Lattice QCD with Applications to B Physics

Lecture 1

Motivation

QCD

Lattice Field Theory

Numerical Methods in QM

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Overall Plan

February 22: Motivation and numerical methods

February 27: Lattice gauge theory, *e.g.*, QCD

March 1: CKM Matrix elements

Motivations for Lattice Field Theory

Lattice field theory is a rigorous way to define quantum field theory, perhaps the only way. Those who aim to "construct" quantum field theory start with a lattice. Their problem then starts out mathematically well-defined (see below), and they try (with the renormalization group) to maintain control over the continuum limit.

Field theory on a lattice is formally the same as classical statistical mechanics. Thus, it provides a new toolkit to carry out practical calculations. *E.g.*, at long distances perturbation theory (the high-energy theorist's favorite tool) breaks down for quantum chromodynamics (QCD).

Indeed there are several problems in high-energy physics, nuclear physics, and astrophysics where non-perturbative information from QCD is needed. Lattice QCD calculations give matrix elements in B decays, information on proton structure, and the equation of state as the universe cools from a quark-gluon soup to hadrons.

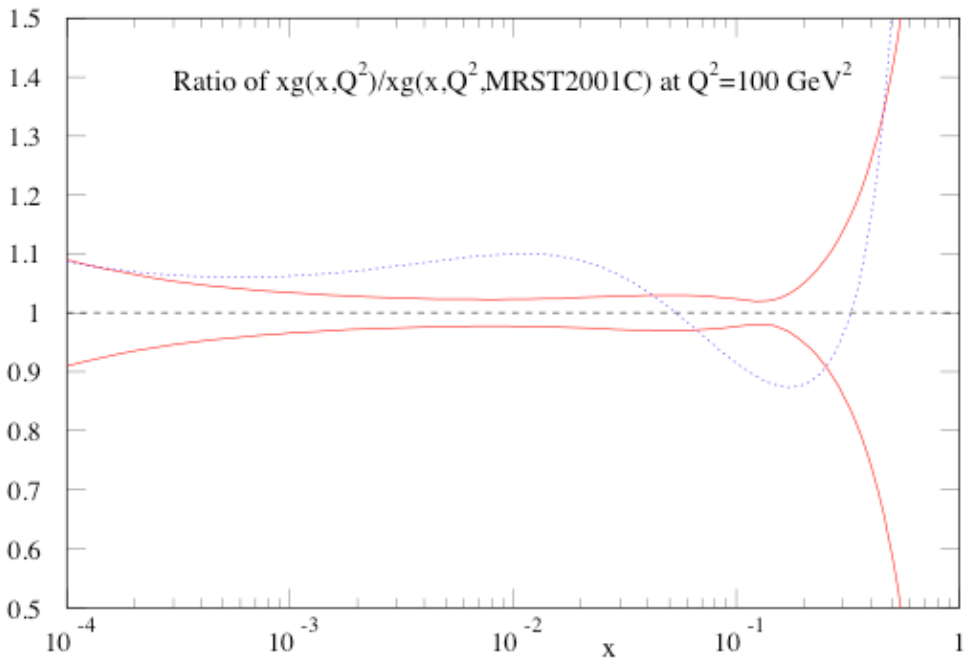
Flavor and Hadron-Collider Physics

There are two places in particle physics where lattice calculations are (or will be) especially important: quark flavor physics and hadron-hadron collisions. Both will help us infer whether there are new phenomena at play in experiments.

At the right we have a plot of the theoretical uncertainty in the gluon density of the proton vs. x.

High mass particles need large x partons and must be seen above background.

Moments of such functions can be calculated in lattice QCD, thereby constraining the large x behavior.

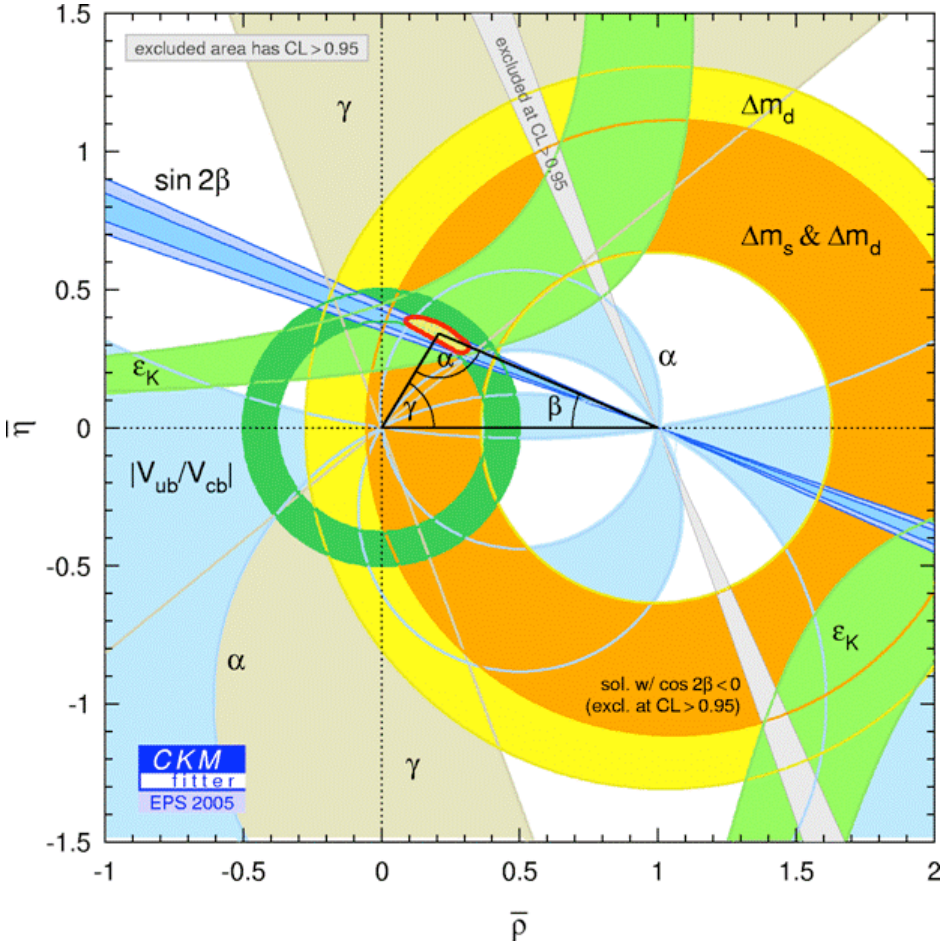


Flavor Physics

CKM unitarity triangle, early 2006

Limit on B_s mixing frequency Δm_s

Watch the orange band!

