LATTICE FIELD THEORY

I think everyone attending this lecture knows that perturbation theory doesn't work in all situations. I want to present lattice field theory (LFT) as a non-perturbative approach to QFT using regularized Euclidean functional integrals, which is what [Montvay-Münster] do. My goals are

(1) To help you see, at least heuristically, why lattice calculations work

(2) To show you the generic steps for carrying out a lattice calculation

(3) Along the way, hopefully show you enough jargon that you can better follow CRC talks showcasing lattice results

I assume you already took a QFT course. To get through my goals in an hour specialize to pure $SU(N_c)$:

$$\mathcal{L} = \frac{1}{4} F^a_{\mu\nu} F^{a,\mu\nu} = -\frac{1}{2g^2} \operatorname{tr} F_{\mu\nu} F^{\mu\nu} \qquad A_\mu \equiv ig A^a_\mu T^a$$

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f^{abc} A^b_\mu A^c_\nu \qquad F_{\mu\nu} \equiv -ig F^a_{\mu\nu} T^a$$

I suppress space-time index sometimes

EUCLIDEAN QFT

Lattice field theories (LFT) work in a Euclidean spacetime. This is achieved through the **Wick rotation**

$$t \to i\tau, \qquad (x^0 \to ix^4) \tag{1}$$

where τ is the **Euclidean** or **imaginary** time. We see that the separation between events becomes

$$ds^2 = -t^2 + \vec{x}^2 \to \tau^2 + \vec{x}^2, \tag{2}$$

which is why we call it Euclidean. With a Euclidean metric, there is no distinction between covariant and contravariant indices, so we will write, e.g. $X_\mu X_\mu$, $F_{\mu\nu} F_{\mu\nu}$, etc.

You can view the Wick rotation as an analytic continuation of correlation functions from real time to imaginary time. It shouldn't be surprising that, in some cases, the Minkowskian correlators can be reconstructed from the Euclidean ones [Osterwalder, Schrader, Wightman, Streater].

What does doing the Wick rotation buy us? Well, the action becomes

$$S = \int dt \, d^3x \, \mathcal{L} \to i \int d\tau \, d^3x \, \mathcal{L} \equiv iS_E, \tag{3}$$

where S_E is the **Euclidean** action. Hence our path integral becomes

$$\mathcal{Z} = \int \prod_{x,\mu} dA_\mu(x) \boxed{e^{iS[A]}} \longrightarrow \int \prod_{x,\mu} dA_\mu(x) \boxed{e^{-S_E[A]}} \quad (4)$$

Highly oscillatory integral.

S pure real $\Rightarrow |e^{iS}| = 1$,

so integral doesn't converge absolutely

In Euclidean space,

now exponentially damped

$X \equiv$ some observable

With $e^{-S_E[A]} > 0$, we see connection with statistical physics:

$$\langle X \rangle = \frac{1}{\mathcal{Z}} \int \prod_{x,\mu} dA_\mu(x) \; e^{-S_E[A]} \; X[A] \quad (5)$$

$$\frac{1}{\mathcal{Z}} e^{-S_E[A]} = pr(A) \quad (6)$$

A final nice thing: It turns out that

$$\langle X(t) X(0) \rangle \sim \sum_n \langle 0|X|n\rangle\langle n|X|0\rangle e^{-tE_n} \quad (7)$$

in Euclidean time, which means we can extract e.g. particle masses through fitting the RHS.

So we see it's nice to do a Wick rotation

- to tame path integrals
- to exploit connections to statistical physics
- to get access to particle masses

<u>A note</u>: Working in a Euclidean does make other kinds of observables more challenging; we lose easy access to real-time observables like transport coefficients and spectral functions. (There are some workarounds but it's tricky.)

LATTICE REGULARIZATION

Take a region of spacetime and discretize it
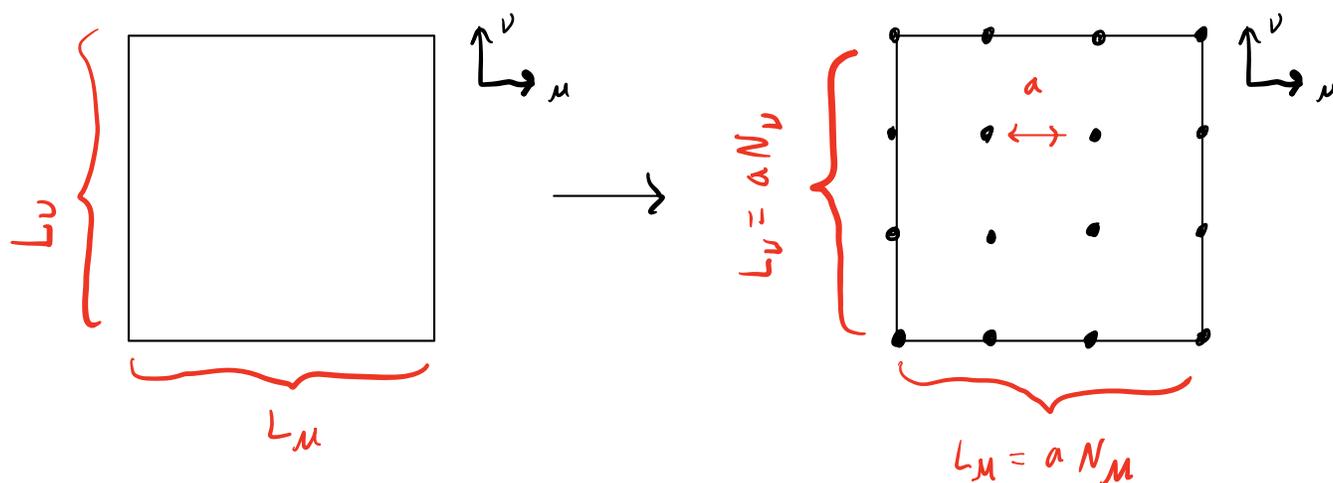
You don't <u>have</u> to use this set up, but it's most common

