for whatever choice of X we can make it symmetric $T_0(X) = T_0(X^{-1})$ by generating X (e.g. w. prev. method) and taking the hermitian adjoint with prob. $1/2$

$$\Rightarrow P_{new}(X) = \frac{1}{2}\left(P_{old}(X) + P_{old}(X^{-1})\right) = P_{new}(X^{-1})$$

LOCAL HEATBATH: GENERAL IDEA

Freeze/fix all fields except one.

$W(\phi_x | \bar{\phi})$

the chosen variable

other variable

e.g. for a real scalar field this is a 1 variable distribution, and in 1 var. we can generate anything directly

for more complicated fields it is still only a few variables:
- $O(N) \to N$ var.s
- $SU(2)$ gauge thy $\to 3$ var.s [3 angles]
- $SU(N)$ gauge thy $\to N^2-1$

FULL DISTR.: $W[\phi] = W(\phi_x | \bar{\phi})\, w(\bar{\phi})$

transition prob. (we only change ϕ_x)

only ergodic if we make a sweep over the whole lattice

$$P([\phi'] \leftarrow [\phi]) = \underbrace{P_x(\phi_x' \leftarrow \phi_x | \bar{\phi})}\, \delta(\bar{\phi}' - \bar{\phi})$$

$\Downarrow$ direct sampling

$$P_x(\phi_x' \leftarrow \phi_x | \bar{\phi}) = W(\phi_x' | \bar{\phi})$$

equivalent to making an ∞ # of Metropolis updates on the same point

HEATBATH FOR SU(2)

ORIGINAL LITERATURE:	
Creutz	1980
Kennedy, Pendleton	1985

$$dP[U_{x,\mu}] \propto \exp\Big(\frac{\beta}{N}\,\mathrm{Re\,Tr}\,U_{x,\mu}\underbrace{A}_{\text{staple sum}}\Big)\,dU_{x,\mu}$$

SU(2) is special: sum of 2 group elements $\propto$ group elem

$$\Rightarrow \quad A = a\underbrace{V}_{\in SU(2)} \qquad \det A = a^2 \det V \Rightarrow a = \sqrt{\det A}$$

$$\Rightarrow dP[U] = dU \exp\Big(\frac{\beta}{2}a\,\mathrm{Re\,Tr}(UV)\Big) \underset{\text{let } X=UV}{=} dX \exp\Big(\frac{\beta}{2}a\,\mathrm{Re\,Tr}\,X\Big) \quad (*)$$

if we generate X with this distribution, we get $U = XV^+ = \frac{XA^+}{a}$

to generate $(*)$ we can use the repr. $U = x_0 \mathbb{1} + i\vec{x}\cdot\vec{\sigma}$

$$\Rightarrow dX = \frac{1}{\pi^2} d^4x\,\underbrace{\delta(x_0^2+|\vec{x}|^2-1)}_{= \frac{\delta(|\vec{x}|-\sqrt{1-x_0^2}) + \cancel{\delta(|\vec{x}|+\sqrt{1-x_0^2})}}{2\sqrt{1-x_0^2}}}$$

will not contrib, since $|\vec{x}| \geq 0$ (not even $|\vec{x}|=0$ contributes, since we have a factor $|\vec{x}|^2 d|\vec{x}|$ in measure)

$$d^4x = d|\vec{x}|\,|\vec{x}|^2\, d^2\Omega \; dx_0 \;\; \Theta(1-x_0^2)$$

spherical angle element in 3D

if I want to extend x_0 integral to $(-\infty,+\infty)$

$$dX \xrightarrow[\text{integrate out } |\vec{x}|]{} \frac{1}{\pi^2} d^2\Omega \; dx_0 \; \frac{(1-x_0^2)\,\Theta(1-x_0^2)}{2\sqrt{1-x_0^2}} = \frac{1}{2\pi^2} d^2\Omega \; dx_0 \sqrt{1-x_0^2}\,\Theta(1-x_0^2)$$

$$\rightarrow \boxed{\vec{x} = \sqrt{1-x_0^2}}$$

$d^2\Omega = d\cos\vartheta \; d\varphi$ $\qquad\qquad$ $\mathrm{Tr}X = 2x_0$

$$\Rightarrow dP(X) = \frac{1}{2\pi^2} d\cos\vartheta \; d\varphi \; dx_0 \sqrt{1-x_0^2}\; e^{a\beta x_0}$$