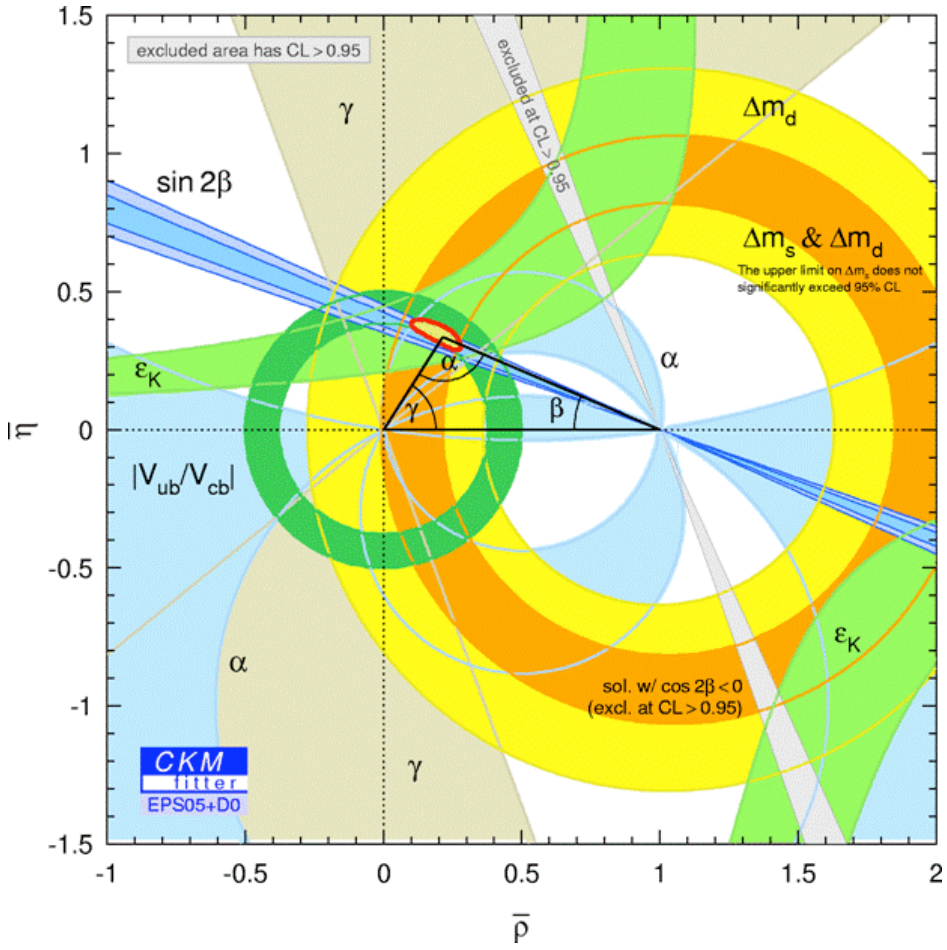


Flavor Physics

CKM unitarity triangle, March 2006

Two-sided bound on Δm_s

Experimental uncertainty 10%



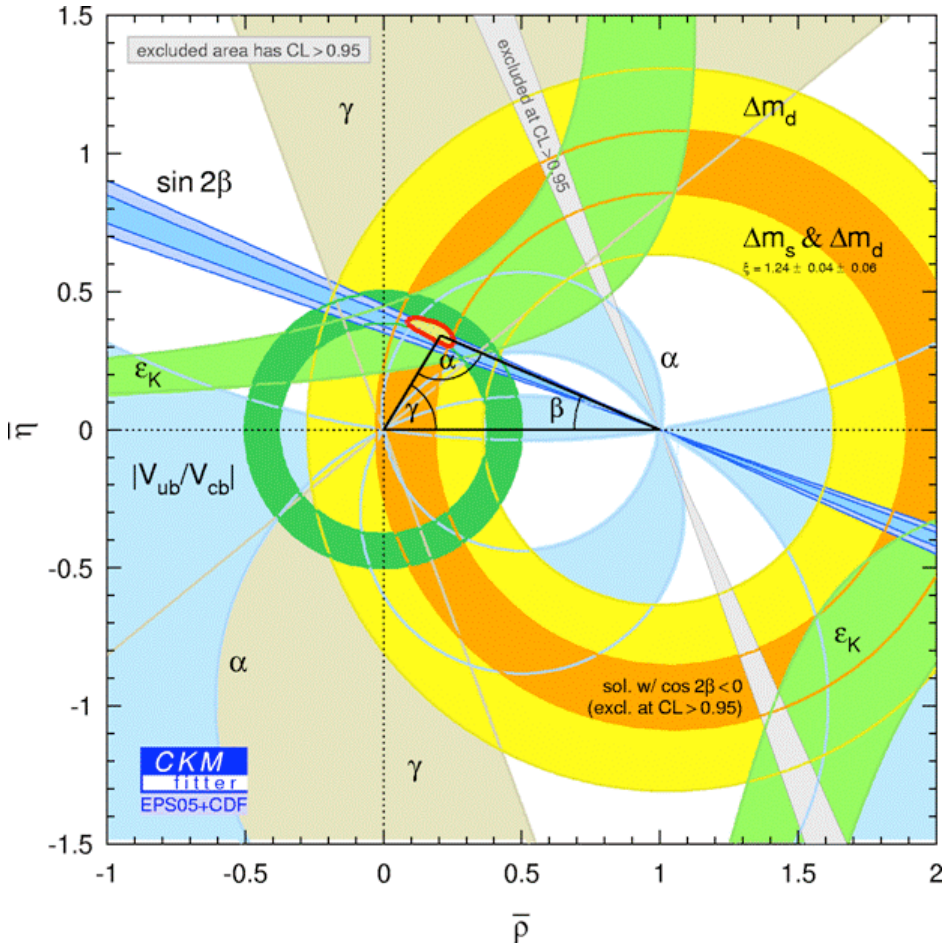
Flavor Physics

CKM unitarity triangle, April 2006

Measurement of Δm_s

Experimental uncertainty 1%

Why is the ring still so BIG? QCD



Quantum Chromodynamics

Quantum chromodynamics (QCD) is the modern theory of the strong interactions: the force that binds quarks and gluons into hadrons, and, in the end, nuclear physics.

"QCD is easily described." The Lagrangian has $1+n_f$ free parameters:

$$\mathcal{L}_{\mathrm{QCD}} = \frac{1}{2g^2}\operatorname{tr} F_{\mu\nu}F^{\mu\nu} - \sum_f \bar{q}_f(\not{D}+m_f)q_f,$$

with gauge coupling (or strong coupling) g^2 and quark masses m_f.

SU(3): $D_\mu = \partial_\mu + A^a_\mu t^a, \qquad F_{\mu\nu} = [D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu]$