a: lattice spacing

$N_\tau \equiv N_4$: Euclidean time extension

$N_\sigma \equiv N_1 = N_2 = N_3$: spatial extension

The lattice is   "site"

$$\mathbb{L} \equiv \{ x \mid x_\mu = a n_\mu, \ 0 \leq n_\mu < N_\mu \} \qquad (8)$$

with $N_\mu \in \mathbb{N}$, $n_\mu \in \mathbb{Z}$, $\mu \in \{1, 2, 3, 4\}$. Unless you believe

We live in a simulation (if you do, please see me after the lecture — I'm looking for a plug), the lattice is a mere calculational crutch that distorts physics a bit. Our hope is that the "real" (Euclidean) world will be recovered in the continuum limit

$$a \to 0$$

OKay, so what kinds of things got "distorted"?

- Poincare symmetry breaks a little. In particular O(4) breaks to hypercube symmetries. We can keep translational symmetries with periodic boundary conditions (PBCs):

$$X + a N_\mu \hat{\mu} = X \qquad (9)$$
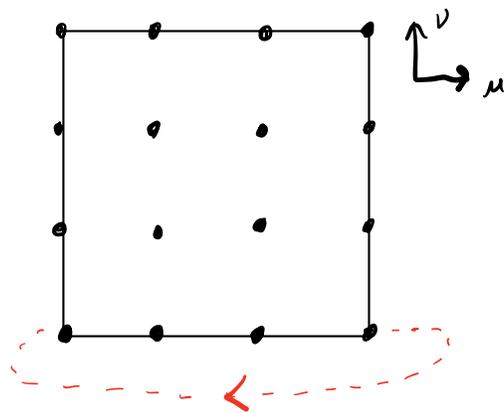
For this reason, often call the lattice a torus.

- Derivatives replaced by finite differences, e.g.

$$\partial_\mu f \to \Delta_\mu^B f \equiv \frac{f(x) - f(x - a\hat{\mu})}{a} \qquad (10)$$

"Backward"

Actually we have some freedom how to discretize things like derivatives. We could have instead defined

$$\partial_\mu f \rightarrow \Delta_\mu^C f = \frac{f(x+a\hat{\mu}) - f(x-a\hat{\mu})}{2a} \qquad (11)$$

"central"

which to pick? You can show by Taylor expansion

balance programming/
computational complexity
against smaller lattice
artifacts

$$\Delta_\mu^B f = \partial_\mu f + \mathcal{O}(a) \qquad (12)$$

$$\Delta_\mu^C f = \partial_\mu f + \mathcal{O}(a^2) \qquad (13)$$

lattice artifacts

This is suggestive of working with small a. Then Δ_μ^C is a better approximation to ∂_μ than Δ_μ^B, and in practice, Δ_μ^C is what's used. Finding discretizations that better suppress lattice artifacts is called improvement. Thinking ahead for a moment, dynamical actions have derivatives in them, so we in general have a choice how to discretize the action.
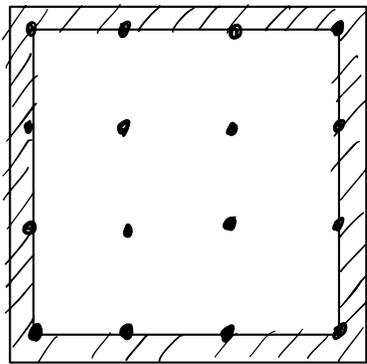
- Integrals replaced with sums:
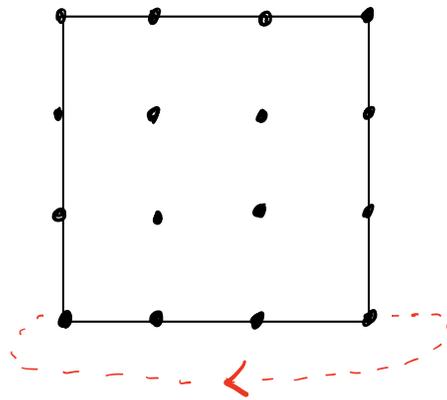
$$\int d^4x \rightarrow a^4 \sum_x$$

- UV and IR regulators automatic. In particular, $\mathbb{1}$ is in some sense "blind" to physics on length scales smaller than a and larger than aN.