$\Rightarrow$ have to generate 3 independent random variables

$x_0 \in [-1,1]$

$\left.\begin{array}{l} \cos\vartheta \in [-1,1] \\ \varphi \in [0,2\pi) \end{array}\right\}$ a uniform random pt. on a spherical surface

e.g. generate $r_1, r_2, r_3 \in [-1,1)$ uniform, accept if $r_1^2+r_2^2+r_3^2 \leq 1$, take direction generating x_0 one way to do it is:

$$dx_0\, e^{a\beta x_0}\sqrt{1-x_0^2} \propto d\lambda\, \lambda^2 \sqrt{1-\lambda^2}\, e^{-2a\beta\lambda^2}$$

$x_0 = 1-2\lambda^2 \Rightarrow \sqrt{1-x_0^2} = \sqrt{1-(1-2\lambda^2)^2} = 2\lambda\sqrt{1-\lambda^2} \propto \lambda\sqrt{1-\lambda^2}$

$x_0 \in [-1,1]$

$\Rightarrow dx_0 \propto \lambda d\lambda$

$\lambda \in [0,1]$

step ① generate λ with $p_1(\lambda) \propto \lambda^2 e^{-2a\beta\lambda^2}$

step ② accept λ with $p_2(\lambda) \propto \sqrt{1-\lambda^2}$

e.g. by noticing that: this is the distribution of the radial variable for a multivariable Gaussian $e^{-2a\beta(x^2+y^2+z^2)}\, dx\,dy\,dz \propto e^{-2a\beta r^2} r^2 dr\, d^2\Omega$ but with the constraint that $0<r\leq 1$ $(r=\lambda)$

For an efficient way to do this:

Kennedy & Pendleton 1985

HEATBATH FOR SU(3) [CABIBBO-MARINARI] (and similarly for SU(N) N≥4)

There is not heat bath algorithm to produce SU(3) links directly.
Use a pseudo heat bath, iterate SU(2) subgroups.

$$R=\begin{pmatrix} r_{11} & r_{12} & 0 \\ r_{21} & r_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad S=\begin{pmatrix} s_{11} & 0 & s_{12} \\ 0 & 1 & 0 \\ s_{21} & 0 & s_{22} \end{pmatrix} \qquad T=\begin{pmatrix} 1 & 0 & 0 \\ 0 & t_{11} & t_{12} \\ 0 & t_{21} & t_{22} \end{pmatrix}$$

$$dP(U) \propto dU \exp\left(\frac{\beta}{3} \operatorname{Re}\operatorname{Tr}(UA)\right)$$

suppose we want to modify U by left mult. with R

$$\frac{\beta}{3}\operatorname{Re}\operatorname{Tr}[R\underbrace{UA}_{W}] = \frac{\beta}{3}\operatorname{Re}\operatorname{Tr}\left[\begin{pmatrix} \boxed{\begin{matrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{matrix}}^{R'} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & 1 \end{pmatrix}\begin{pmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{pmatrix}\right] = \frac{\beta}{3}\operatorname{Re}\left(r_{11}w_{11}+r_{12}w_{21}+r_{21}w_{12}+r_{22}w_{22}\right)$$

$+ \; r_{ij}$ independent

so 

This block of W plays the role of A in our discussion of the SU(2) heat bath algorithm. It is not an element of SU(2), an not even prop. to one, but

if $W' = w_0 \mathbb{1} + i\vec{w}\cdot\vec{\sigma}$, $w_0, w_1, w_2, w_3 \in \mathbb{C}$ $\Longrightarrow$ [exercise] $\operatorname{Re}\operatorname{Tr}(RW) = \operatorname{Re}\operatorname{Tr}(R'(\underbrace{\operatorname{Re} w_0 \mathbb{1} + i(\operatorname{Re}\vec{w})\cdot\vec{\sigma}}))$ prop. to an SU(2) element

projection by taking real parts of coeffs. w_i

OVERRELAXATION

$\Delta S = 0$ <u>microcanonical</u> algorithm (Metropolis would always accept)
$\hookrightarrow$ <u>not ergodic</u> (combine w. Metropolis or heatbath to make it ergodic)

