Lecture 2: Lattice Quantum Chromodynamics

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Outline

- ▶ Introduction to Lattice QCD
- ▶ Constructing a LQCD Computation
- ▶ Systematics in LQCD Calculations
- ► Future Prospects
- Conclusions

Note: all references in online slides are hyperlinked

Introduction

The Strong Force, Quantum Chromodynamics (QCD)



Quarks and gluons bind into hadronic matter

Form into $q-\bar{q}$ pairs (mesons), or qqq triplets (baryons)

Mass gluon	0
Mass up quark	$2 { m MeV}$
Mass down quark	5 MeV
Mass pion	$140 { m MeV}$
Mass nucleon	$940 \mathrm{MeV}$

 $\begin{array}{ll} {\rm Mass \ of \ constituents \ll mass \ of \ hadrons} \\ \implies {\rm a \ lot \ of \ energy \ stored \ in \ gluon \ field!} \end{array}$

-

String Breaking

Not possible to isolate free quarks

V(r) grows proportional to quark separation r \implies requires energy to pull quarks apart \implies quarks connected by flux tube "string"

Large r: string breaks, forms 2-meson state



QCD and Confinement

$$\begin{split} &\alpha_s \approx \frac{g^2}{4\pi} \text{ runs with center of mass energy } Q \\ &Q \rightarrow \infty \implies \alpha_s \rightarrow 0 \text{ (asymptotic freedom)} \end{split}$$

Perturbative QCD with expansion parameter $\alpha_s \ll 1$ for a generic observable f:

$$f_{\rm QCD} = f_0 + f_1 \alpha_s + f_2 \alpha_s^2 + \dots$$

Use Feynman diagram technology up to $N\operatorname{-loop}$ order



QCD and Confinement

Coupling gets strong $(\alpha_s \sim 1)$ at small Q

 \implies quarks confined to hadrons

 \implies perturbative expansion strategy fails

Need different technique to tackle nonperturbative regime: Lattice QCD



What is Lattice Quantum Chromodynamics (LQCD)?

 \mbox{LQCD} is the only known mathematically rigorous method

to compute properties of hadrons in nonperturbative QCD

Constructed from $\mathbf{quark}\ \mathbf{and}\ \mathbf{gluon}\ \mathrm{degrees}\ \mathrm{of}\ \mathrm{freedom}$

After removing systematic biases, predictions of QCD (not an approximation!)

- $\checkmark~$ Complementary to experiment
- $\checkmark~$ Controlled nuclear effects
- $\checkmark~$ Realistic, robust uncertainty estimates
- $\checkmark~$ Systematically improvable
- $\checkmark~$ Computers are (relatively) in expensive



Successes of Lattice QCD



(Very) few inputs, (very) many outputs

▶ Heavily constrained by SM

▶ Widely used in flavor physics (CKM matrix elements)

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Constructing a LQCD Computation

The (Minkowski) Path Integral (1/2)

The **bold nomenclature** will appear again later...

Starting with the time-dependent Schrödinger equation: $\frac{\partial}{\partial t} \left| \psi \right\rangle = -\frac{i\hat{H}}{\hbar} \left| \psi \right\rangle$, $(\hbar = 1)$

Solve the differential equation to relate time 0 to time t

$$\begin{aligned} \left|\psi(t)\right\rangle &= \exp\left[-i\hat{H}t\right] \left|\psi(0)\right\rangle \\ \implies \left\langle x \left|\psi(t)\right\rangle &= \int dx' \underbrace{\left\langle x \left|\exp\left[-i\hat{H}t\right] \left|x'\right\rangle\right\rangle}_{D^{-1}(x,x';t)} \left\langle x' \left|\psi(0)\right\rangle\right. \end{aligned}$$

with the **propagator** defined by $D^{-1}(x, x'; t) = \langle x | \exp[-i\hat{H}t] | x' \rangle$.

The (Minkowski) Path Integral (2/2)

The **bold nomenclature** will appear again later...