  Let's understand a bit better. We took PBCs to get translational symmetry. These PBCs help also to

milden systematic error due to loss of IR physics:

So in general we like PBCs. But they discretize the momenta. Can be seen through Fourier transforms:

$$f(x) = f(x + aN) \implies \int dp\, f(p) e^{ipx} = \int dp\, f(p) e^{ip(x+aN)}$$

for simplicity focus on one dimension

$$\implies e^{ipx} = e^{ip(x+aN)}$$

$$\implies ipaN = 2\pi i n \qquad n \in \mathbb{Z}$$

$$\implies p = \frac{2\pi n}{aN} \qquad\qquad (14)$$

which tells us momentum-space integrals should also be discretized. Moreover, introducing a lattice spacing directly regulates momenta. For

$$f(p + \tfrac{2\pi}{a}) = a^4 \sum_{x} e^{-ipx} e^{-\frac{2\pi i}{a}x} f(x) \qquad x = an, \quad n \in \mathbb{Z}$$

$$= e^{-\frac{2\pi i}{a} a n} f(x)$$

$$= f(p) \tag{15}$$

This shows us functions are periodic in momentum space, so we can restrict momenta WLOG to first Brillouin zone

$$-\frac{\pi}{a} < p_\mu \leq \frac{\pi}{a} \tag{16}$$

What we have achieved is a non-perturbative regularization, to be contrasted with e.g. Pauli-Villars or dimensional regularization, which rely on perturbation theory.

- Systematic effects due to a (UV) are expected to be removed in continuum limit. Effects due to the finite box size expected to die out in thermodynamic limit, $L \to \infty$.

BUILDING BLOCKS OF LATTICE GAUGE THEORY

The discussion of the last section was quite generic, but now we want to introduce some gauge fields. We want $\mathcal{L}$ to be invariant under local gauge transformations

$$U_\mu(x) \to \Lambda(x) U_\mu(x) \Lambda^{-1}(x + a\hat{\mu}), \qquad \Lambda \in SU(N_c) \tag{17}$$

As you know, local gauge invariance requires the introduction of covariant derivatives; in other words, taking derivatives by comparing two points x and y requires you to parallel transport e.g. your field at y to x. The parallel transporter along the curve C_{yx} can be reconstructed in the continuum from the gauge field A_μ using **Dyson's formula**

$$U(C_{xy}) = P \exp \left\{ - \int_{C_{xy}} A_\mu \, dx^\mu \right\} \qquad (18)$$

This can be viewed as a motivation for the shortest parallel transporter on the lattice

$$U_\mu(x) \equiv e^{-a A_\mu(x)}, \qquad \overset{\textstyle U_\mu(x)}{\underset{\textstyle x \qquad x+a\hat{\mu}}{\bullet \longrightarrow \bullet}} \qquad (19)$$

the **link variable** or simply **link**. For this reason, you sometimes hear people say "the gluons live on the links".

If we follow a path then reverse our steps, we should end up back where we started:

$$U_{-\mu}(x + a\hat{\mu}) \, U_\mu(x) = \mathbb{1}. \qquad (20)$$

Since $U_\mu^\dagger(x) U_\mu(x) = \mathbb{1}$, we see

$$U_\mu^\dagger(x) = U_{-\mu}(x + a\hat{\mu}) \qquad (21)$$

For pure $SU(N_c)$, the U_μ are the only objects we have

for constructing observables. Elitzur's theorem tells us observables have to be gauge-invariant. A large class of gauge-invariant observables are the Wilson loops

$$W_{\mu\nu\dots\rho}(x) = tr \; U_\mu(x) \, U_\nu(x+a\hat{\mu}) \; \dots \; U_\rho(x-a\hat{\rho}), \qquad (22)$$

i.e. the product of links around a closed path. In particular from eq (18) we see that under a local gauge transformation
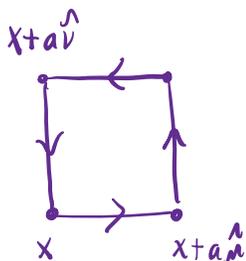
example Wilson loop
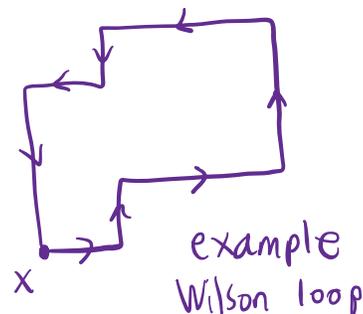
$$W_{\mu\nu\dots\rho}(x) \rightarrow tr \; \Lambda(x) U_\mu(x) \Lambda^{-1}(x+a\hat{\mu}) \Lambda(x+a\hat{\mu}) U_\nu(x+a\hat{\mu})$$