<u>idea:</u> use a symmetry (e.g. a "reflection"), it leaves the action unchanged but allows you to take bigger steps $\Rightarrow$ smaller autocorrelation

in gauge thy:

$$S = c \sum_P \square = c\, \mathrm{Re}\, \mathrm{Tr}\, U_{x\mu} A$$ staple sum

if $U \to U' = A U A^{-1} \Rightarrow \mathrm{Tr}(UA) = \mathrm{Tr}(AU) = \mathrm{Tr}(AUA^{-1}A) = \mathrm{Tr}(U'A)$

U' not necessarily an $SU(N)$ matrix, but in $SU(2)$ it is

[<u>exercise</u>: show that sum of two $SU(2)$ matrices $=$ (number $\cdot$ $SU(2)$) matrix]

$\Rightarrow P(U' \leftarrow U)\, e^{-S[U]} DU = P(U \leftarrow U')\, e^{-S[U']} DU'$ since $d(AUA^{-1}) = d(VUV^{-1}) = dU$ (Haar m.) $V \in SU(2)$

$SU(N)$ $N \geq 3$: can work with $SU(2)$ subgroups

state-of-the-art for pure gauge: combination of heatbath & overrelaxation

CORRELATION FUNCTIONS

e.g. correlator of Polyakov loops $P(\vec{x}) = \prod_{\tau=0}^{N_\tau - 1} U_4(\vec{x},\tau)$

$$\langle \mathrm{Tr}\, P(\vec{r})^\dagger \; \mathrm{Tr}\, P(\vec{0}) \rangle \sim e^{-F_{Q\bar{Q}}(|\vec{r}|)/T}$$

static quark-antiquark pair free energy

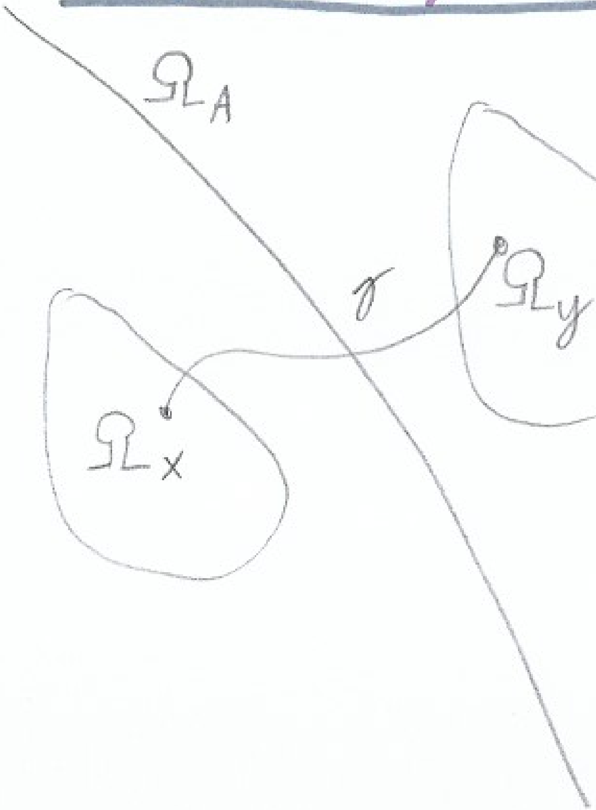
$$F_{Q\bar{Q}}(r) \xrightarrow[T \to 0]{} V_{QQ}(r)$$

other examples:
- correlator of plaquettes
- correlator of energy-momentum tensor elements etc.

can be evaluated directly, but for pure gauge thy there is a simple but efficient trick to do this, called the multilevel algorithm hep-lat/0108014

hep-lat/0209145

LOCALITY OF PROB. DISTRIBUTIONS



$\mathcal{C}$: configuration of fields

$\mathcal{X}, \mathcal{Y}, \mathcal{A}$: mutually disjoint subsets of $\mathcal{C}$