t^a_{ij}: 3×3 traceless anti-Hermitian matrices, $t^{a\dagger} = -t^a$.

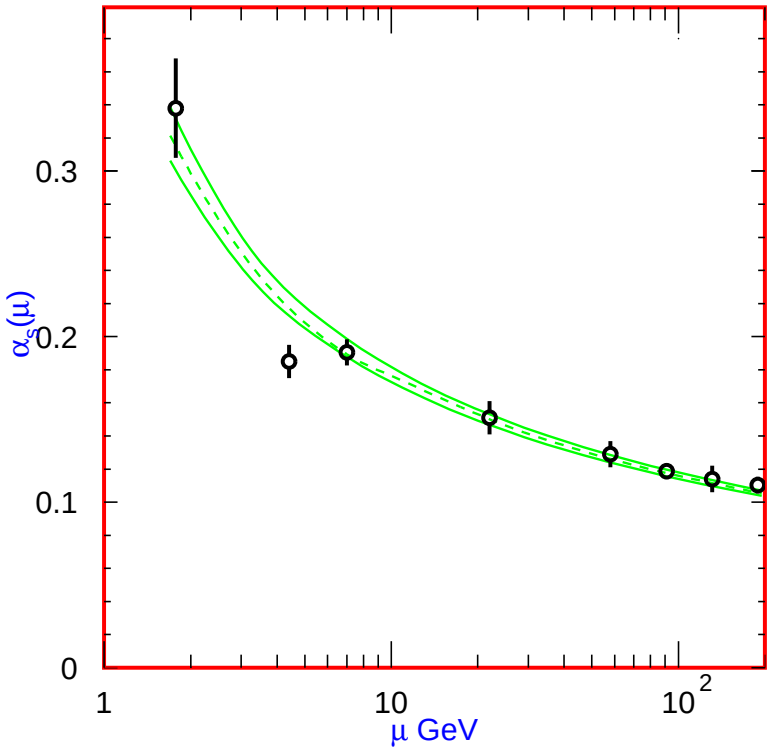
q^j_f: transform under 3 representation of SU(3).

Set the parameters with $1+n_f$ experimental measurements; predict everything else.

Different conventions for factors of i. Perturbative QCD: $A_\mu \to gA_\mu$.

Asymptotic Freedom

Renormalized coupling $g^2(Q)$ decreases as the momentum scale Q increases:



PDG 2006

$\Rightarrow$ perturbative QCD at short-distances/high energies.

Renormalized QCD remains logically sound at the highest energies.

Long Distances—Color Singlets

At long distances QCD does not break down.

Perturbation theory does. $\Longrightarrow$

Quarks and gluons are confined into color singlets:

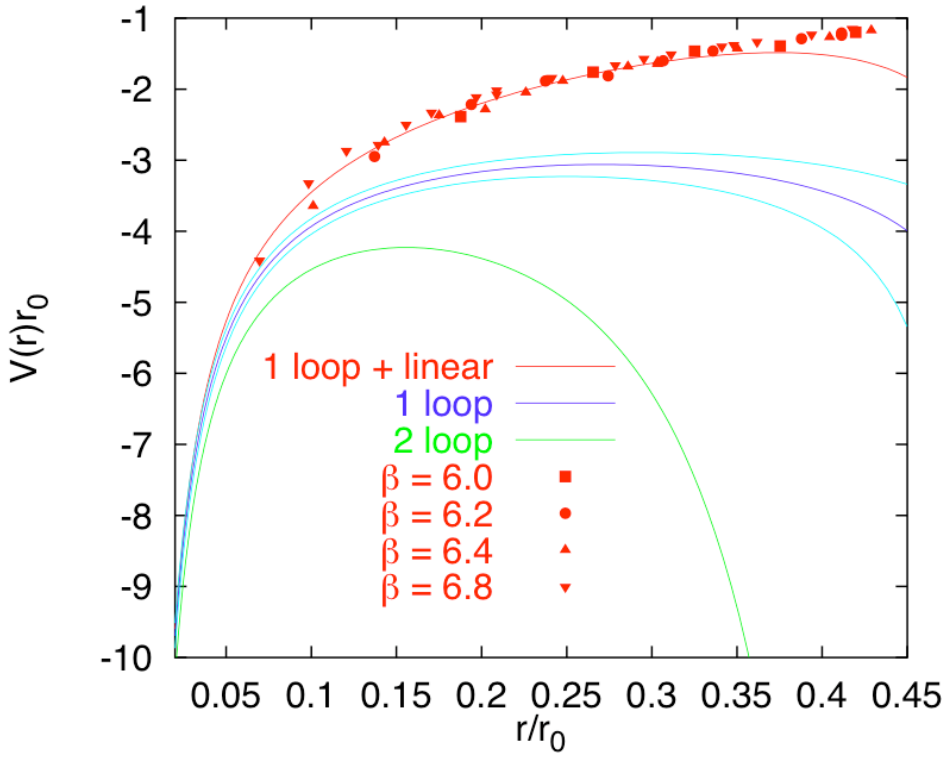
mesons $\bar{q}^i_f q^i_g$,

baryons $\varepsilon_{ijk} q^i_f q^j_g q^k_h$,

glueballs FF and FFF,

hybrids $\bar{q}qF$, deuterons, etc.