$$\dots \; U_\rho(x-a\hat{\rho}) \Lambda^{-1}(x),$$

and the final $\Lambda(x)$ cancels from cyclicity of the trace. The smallest Wilson loop is the plaquette

$$tr \; U_{\mu\nu}^{\square}(x) = tr \; U_\mu(x) \, U_\nu(x+a\hat{\mu}) \, U_\mu^\dagger(x+a\hat{\nu}) \, U_\nu^\dagger(x) \qquad (23)$$

$x+a\hat{\nu}$

x $\quad x+a\hat{\mu}$

When one wants to probe some physical observable, one needs to use lattice objects to build an object that has the same quantum numbers as a physical observable. That composite object is called an interpolator. Looking at the indices of the plaquette, you may guess it interpolates $F_{\mu\nu}$. And you would be right in the sense that

$$U_{\mu\nu}^{\square} = \exp\left\{-a^2 F_{\mu\nu} + O(a^3)\right\}, \qquad (24)$$

which can be shown either by expanding the exponentials or using the Campbell-Baker-Hausdorff formula

$$\exp(\varepsilon X)\exp(\varepsilon Y) = \exp\left\{\varepsilon X + \varepsilon Y + \frac{1}{2}[\varepsilon X, \varepsilon Y] + O(\varepsilon^3)\right\}. \qquad (25)$$

Either way, you exploit

$$A_\mu(x+a\hat{\nu}) = A_\mu(x) + a\,\partial_\nu A_\mu(x) + O(a^2) \qquad (26)$$

The entire lattice formalism is due to [Wilson], and in this paper, he proposes a discretization of the gauge action, commonly called the Wilson action:

$$S_W = \beta \sum_{x,\mu<\nu} \left(1 - \frac{1}{N_c}\operatorname{Re}\operatorname{tr} U_{\mu\nu}^{\square}\right). \qquad (27)$$

If one keeps higher-order terms in (24), one finds

$$S_W = \beta \sum_{x,\mu<\nu} \left(1 - \frac{1}{N_c}\operatorname{Re}\operatorname{tr} U_{\mu\nu}^{\square}\right)$$

$$= \qquad \left(\quad -\frac{1}{2N_c}\operatorname{tr}\left(U_{\mu\nu}^{\square} + U_{\mu\nu}^{\square\dagger}\right)\right)$$

$$= \qquad \left(\qquad \operatorname{tr}\left(2\mathbb{1} + \frac{a^4}{2}F_{\mu\nu}^2 + O(a^6)\right)\right)$$

$\bullet\ F_{\mu\nu} = -F_{\mu\nu}^\dagger \Rightarrow a^2$ terms cancel

- other terms $a^p f_{\mu\nu}^{p-2}$ cancel for odd p since $F_{\mu\nu}^{p-2}$ antisymmetric under $\mu \leftrightarrow \nu$, and all μ, ν combinations are summed over

- $-\frac{1}{2N_c} \text{tr } 2\mathbb{1} = -1$, cancelling leading 1

$$= -\frac{\beta}{2N_c} a^4 \sum_{x, \mu < \nu} \text{tr } F_{\mu\nu}^2 + O(a^6)$$

$$= -\frac{\beta}{4N_c} a^4 \underbrace{\sum_x \text{tr } F_{\mu\nu}(x) F_{\mu\nu}(x)} + \underbrace{O(a^6)} \qquad (28)$$

$a \to 0$, converges to

$\int d^4x \ \text{tr } F_{\mu\nu}(x) F_{\mu\nu}(x)$

$O(a^2)$ lattice artifact relative to gauge action

In other words we see S_W discretizes the Yang-Mills action if we identify

"coupling constant" $\beta \equiv \frac{2N_c}{g^2}$ $\qquad (29)$

A couple notes are in order: The β symbol is chosen here in analogy to $1/k_B T$ in statistical physics. g is the bare coupling: Again, we haven't done any perturbative renormalization. Owing to the lattice regularization, we will find $g(a)$.

Now that we have an action, we can compute expectation values:

$$\langle X \rangle = \frac{1}{Z} \int \prod_{x, \mu} dU_\mu(x) \ e^{-S_W[U]} X[U] \qquad (30)$$

- Imagine fixing $U_\mu(x) \; \forall x, \mu$. We call that a configuration, which is a possible realization of the field U. $f[U]$ here then just means f is a functional of the configuration.

- We traded A_μ for U_μ in the measure. U_μ is more convenient notationally

- The integral is seen to run over all possible configurations weighted by a Boltzmann factor

- The measure   "Haar measure"

$$\mathcal{D}U \equiv \prod_{x, \mu} dU_\mu(x) \qquad\qquad (31)$$

is finite-dimensional at $a > 0$: This really is a well defined integral!