Use an operator $\hat{\chi}$ to create \hat{H} eigenstates $|\psi\rangle$ out of the vacuum $|0\rangle$:

$$\begin{split} \hat{\chi}(t) \left| 0 \right\rangle &= \sum_{\psi} \left| \psi(t) \right\rangle \underbrace{\left\langle \psi(t) \left| \hat{\chi}(t) \right| 0 \right\rangle}_{z_{\psi}} = \sum_{\psi} \int dx \left| x \right\rangle \left\langle x \left| \psi(t) \right\rangle z_{\psi} \\ \text{with overlap } z_{\psi} &= \left\langle \psi(t) \left| \hat{\chi}(t) \right| 0 \right\rangle = \left\langle \psi(0) \left| \hat{\chi}(0) \right| 0 \right\rangle \quad \text{(for example: pion decay constant } f_{\pi} &= \left\langle \pi | \mathcal{P} | 0 \right\rangle) \end{split}$$

Combine the operator and the state propagator into a correlation function

$$\underbrace{\left\langle \hat{\chi}(t)\hat{\chi}(0)\right\rangle}_{\psi} = \mathcal{Z}^{-1}\left\langle 0\left|\hat{\chi}(t)\hat{\chi}(0)\right|0\right\rangle = \mathcal{Z}^{-1}\sum_{\psi}\int dxdx'\left|z_{\psi}\right|^{2}\left\langle \psi\left|x\right\rangle\left\langle x\right|\exp\left[-i\hat{H}t\right]\left|x'\right\rangle\left\langle x'\right|\psi\right\rangle$$

(Vacuum polarization $\mathcal{Z} = \text{Tr}\left[\exp[-i\hat{H}t]\right]$)

The remaining terms are eigenstate wavefunctions, such as a plane wave $\langle x'|\psi\rangle \sim e^{-ip\cdot x'}$

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Path Integral for LQCD

LQCD is a numerical evaluation of the path integral, with additional (well-controlled) modifications:

- ▶ Finite compute power ⇒ finite spacetime lattice introduces ultraviolet, infrared regulators (lattice spacing a, lattice volume L/a)
- ► Preserve gauge symmetry quarks → lattice sites q(x)gluons → lattice links $U_{\mu}(x) = e^{-ig \int_{x}^{x+a\hat{\mu}} A_{\mu}(x')dx'}$



- Sign problem from propagator phase $\sim \exp[-i\hat{H}t]$
 - \implies change to Euclidean time $(t \rightarrow -i \tau)$ and partition function $Z = \exp[-\hat{H} \tau]$
 - \implies cannot compute dynamics/cross sections directly in LQCD

In QCD, the path integral is an expectation value of a combination of operators \mathcal{O}_{ψ} :

$$\left\langle \mathcal{O}_{\psi} \right\rangle = \mathcal{Z}^{-1} \int \overset{\text{gluon}}{\overbrace{\mathcal{D}A}} \overset{\text{quark}}{\overbrace{\mathcal{D}\psi\mathcal{D}\overline{\psi}}} \overset{\text{action}}{\underset{\exp[-S]}{\exp[-S]}} \mathcal{O}_{\psi}$$

In QCD, the path integral is an expectation value of a combination of operators \mathcal{O}_{ψ} :



 $\left\langle \mathcal{O}_{\psi} \right\rangle = \mathcal{Z}^{-1} \int \mathcal{D}A \, \det \left[\mathcal{D} + m \right] \exp[-S] \, \mathcal{O}_{\psi}$

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integrate out by hand

Markov Chain Monte Carlo (MCMC) & importance sampling Generate ensemble of gauge configurations U_n

In QCD, the path integral is an expectation value of a combination of operators \mathcal{O}_{ψ} :



integrate out by hand

Markov Chain Monte Carlo (MCMC) & importance sampling Generate **ensemble of gauge configurations** U_n "valence quark" propagators computed on each gauge configuration contracted to have hadron quantum numbers

$$[\overline{\psi}\psi]_n = (\not\!\!D[U_n] + m)^{-1}$$

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integrate out by hand

Markov Chain Monte Carlo (MCMC) & importance sampling Generate **ensemble of gauge configurations** U_n "valence quark" propagators computed on each gauge configuration contracted to have hadron quantum numbers $[\overline{\psi}\psi]_n = (D [U_n] + m)^{-1}$