pentaquarks $uudd\bar{s}u$?



Non-perturbative methods needed to understand long-distance QCD.

Non-Perturbative Tools

There are some general purpose tools: unitarity, analyticity, symmetry . . . .

Renormalization group tools: separate long- and short-distance dynamics, solve each part separately. Or solve one part and take the other from experiment.

Three decades ago, Kenneth Wilson returned from a scientific excursion into condensed matter physics. He had taken ideas of renormalization field theory as gifts, and returned with their tool-kit, including strong coupling expansions.

These tools exploited the formal similarity between the functional integral of quantum field theory and the partition function of statistical mechanics.

Fields on a lattice are obvious in crystals. The trick was to do the same for gauge theories such as QCD.

Path Integrals, Functional Integrals

Richard Feynman devised a path integral formulation of quantum mechanics:

$$\langle x_T | Q(x,T) | x_0 \rangle = \int \mathcal{D}x \, Q(x) e^{iS}$$

where S is the classical action for a path from x_t to x_0. We'll define $\mathcal{D}x$ later today.

The analogous expression for gauge field theory is the functional integral

$$\langle 0 | Q(q,\bar{q},A) | 0 \rangle = \frac{1}{Z} \int \prod_{\mu,a,x} dA^a_\mu(x) \prod_{\alpha,f,i,x} dq^i_{f,\alpha}(x) \prod_{\alpha,f,i,x} d\bar{q}^i_{f,\alpha}(x) \, Q(x) e^{iS}$$

where gauge bosons A carry a Lorentz index μ & a color index a, and (anti-)quarks q ($\bar{q}$) carry a Dirac index α, flavor index f, & color index i.

In field theory, the spacetime coordinate x is a label. But what does a product over x mean? x is a 4-vector of real numbers!!!

Make x discrete, and see if a continuum limit can be defined.

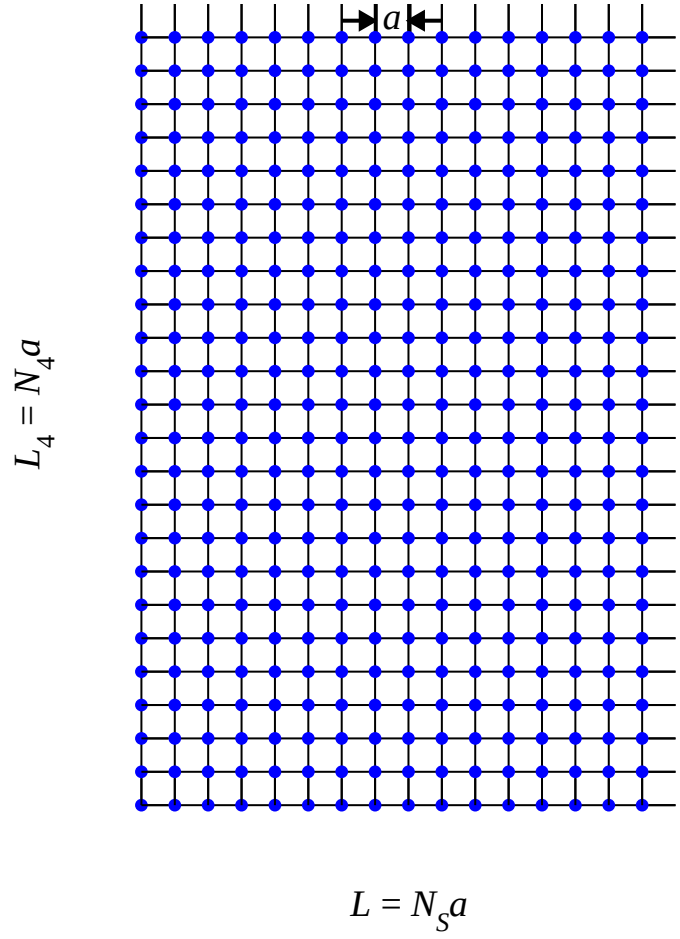
Lattice Field Theory

Lattice field theory (*e.g.*, for a magnet) associates the degrees of freedom with the sites, links, etc., of a lattice.

For particle physics it is a (Euclidean) space-time lattice.

Wilson's idea was that the lattice fields represent aggregate degrees of freedom of the neighborhood of the sites (etc.).

Mathematical advantages: lattice provides ultraviolet cutoff from the outset; functional integral is well-defined.



What does the lattice do to the field theory?

In the spatial directions, let $L = Na$ be the physical size of the box. Then

continuum $a \to 0$		continuum $a \to 0$
infinite volume $L \to \infty$	$\Longleftarrow$	finite volume (L finite)
$N_{\mathrm{d.o.f.}}$ is uncountably infinite		$N_{\mathrm{d.o.f.}}$ is infinite, but countable
		$\Uparrow$
lattice (a non-zero)		lattice (a non-zero)
infinite volume $L \to \infty$		finite volume (L finite)
$N_{\mathrm{d.o.f.}}$ is infinite, but countable		$N_{\mathrm{d.o.f.}}$ is finite

No divergences if $N_{\mathrm{d.o.f.}}$ is finite, *i.e.*, if a non-zero and L finite.