- In practice, you can't just use (30) directly. Consider a $N_\sigma^3 \times N_t = 2^4$ lattice. (As small as possible) The dimension of the integral is

$$2^4 \quad \times \quad 4 \quad \times \quad N_c^2 - 1 \quad = 512$$

   sites   directions   Haar   for SU(3)

If I support each integral with only 2 points, my computation has

$$2^{512} \quad \approx \quad 1.3 \times 10^{154} \quad \text{terms}$$

You only get $\sim 6 \times 10^9$ cycles/second on the best CPUs, so we need to find some trick.

I've been hinting at using LFT to put a QFT on a computer, but that's not the only use. In fact, [Wilson] uses this framework to do a purely analytic calculation. He argues in the strong-coupling limit, i.e. for $\beta \ll 1$, that the static quark-antiquark potential should assume the form

"Cornell potential"
$$V_{\bar{q}q}(r) = A + \frac{B}{r} + \sigma r \qquad (32)$$

i.e. he derives the σr term in the strong-coupling limit, which proffers an explanation for confinement. A very readable derivation is in [Gattringer-Lang].

THE CONTINUUM LIMIT

In $a \to 0$ limit, physical quantities X should agree with experiment, which means X should become independent of a, "forgetting" about the lattice. Looking at e.g. (28), the two parameters at our disposal are a and g, so

$$\lim_{a \to 0} X(a,g) = X^{phys} \qquad (33)$$

In order for (33) to work, changes in a must be

compensated by changes in g. Thus $g(a)$. One can play the same game as when determining how a coupling changes with the cutoff for QCD in the continuum, namely we formulate (33) as

$$\left(\frac{\partial}{\partial \log a} + \frac{\partial g}{\partial \log a} \frac{\partial}{\partial g} \right) X = 0 \qquad (34)$$

with β function

$$\beta \equiv - \frac{\partial g}{\partial \log a} \qquad (35)$$

One can even take over

$$\beta(g) = -b_0 g^3 - b_1 g^5 + O(g^7) \qquad (36)$$

from perturbation theory, as b_0 and b_1 do not depend on the regularization scheme. Thus we have the standard result that (35) is solved at two-loop order by

$$a \Lambda_L = \exp\left(- \frac{1}{2 b_0 g^2} \right) (b_0 g^2)^{-b_1/2b_0^2} \qquad (37)$$

or

$$\frac{1}{g(a)^2} = b_0 \log\left(a^{-2} \Lambda_L^{-2} \right) + \frac{b_1}{b_0} \log \log \left(a^{-2} \Lambda_L^{-2} \right) + O\left(\frac{1}{\log(a^2 \Lambda_L^2)} \right) \qquad (38)$$

You recall that $b_0(N_c, N_f)$ and $b_1(N_c, N_f)$. For SU(3), as long as you have fewer than 17ish quark flavors, we see

$a \to 0$ drives $g \to 0$ and vice versa. Thus the continuum limit can be achieved by

$$\beta = \frac{2N_c}{g^2} \longrightarrow \infty, \qquad (39)$$

which for pure $SU(N_c)$ is the only input parameter.

Now we see an issue: We can't take $a \to 0$ with $N_\sigma^3 \times N_\tau$ fixed: The box would evaporate. Thus one should try to keep the physical volume

$$V = a^4 N_\sigma^3 N_\tau \qquad (40)$$

approximately fixed, which translates to increasing N_σ and N_τ, i.e. the number of sites. Thus one can intuitively think about $a \to 0$ in this manner as increasing the resolution of your configurations.

In practice, $a \to 0$ is carried out using continuum-limit extrapolations. Say we found a way to do the integral in (30). Then we would get at a particular spacing

$$\langle X(a) \rangle$$

The idea is to repeat this process for many spacings, yielding schematically
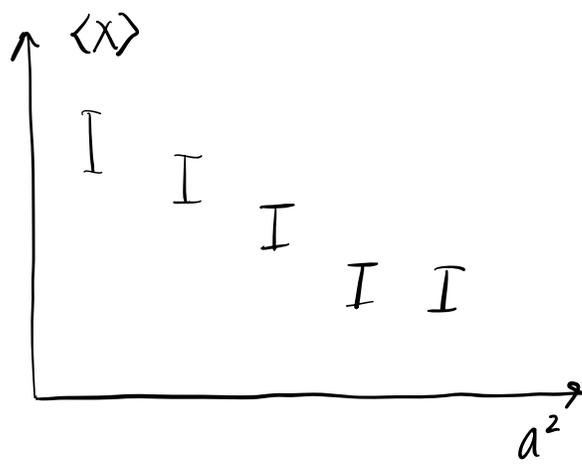
we want to fit those data to estimate $\langle X(0)\rangle$. What should the fit form be? We just argued