$\Omega_{\mathcal{X}}, \Omega_{\mathcal{Y}}, \Omega_{\mathcal{A}}$: their support

suppose any continuous path from $\Omega_{\mathcal{X}}$ to $\Omega_{\mathcal{Y}}$ goes through $\Omega_{\mathcal{A}}$

we call a prob. distr. <u>local</u> if for any setup w. this topology

$$P(\mathcal{X}, \mathcal{Y}) = \sum_{\mathcal{A}} p(\mathcal{A})\, P_{\mathcal{A}}(\mathcal{X})\, \tilde{P}_{\mathcal{A}}(\mathcal{Y})$$

i.e. $\mathcal{X}$ and $\mathcal{Y}$ influence each other only through $\mathcal{A}$

obviously satisfied for

- continuum QFT w $\mathcal{L}$ containing only finite num. derivatives
- lattice field thy w. nearest neighbour, next-to-nearest etc. (finite range) couplings etc. (not true for dynamical fermions that are integrated out)

MULTILEVEL INTEGRATION (GENERAL IDEA)

O_x : function of fields on Ω_x [2-level here]

O_y : function of fields on Ω_y

$$\langle O_x O_y \rangle \equiv \sum_C p(C)\, O_x(C)\, O_y(C) = \sum_x \sum_y p(x,y)\, O_x(x)\, O_y(y)$$

$$= \sum_A \sum_x \sum_y p(A)\, p_A(x)\, \tilde{p}_A(y)\, O_x(x)\, O_y(y) = \sum_A p(A) \langle O_x \rangle_A \langle O_y \rangle_A$$

where $\langle O_x \rangle_A = \sum_x p_A(x)\, O_x(x)$ and $\langle O_y \rangle_A = \sum_y \tilde{p}_A(y)\, O_y(y)$

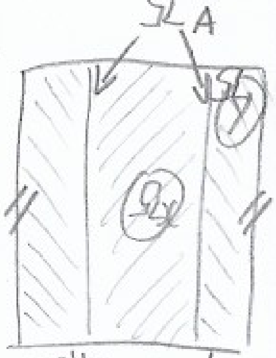
we have 2 subvolumes and 1 boundary

n updates N updates

$\Rightarrow$ Nn MC updates in total

but in effect we have Nn^2 measurements

$\Rightarrow$ stat error $\propto \frac{1}{\sqrt{N}\, n}$



with periodic boundary conds

LATTICE FIELD THY II "TOC"

① UNIVERSALITY AND THE RENORMALIZATION GROUP

(~ 4 lectures)

Why do we expect different discretizations to give the same cont. lim.?

intimately related to

Why is behavior near 2nd order phase transitions universal?

⇝ renormalization group à la Wilson

- the renormalization group & universality
- the field theoretical RG, β-functions, triviality, asymptotic freedom
- Banks-Zaks fixed point, conformal window
- "exploiting universality" constructing improved actions

② CHIRAL SYMMETRY

(~ 4 lectures)

symmetry in the limit $\boxed{m_q \to 0}$

spontaneously broken ⇒ π as Goldstone boson

but also explicitly broken by $m_q \neq 0$

- chiral symmetry in continuum QCD
- lattice chiral symm. & Ginsparg-Wilson fermions
  - overlap fermions
  - domain wall fermions
- topology of gauge fields, index thm
- axial anomaly
- the chiral condensate & the Banks-Casher relation
- the chiral phase transition at finite temperature

③ HADRON SPECTROSCOPY

(~ 2 lectures)

- hadron interpolators and correlators
- calculation of quark propagators (solving the discretized Dirac equation)

  ⇝ iterative methods in linear algebra (conjugate gradient)
- extracting the hadron masses: ground & excited states
- resonances, unstable particles in a finite volume

④ SIMULATIONS W. DYNAMICAL FERMIONS

(~2 lectures)

How to deal with $\det M[U]$?

difficulty: long-range interactions in gluonic effective action

- pseudofermions
- hybrid Monte Carlo (HMC) (also called Hamiltonian Monte Carlo)
- approximation thy, best polynomial and rational approximations of a given order
- rational Hybrid Monte Carlo (RHMC)