Ultraviolet and infrared divergences do not appear in *physical* quantities.

IR: must happen if theory is sensible.

UV: Renormalization: $g_0^2 = g_0^2(a)$, $m_0 = m_0(a)$, such that physics is a independent.

Numerical Lattice Field Theory

With the lattice formulation there are many things you could do: strong coupling expansions, abstract renormalization arguments, etc.

But usualy when people say "lattice QCD," they mean a numerical approach, in which the path integral is evaluated on a computer.

It practice that is not enough. QCD is a multi-scale problem: the scale of non-perturbative physics, Λ_{QCD}, is 250–2500 MeV; the u, d, and s quarks have mass smaller than this, and the c (?), b, and t quarks have mass larger than this.

In practice, the computer generates a lot of "data," and we exploit other tools to help us understand the effects of $a > 0$, $L < \infty$, $m_q > m_d$, $m_b \sim a^{-1}$.

To "analyze the data" we use effective field theories, conceptually similar to the effective 4-quark Hamiltonian, HQET,.... N.B., HQET was invented to handle $a^{-1} \sim m_b$.

Numerical Methods

The numerical work mystifies many people, but it is easy to learn the basic concepts using quantum mechanics.

For the rest of this lecture, we will see how this is done. By the end, you should be able to write a program to compute energy levels in quantum mechanics.

Consider the propagator in quantum mechanics, with Hamiltonian $H = p^2/2m + V(x)$:

$$\langle x(T)|x(0)\rangle = \langle x_T|e^{-i\hat{H}T}|x_0\rangle = \sum_n \langle x_T|n\rangle e^{-iE_nT}\langle n|x_0\rangle,$$

To derive the path integral, split the time T into many little intervals $\delta = T/N$. Then

$$\langle x_T|e^{-i\hat{H}T}|x_0\rangle = \int \prod_{i=1}^{N-1} dx_i \prod_{i=0}^{N-1} \langle x_{i+1}|e^{-i\hat{H}\delta}|x_i\rangle,$$

repeatedly inserting $1 = \int dx_i |x_i\rangle\langle x_i|$.

We would like to derive an expression for

$$\langle x_{i+1}|e^{-i\hat{H}\delta}|x_i\rangle \approx \langle x_{i+1}|e^{-i\hat{V}(x)\delta/2}e^{-i\hat{p}^2\delta/2m}e^{-i\hat{V}(x)\delta/2}|x_i\rangle = e^{-iV(x_{i+1})\delta/2}\langle x_{i+1}|e^{-i\hat{p}^2\delta/2m}|x_i\rangle e^{-iV(x_i)\delta/2}.$$

With analysis, this is possible through analytical continuation

$$\langle x_{i+1}|e^{-\hat{p}^2 a/2m}|x_i\rangle = \sqrt{\frac{m}{2\pi a}}e^{-m(x_{i+1}-x_i)^2/2a}.$$

with $a = \varepsilon + i\delta$, $\varepsilon \to 0^+$.

For numerical work, the analytical continuation is not feasible. We simply make do with propagation through imaginary time.

This "Euclidean field theory" is common in mathematical physics, for the same reason. It is better to work with well-defined expressions, and continue as a last resort.

Minkowski has metric $\mathrm{diag}(-1,1,1,1)$; Euclidean has metric $\mathrm{diag}(+1,1,1,1)$.

Then one has (for imaginary time, $T \to -iT$)

$$\langle x_T | e^{-\hat{H}T} | x_0 \rangle = \lim_{N\to\infty} \int \mathcal{D}x_N \, \exp\left(a \sum_{i=0}^{N-1} L_i \right), \qquad \mathcal{D}x_N = \prod_{i=1}^{N-1} dx_i \sqrt{\frac{m}{2\pi a}},$$

where the limit is taken with T fixed, $a = T/N$.

The (discrete time) Lagrangian is

$$L_i = -\tfrac{1}{2} m \left(\frac{x_{i+1} - x_i}{a} \right)^2 - \tfrac{1}{2} V(x_{i+1}) - \tfrac{1}{2} V(x_i),$$

which one recognizes as a discrete approximation to the kinetic energy and the average of the potential energy over two times.

In numerical work, one uses a sequence of Ns and extrapolates.

As we shall discuss in subsequent lectures, one has theoretical control over the extrapolation, even for field theory where issues of renormalization must be addressed.

More on Path Integrals

Let us look some more at the (imaginary time, $T \to -iT$) propagator

$$\langle x_T | e^{-\hat{H}T} | x_0 \rangle = \lim_{N\to\infty} \int \mathcal{D}x_N \, e^{-S(\{x_i\}_N)}, \qquad \mathcal{D}x_N = \prod_{i=1}^{N-1} dx_i \sqrt{\frac{m}{2\pi a}},$$

$$S = a \sum_{i=0}^{N-1} \left[\tfrac{1}{2} m \left(\frac{x_{i+1} - x_i}{a} \right)^2 + V(x_i) \right].$$

The left-hand side obeys a composition law when tacking two paths together:

$$\langle x_{T'+T} | e^{-\hat{H}(T'+T)} | x_0 \rangle = \int dx_T \langle x_{T'+T} | e^{-\hat{H}T'} | x_T \rangle \langle x_T | e^{-\hat{H}T} | x_0 \rangle$$

So does the right-hand side:

$$\int \mathcal{D}x_{N'+N} \, e^{-S(\{x_i\}_{N'+N})} = \int dx_N \int \mathcal{D}x_{N'} \, e^{-S(\{x_i\}_{N'})} \int \mathcal{D}x_N \, e^{-S(\{x_i\}_N)},$$

even without taking the limit of infinite N, N'.

Furthermore, an operator $\hat{Q} = Q(\hat{x}) = \int dx |x\rangle Q(x) \langle x|$, acting at time t, $0 < t < T$,

$$\langle x_T | e^{-\hat{H}(T-t)} Q(\hat{x}) e^{-\hat{H}t} | x_0 \rangle = \int \mathcal{D}x \, Q(x_t) \, e^{-S(\{x_i\})}$$

and similarly for several operators inserted at various different times.