$$S_W(a) = S_{YM} + O(a^p) \tag{41}$$

With $p = 2$. A different (improved) discretization of S_{YM} would deliver $p > 2$. Interpolators are also subject to these corrections. Lets say
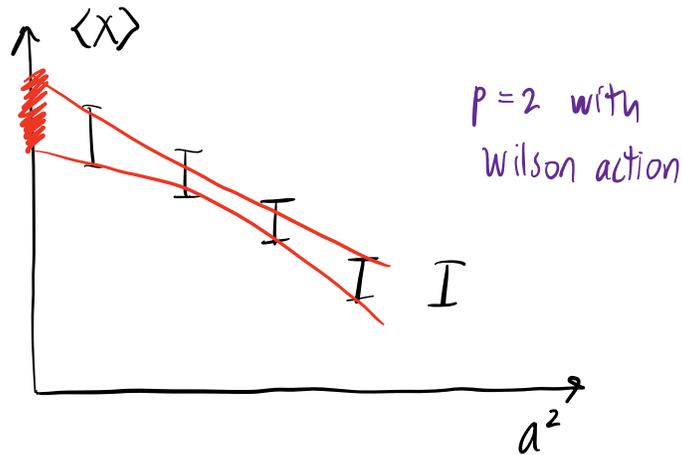
$$X(a) = X_{phys} + O(a^q) \tag{42}$$

Plugging (41) and (42) into (30) yields

$$\langle X(a)\rangle = \frac{1}{Z} \int \mathcal{D}U \, e^{-S_W[U]} X[U]$$

$$= e^{-S_{YM} + O(a^p)} \left(X_{phys} + O(a^q)\right)$$

$$= e^{-S_{YM}} \left(1 + O(a^p)\right) \left(X_{phys} + O(a^q)\right)$$

$$= \langle X_{phys}\rangle + O(a^p, a^q). \tag{43}$$

Thus if we are in a situation where $p \leq q$, we can do a linear fit in a^p:

$$\langle X(a) \rangle = \langle X_{phys} \rangle + m a^p \qquad (44)$$

$p=2$ with Wilson action

It is a bit delicate picking the fit form (e.g. should I include higher-order terms?) and where to start the fit (is my lattice too coarse given the number of terms in the fit?) Safest approach is to do model weighting.

One last note about the continuum limit. Earlier we wrote

$$\langle X(t) X(0) \rangle \sim \sum_n \langle 0 | X | n \rangle \langle n | X | 0 \rangle e^{-t \epsilon_n}$$

in Euclidean spacetime. This tells us that for a given Euclidean time separation t, the two-point function dies off like

$$\langle X(t) X(0) \rangle \sim e^{-t \epsilon_0} \qquad (45)$$

This ϵ_0 is related in the usual way to a length

$$\xi \equiv \frac{1}{E_0} \qquad (46)$$

This correlation length controls the rate of exponential decay, and is not dependent on a; it comes from the Hamiltonian in the continuum theory. In the continuum limit,

$$\frac{\xi}{a} \to \infty \qquad (47)$$

i.e. the correlation length effectively diverges. A divergent correlation length is a hallmark of a 2nd order phase transition, so in that sense, the continuum limit corresponds to a 2nd order transition.

FINITE TEMPERATURE

We have discussed quite a bit now the factor

$$Z = \int \mathcal{D}U \, e^{-S_E[U]} \qquad (48)$$

and how it's involved in Boltzmann factors. This path integral can be constructed in the usual way, with a starting point (in one dimension, for generic field $\varphi_0 \equiv \varphi(\tau=0)$) 1D just to heuristically remind ourselves how it worked

$$Z = tr \, e^{-a N_\tau H} = \int d\varphi_0 \, \langle \varphi_0 | e^{-a N_\tau H} | \varphi_0 \rangle \qquad (49)$$

One breaks up the dimension (and exponential) into discrete steps, inserting $\int d\varphi_n \, |\varphi_n\rangle\langle\varphi_n|$ between them, to arrive at

$$\mathcal{Z} = \int \mathcal{D}\varphi \, e^{-S_E[\varphi]}. \tag{50}$$

In that context (now going back to 4D) we had

$$S_E = \int_0^{aN_\tau} d\tau \int d^3x \, \mathcal{L} \tag{51}$$

What if we were instead looking at a static 3D system in thermal equilibrium at temperature T? Statistical physics tells us the partition function is

$$\mathcal{Z} = tr \, e^{-\beta H} \tag{52}$$

Formally, we could do the same steps to construct the path integral with this partition function. It would look the same as (48), only now we would have

$$S_E = \int_0^\beta d\tau \int d^3x \, \mathcal{L} \tag{53}$$

Thus the whole 4D and 3D at finite T theories are the same, with the correspondence

$$\beta = \frac{1}{T} = aN_\tau \quad \Rightarrow \quad T = \frac{1}{aN_\tau} \tag{54}$$

So a lattice simulation can always be interpreted as a

3D simulation at finite T. This is exactly what lattice practitioners do when doing phase diagram calculations.