In field theories, we do not have just 1 degree of freedom. We have zillions.
It is impractical to study the dependence of the wave function on all of them.

So let us set $x_T = x_0$ and integrate over x_0, yielding the "partition function"

$$Z = \int \mathcal{D}x \, e^{-S} = \int dx \, \langle x | e^{-\hat{H}T} | x \rangle, \qquad \mathcal{D}x = \prod_{i=0}^{N-1} dx_i \sqrt{\frac{m}{2\pi a}},$$

now with N integrations.

The parallel with statistical mechanics can be pursued further by introducing

$$\langle Q(x_t)\rangle = \frac{1}{Z}\int \mathcal{D}x\, Q(x_t)\, e^{-S(\{x_i\})}$$
$$\langle Q_1(x_{t_1})Q_2(x_{t_2})\rangle = \frac{1}{Z}\int \mathcal{D}x\, Q_1(x_{t_1})Q_2(x_{t_2})\, e^{-S(\{x_i\})}$$
$$\langle Q_1(x_{t_1})Q_2(x_{t_2})\rangle_c = \langle Q_1(x_{t_1})Q_2(x_{t_2})\rangle - \langle Q_1(x_{t_1})\rangle\,\langle Q_2(x_{t_2})\rangle$$

The clash of the notation $\langle\bullet\rangle$ with Dirac notation is unfortunate, but conventional.

For large T Proofs as exercises: use $1 = \sum_n |n\rangle\langle n|$ ruthlessly.

$$Z \overset{\text{large } T}{\longrightarrow} e^{-E_0 T}$$
$$\langle Q(x_t)\rangle \overset{\text{large } T}{\longrightarrow} \langle 0|Q(\hat{x})|0\rangle$$

gives you the vacuum energy E_0 and vacuum expectation value (vev).

Not miraculous. The same manipulations enter scattering theory, with propagators out to $T(1-i\varepsilon)$, $T\to\infty$.

For large T (and $t_1 - t_2 = ja$) Proof as exercise.

$$\langle Q_1(x_{t_1}) Q_2(x_{t_2}) \rangle_c \overset{\text{large } T}{\longrightarrow} \sum_{n \neq 0} \langle 0|Q_1(\hat{x})|n\rangle \langle n|Q_2(\hat{x})|0\rangle e^{-(E_n - E_0)ja} + \sum_{n \neq 0} \langle 0|Q_2(\hat{x})|n\rangle \langle n|Q_1(\hat{x})|0\rangle e^{-(E_n - E_0)(T-ja)},$$

gives you the excited-state energies E_0 and vacuum $\longrightarrow$ 1-particle matrix elements.

For large ja and/or $T - ja$ Proof as exercise.

$$\langle Q_1(x_{t_1}) Q_2(x_{t_2}) \rangle_c \overset{\text{large } T}{\longrightarrow} \langle 0|Q_1(\hat{x})|1\rangle \langle 1|Q_2(\hat{x})|0\rangle e^{-(E_1 - E_0)ja} + \langle 0|Q_2(\hat{x})|1\rangle \langle 1|Q_1(\hat{x})|0\rangle e^{-(E_1 - E_0)(T-ja)},$$

thus isolating properties of the first excited-state $|1\rangle$.

If (by symmetry or clever design) $Q_i(\hat{x})|1\rangle = 0$, then $|n\rangle$, $n \geq 2$, can be isolated.

So, if you know how to compute the path integrals numerically, a fit to the T dependence of Z give E_0, and the j dependence of 2-point correlators gives $E_n - E_0$.

Hadron Masses

In field theory (*e.g.*, QCD), $E_n - E_0$ is what we identify with a particle's energy. If the 3-momentum is zero, that yields the rest mass.

It's worth writing it in particle-physics notation.

The operator $\Pi^+ = \bar{d}\gamma_5 u$ annihilates π^+ (and all its radial excitations); similarly, the operator $\Pi^- = \bar{u}\gamma_5 d$ annihilates π^-. For large times T and x_4 [$x = (\boldsymbol{x}, x_4)$]

$$\int d^3x \langle \Pi^+(x)\Pi^-(0)\rangle_c \to \langle 0|\hat{\Pi}^+|\pi_0^+\rangle\langle\pi_0^+|\hat{\Pi}^-|0\rangle \exp\left[-m_{\pi^+}x_4\right] + \langle 0|\hat{\Pi}^-|\pi_0^-\rangle\langle\pi_0^-|\hat{\Pi}^+|0\rangle \exp\left[-m_{\pi^-}(T-x_4)\right],$$

is how we compute the pion mass, and similarly for any other hadron mass.

Replace Π^- with $A_4^- = \bar{u}\gamma_4\gamma_5 d$, and then $\langle 0|\hat{A}_4^-|\pi^-\rangle =: f_\pi m_\pi$ appears.

Monte Carlo Integration for QM

Choose C random configurations of $\{x_i | i = 0, \ldots, N-1\}$, denoting individual configurations as $\{x_i\}^{(c)}$, $c = 0, \ldots, C-1$. Then

$$Z = \int \mathcal{D}x\, e^{-S} = \lim_{C\to\infty} \left(\frac{m}{2\pi a}\right)^{N/2} \sum_{c=0}^{C-1} \exp\left[-S\left(\{x_i\}^{(c)}\right)\right],$$

$$\int \mathcal{D}x\, f(\{x_i\}) e^{-S} = \lim_{C\to\infty} \left(\frac{m}{2\pi a}\right)^{N/2} \sum_{c=0}^{C-1} f(\{x_i\}^{(c)}) \exp\left[-S\left(\{x_i\}^{(c)}\right)\right].$$

An estimate of the left-hand side is achieved for C finite.

From now on we use finite C, and omit the normalization factor $(m/2\pi a)^{N/2}$, which drops out of correlation functions.

This method is hopeless for large N. S is extensive, many configurations have $S \sim N$; they are a waste of time.

The remedy is called importance sampling.

Don't choose all configurations with equal weight, choose them with weight e^{-S}.

This is possible because S is real and bounded below. Hence imaginary time!

Then

$$\frac{1}{Z}\int \mathcal{D}x\, f(\{x_i\})e^{-S} \approx \frac{1}{C}\sum_{c=0}^{C-1} f(\{x_i\}^{(c)}).$$

converging to be exact as $C \to \infty$. $C =$ # of configurations in ensemble.

Quantum theory has been reduced to the design of random number generators, for many variables, with distribution e^{-S}.

Necessary *vs.* Sufficient for Monte Carlo

The aim of any algorithm is to generate a transition rule $T(\{x\} \to \{y\})$ so that the probability density is (eventually) $P(\{x\}) \propto e^{-S(\{x\})}$.

Start with an initial distribution $P(\{x\},0)$. The transition rule $T(\{x\} \to \{y\})$ changes the distribution from $P(\{x\},c)$ to $T(\{x\} \to \{y\})$ independent of c.

$$P(\{x\},c+1) = P(\{x\},c) - \int \mathcal{D}y P(\{x\},c) T(\{x\} \to \{y\}) + \int \mathcal{D}y P(\{y\},c) T(\{y\} \to \{x\})$$

The steady state (if it exists) has $P(\{x\},c)$ independent of c.

$$\int \mathcal{D}y P(\{x\}) T(\{x\} \to \{y\}) = \int \mathcal{D}y P(\{y\}) T(\{y\} \to \{x\}) \qquad \text{necessary}$$

$$P(\{x\}) T(\{x\} \to \{y\}) = P(\{y\}) T(\{y\} \to \{x\}) \qquad \text{sufficient}$$

The last (unintegrated) condition is called detailed balance. It is easier to solve.

A Simple Method

Perhaps the simplest method to generate the desired distribution is the Metropolis method.

Requires only $e^{-S} \geq 0$.

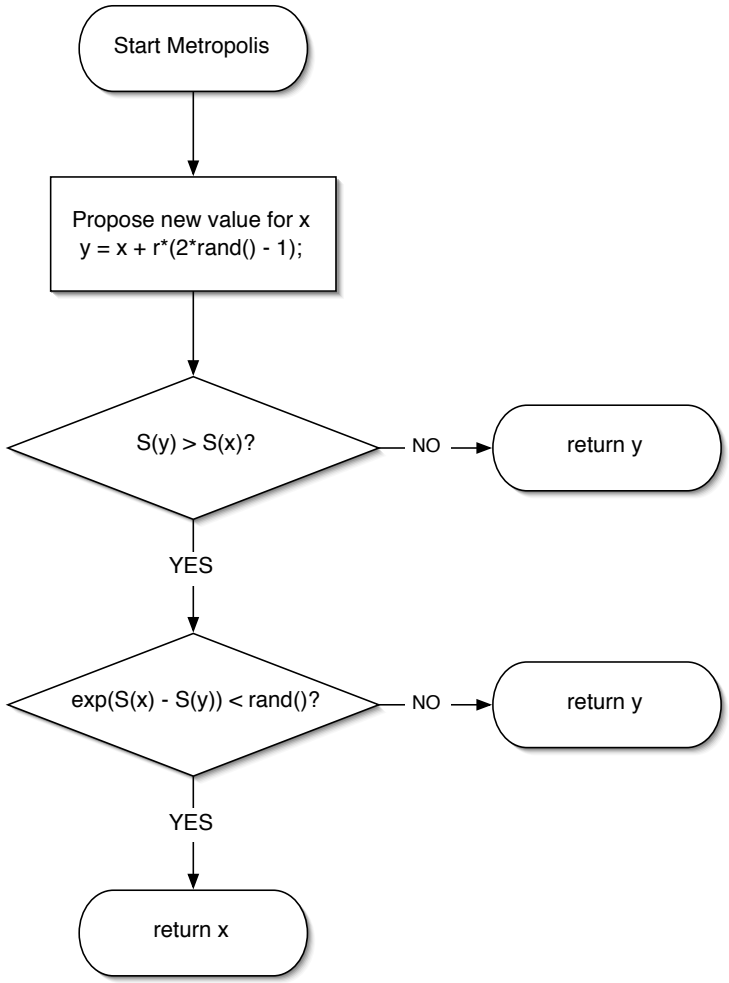
Visit each x_i in turn, and follow the flow chart.

$\texttt{rand}() \in [0, 1)$

Choose r to accept ~ 40–50% of updates.

For more complicated (sets of) degrees of freedom only the proposed update must change.

May also update x_i several times, before proceeding to $i + 1$.



Metropolis and Detailed Balance

We now check the Metropolis satisfies detailed balance, re-written

$$\frac{T(\{x\}\to\{y\})}{T(\{y\}\to\{x\})} \stackrel{!}{=} \frac{P(\{y\})}{P(\{x\})} = e^{-[S(\{y\})-S(\{x\})]} = e^{-\Delta S}$$

Three cases:

$S(\{y\}) = S(\{x\})$

always accept

both Ts $= 1$

$e^{-\Delta S} = 1$

$S(\{y\}) > S(\{x\})$

$0 < e^{-\Delta S} < 1$

"accept if $R \leq e^{-\Delta S}$"

accepts fraction $e^{-\Delta S}$

$T(\{x\}\to\{y\}) = e^{-\Delta S}$

$T(\{y\}\to\{x\}) = 1$

$S(\{y\}) < S(\{x\})$

$0 < e^{\Delta S} < 1$

$T(\{x\}\to\{y\}) = 1$

$T(\{y\}\to\{x\}) = e^{\Delta S}$

In all three cases, Metropolis satisfies detailed balance.

Statistical Uncertainties

With Monte Carlo integration, there are statistical errors that fall as $C^{-1/2}$.