Note that at fixed T, (54) tells us that $N_\tau \to \infty$ drives $a \to 0$. Thus for phase diagram calculations, it's common to see N_τ represent the lattice spacing, with smaller N_τ corresponding to coarser lattices and larger N_τ to finer. We see conversely that at fixed a, $N_\tau \to \infty$ drives $T \to 0$. For this reason, zero-temperature calculations are carried out with $N_\tau \gg N_\sigma$, so T is negligible.

While we're on the subject, since $\mathcal{Z}$ can be interpreted as the partition function of a 3D statistical physics system, we can use standard thermodynamic relations. For example in the grand canonical ensemble, we can get in principle the pressure

$$p = \lim_{V \to \infty} \frac{T}{V} \log \mathcal{Z} \qquad (55)$$

and derive other thermodynamic observables from there.

The tricky part is the chemical potential. The chemical potential couples to γ_4 (γ_0 in Minkowski). The Wick rotation doesn't get rid of the i in this part of the action, rendering the Boltzmann factor complex. That is the sign problem, and it prevents direct simulations at $\mu \in \mathbb{R}$.

One workaround is to simulate at pure imaginary μ,

like the Wick rotation, and try to analytically continue back to $\mu \in \mathbb{R}$. A highly successful trick expands P in $\mu/T \equiv \hat{\mu}$:

$$P(\mu, T) = \sum_{ijk} \frac{\hat{\mu}_B^i \; \hat{\mu}_Q^j \; \hat{\mu}_S^k}{i! \, j! \, k!} \boxed{\frac{\partial^{i+j+k} \; P(0, T)}{\partial \hat{\mu}_B^i \; \partial \hat{\mu}_Q^j \; \partial \hat{\mu}_S^k}}$$

defined at $\mu = 0$ so avoids the sign problem

SCALE SETTING

As we saw, $g \to 0$ formally sends $a \to 0$. If we want to put the lattice on a computer, nothing we have done so far really tells us how to get anything in physical units.

Scale setting is the process of attaching physical units. Roughly it goes like this: Suppose I have some observable X I am interested in. I choose another observable Y where I know its real-world value, Y_{phys}, say from experiment. Y is called the reference scale. We assume X and Y have units of MeV. From our discussion about the continuum limit, it should be that

$$\frac{X^{phys}}{Y^{phys}} = \lim_{a \to 0} \left\langle \frac{X(a)}{Y(a)} \right\rangle \equiv R \qquad (56)$$

We determine R from our continuum-limit extrapolation and obtain

$$X^{phys} = R \, Y^{phys}. \tag{57}$$

This also gives us a way to estimate a in physical units. Everything directly coming out of the computer is unitless, so I should be able to write something like

$$Y(a) = a \left(Y^{phys} + O(a\Lambda_L) \right) \tag{58}$$

Thus a first estimate for a could be

$$a \approx \frac{Y(a)}{Y^{phys}} \tag{59}$$

In practice, scale setting is a bit delicate. A good choice for Y^{phys} depends on, e.g.

- the theory being considered, i.e. does it make sense to use $Y^{phys} = M_\Omega$ from experiment for an $N_f = 5$ (5 degenerate quarks) theory?
- how noisy the interpolator Y is
- how badly distorted is Y by e.g. finite box size

HOW TO GET $\langle X \rangle$: USING COMPUTERS

At this point, I think I have discussed the necessary ingredients of a lattice calculation, except

one: We already mentioned that computing

$$\langle X \rangle = \frac{1}{Z} \int \mathcal{D}U \, e^{-S_W[U]} X[U] \tag{60}$$

directly is not really tractable. What to do?

   The crucial point is that (60) shows us configurations U are distributed according to

$$\mathrm{pr}(U) \sim \frac{1}{Z} \mathcal{D}U \, e^{-S_W[U]} \tag{61}$$

Configurations U with crazy $S_W[U]$ are exponentially suppressed, and hence are negligible. Thus we can get $\langle X \rangle$ to a good approximation by drawing N configurations according to (61), estimating

$$\overline{X} \equiv \frac{1}{N} \sum_i X_i \approx \langle X \rangle \tag{62}$$

The estimator $\overline{X}$ should approach $\langle X \rangle$ as $N \to \infty$, and for finite N, assuming the X_i are drawn independently, the central limit theorem guarantees

$$\sigma_{\overline{X}}^2 = \frac{1}{N(N-1)} \sum_i (X_i - \overline{X})^2 \tag{63}$$

   OK how do we draw the configurations? Well, a configuration will be saved in the computer as a large array

$$U = \left[U_1(x), U_1(x+a\hat{1}), \dots, U_2(x), U_2(x+a\hat{1}), \dots \right] \quad (64)$$