Let the average in the finite ensemble be written

$$\overline{f(\{x_i\})} := \frac{1}{C} \sum_{c=0}^{C-1} f(\{x_i\}^{(c)}).$$

so $\overline{f(\{x_i\})}$ estimates $\langle f(\{x_i\}) \rangle$.

The central limit theorem says that $\overline{f(\{x_i\})}$ fluctuates around $\langle f(\{x_i\}) \rangle$ with variance

$$\sigma^2(f) = \frac{1}{C-1} \left[\overline{f^2} - \overline{f}^2 \right].$$

(Think of repeating a Monte Carlo of C configurations many times, and drawing the histogram of $\overline{f}$.)

Indeed, statistical fluctuations are correlated

$$\sigma^2(f_i, f_j) = \frac{1}{C-1}\left[\overline{f_i f_j} - \overline{f_i}\,\overline{f_j}\right].$$

For example, $f_t = Q(x_t)Q(x_0)$ and f_{t+u}.

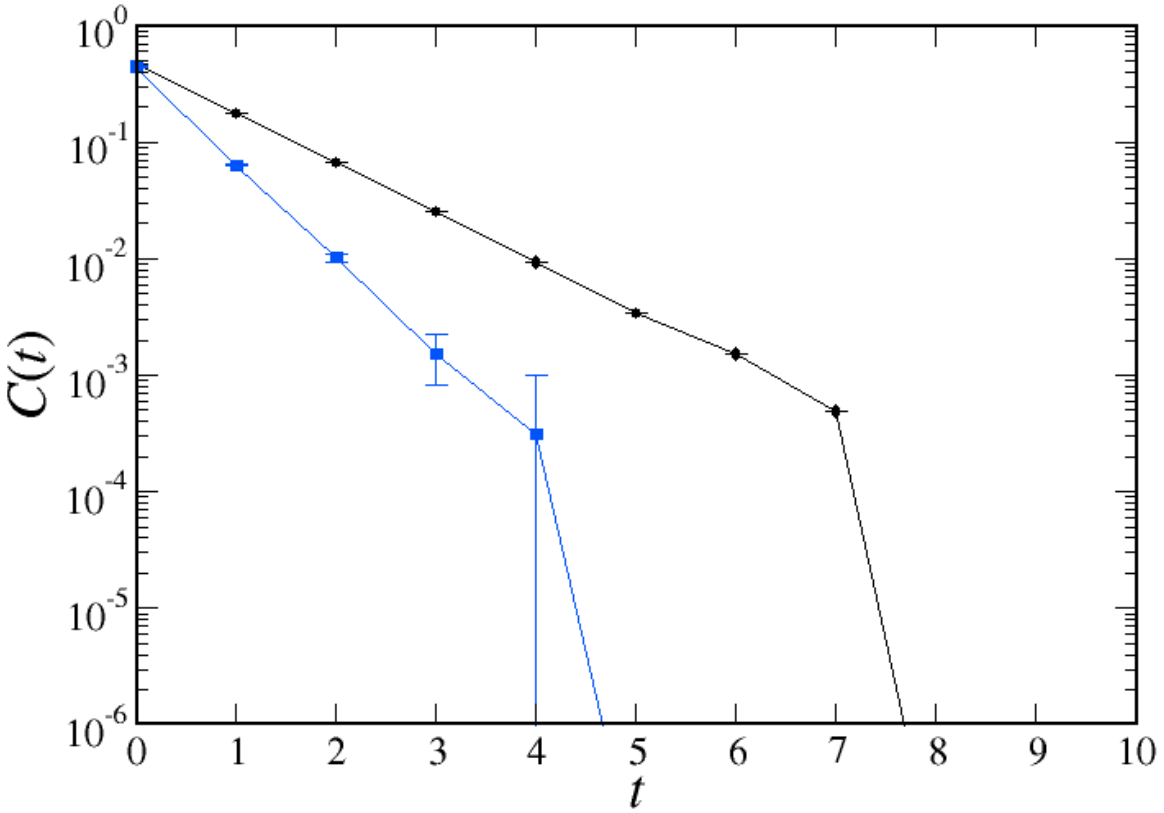
In field theory, we can gain some intuition about the fluctations, because

$$\overline{f_i f_j} - \overline{f_i}\,\overline{f_j} \approx \langle f_i f_j \rangle - \langle f_i \rangle \langle f_j \rangle.$$

In practice, similar quantities (like successive times of a correlation function) fluctuate together.

Statistical errors often cancel somewhat when forming ratios and differences.

Exercise: What is "easier" (statistically)—the mass (gap) (or energy) $E_1 - E_0$, or the overlaps $\langle 0|Q_1|1\rangle\langle 1|Q_2|0\rangle$?


10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
$C(t)$
0
1
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7
8
9
10
t

Statistical Errors for Masses, etc.

Usually we are interested in energies or quantum-mechanical matrix elements.

For example, the energy difference can be extracted from

$$m_{\mathrm{eff}}(t) = -\ln \frac{\langle Q_1(x_{t+1}) Q_2(x_0) \rangle_c}{\langle Q_1(x_t) Q_2(x_0) \rangle_c}$$

Independent of $t \Leftrightarrow$ one state dominates.

Logarithm does not commute with $\langle \bullet \rangle$.

To estimate the statistical error on m_{eff}, we really need many ensembles.

In the bootstrap method, new pseudo-ensembles are generated from the original, by drawing configurations at random, allowing repeats.

Bootstrap can be wrapped around an arbitrarily complicated analysis.

Summary

From this simple example, several general features emerge.

Energy levels (*aka* masses) and simple matrix elements are straightforward: no complication from imaginary time whatsoever.

Excited states are more complicated than the lowest-lying state (of given quantum numbers).

The complications of numerical methods for field theory stem from the zillions of variables (and also from fermions).

Statistical errors and discretization errors are (in principle) always reducible by brute force: increase C and N; CPU time $\propto CN$.