Each $SU(N_c)$ matrix $U_\mu(x)$ is represented as a matrix with N_c^2 complex elements, i.e. with $2N_c^2$ real numbers. Being thoughtful about the order in which you store the $U_\mu(x)$ in the array U generally helps the code access elements of U more quickly. The most common technique to draw configurations is to use a Markov chain

$$U^{(0)} \rightarrow U^{(1)} \rightarrow U^{(2)} \rightarrow \dots \quad (65)$$

Here $U^{(n)}$ is generated by deforming $U^{(n-1)}$ in some way. It can also be $U^{(n)} = U^{(n-1)}$ (trivial). Here $U = U^{(n-1)}$ ↘

The generation can be decomposed into two steps:

i) A trial configuration U' is proposed with probability $T(U'|U)$.

ii) The trial is accepted with likelihood "Metropolis step"

$$A(U \rightarrow U') = \min\left[1, \frac{T(U|U')}{T(U'|U)} \frac{e^{-S[U']}}{e^{-S[U]}} \right] \quad (66)$$

If accepted, $U^{(n)} = U'$; otherwise $U^{(n)} = U^{(n-1)}$.

We see that if the trial lowers the action, it is always accepted. Otherwise it's accepted based on the action difference, which we see is the ratio of Boltzmann factors.

this procedure is common also in statistical physics simulations

To transition from U to U' we need to propose U' then accept it. Thus

$$pr(U \to U') = T(U'|U) A(U \to U')$$

$pr(U \to U')$ can be viewed as the U, U' element of a transition matrix. It turns out that if your transition matrix (which depends on the algorithm— doesn't have to be Metropolis) satisfies

- **ergodicity**: Every configuration is accessible from every other configuration in finitely many steps

- **normalization**: The transition probabilities are normalized appropriately

$$\sum_{U'} pr(U \to U') = 1 \qquad (67)$$

- **balance**: The probability of jumping into a configuration equals the probability to jump out of it

$$\sum_U pr(U \to U') pr(U) = \sum_U pr(U' \to U) pr(U') \qquad (68)$$

then the Markov process is guaranteed to bring the ensemble to $pr(U)$. In particular by plugging (67) into (68) we see that

$$\sum_U pr(U \to U') pr(U) = pr(U') \sum_U pr(U' \to U)$$

$$= pr(U'), \qquad (69)$$

i.e. pr is a fixed point. If you use the Metropolis algorithm, the ensemble converges to $pr(U) = Z^{-1} e^{-S[U]}$, i.e. Boltzmann.

Intuitively, you can believe the Metropolis step brings us to Boltzmann: We always move when the configuration is more probable (in Boltzmann sense) and if it's less probable, the acceptance probability is still dictated by the ratio of Boltzmann factors. More rigorously, you can show that (66) satisfies balance (actually an even stronger condition called detailed balance).

In principle one can choose the trial uniformly at random, but owing to Metropolis, the acceptance will be poor, which means it takes longer to get representative samples. As long as you use the Metropolis prescription (66), you have some freedom in how you generate the trial. It's efficient to suggest configurations that have reasonable probabilities to begin with, which is called importance sampling.

A final note: Since $U^{(n)}$ is generated based on $U^{(n-1)}$, $U^{(n)}$ and $U^{(n-1)}$ are in general correlated. This can be dealt with in many ways, but the easiest is to find an $m \in \mathbb{N}$ large enough such that $U^{(n)}$ and $U^{(n+m)}$ are effectively uncorrelated, keeping

only every m^{th} measurement. One way to judge what m should be is to estimate the integrated autocorrelation time, but I don't have time to get into that.

SUMMARY

- Euclidean spacetime useful for getting particle masses. Also improves path integral convergence.
- Lattice regulates integral, rendering it well defined.
- Strong connections with statistical physics.
- Lattice lets us use computers to compute path integrals efficiently through Markov chains.

To do a lattice calculation at finite T, (very roughly)

1. Get your software
2. Pick T, N_τ (fixes a since $T = \frac{1}{a N_\tau}$)
3. Generate Markov chain of configurations
4. Estimate $\overline{X(a)} \approx \langle X(a) \rangle$ by measuring X on the configurations
5. Repeat 3 & 4 for a larger N_τ
6. Fit $\overline{X(a)}$ and extrapolate $a \to 0$

There was a lot I couldn't cover. See [Gattringer-Lang] and [Montvay-Münster] for a more complete introduction. I also keep a [Github] where I keep detailed notes about topics in lattice QCD.

THANKS FOR READING

[Montvay-Münster]: "Quantum fields on a lattice" (1994)

[Osterwalder, Schrader, Wightman, Streater]:

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[Wilson]: "Confinement of quarks", Phys. Rev. D. 10, 8 (1974)

[Gattringer-Lang]: "Quantum Chromodynamics on the lattice: an introductory presentation" (2010)

[Github]: github.com/clarkedavida/researchNotes