Computation is "just" an average of correlation functions computed on sampled gauge snapshots

Computationally expensive:

- generate gauge ensembles/configurations (MCMC)
- valence quark propagators (large sparse matrix inversions)

Once these done, lots of potential data reuse

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LQCD Computation Anatomy

Write correlation functions with complete set of states $1 = \sum_n |n\rangle \langle n|$, including ground state and **excited states**



only valence quarks drawn in diagrams implicit $q\bar{q}$ loops+gluons to all orders

Extract masses from 2-point

Source/sink operators $(\blacksquare, \blacktriangle)$ have different overlaps onto states m, n

LQCD Computation Anatomy

Write correlation functions with complete set of states $1 = \sum_n |n\rangle \langle n|$, including ground state and **excited states**



Extract masses from 2-point, matrix elements from 3-point

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LQCD Computation Anatomy

Write correlation functions with complete set of states $1 = \sum_n |n\rangle \langle n|$, including ground state and **excited states**



Extract masses from 2-point, matrix elements from 3-point Source/sink operators $(\blacksquare, \blacktriangle)$ have different overlaps onto states m, n

Extracting Physics from LQCD

Numerical values are all dimensionless ("lattice units," $a \cdot M_X$), must be matched to physical world

LQCD Inputs: $am_{(u,d),\text{bare}}$ $am_{s,\text{bare}}$ $\beta = 6/g_{\text{bare}}^2$

 $\begin{array}{ll} \text{Scale setting } (\beta \rightarrow a) \text{:} & \text{e.g. } a^{-1} \; [\text{GeV}] = \frac{M_\Omega}{aM_\Omega} \frac{[\text{expt}]}{[\text{LQCD}]} \\ \\ \text{Quark mass tuning:} & \text{e.g. } M_\pi/M_\Omega, \; M_K/M_\Omega \end{array}$



Each gauge ensemble generated with fixed $a, L/a, aM_{\pi}...$

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Each gauge ensemble generated with fixed $a, L/a, aM_{\pi}...$

"Complete" error budget \implies extrapolation in a, L, M_{π} ; guided by EFT, FV χ PT

- $\blacktriangleright \quad a \to 0 \qquad \qquad (\text{continuum limit})$
- $L \to \infty$ (infinite volume limit)
- $M_{\pi} \to M_{\pi}^{\text{phys}}$ (chiral limit)

Additional Peculiarities about LQCD

Some tricks & quirks about LQCD computations:

- ▶ Boundary Conditions ⇒ directly related to finite-volume effects
 - spatial, temporal boundaries can be manipulated
 - periodic or open boundaries are most common, but some exotics (e.g. G-parity)
- ▶ Partial quenching, mixed action
 - action for generating gauge ensemble \neq action for producing quark propagators
 - usually saves computing time, but sometimes spoils physics interpretation

Fermion Doubling –

- No-go theorem: cannot have a *doubler-free* theory of lattice fermions with good chiral symmetry
- **doublers**: 2^D copies of all fermions in a D-dimensional spacetime
- correspond to maximum lattice momenta $p_{\mu} = \pm \frac{\pi}{a}$ in Dirac equation: $\tilde{p}_{\mu} = \frac{1}{a} \sin(p_{\mu}a)$



Types of Lattice Fermions

Introduce $O(a^N)$ effective terms into fermion action to address problem of doublers

Most common listed below, but many more not listed:

- ► Staggered keep doublers ("tastes") and chiral symmetry
 - Diagonalize action: 4-spinors $\rightarrow 4\times$ 1-spinors, drop $\times 3$
 - Spin/taste components spread out over unit hypercubes
- ▶ Wilson break chiral symmetry with additional mass term
 - add term $ar\partial^2$ to action $\implies am_q(p) = am_{q,0} + \frac{2}{a}\sin\frac{p_\mu a}{2}$
- Domain Wall isolate chirality in extra 5th dimension
 - uses Wilson term to remove doublers
 - chiral symmetry breaking $\propto e^{-\alpha L_5}$

"Universality": no matter the action, must reproduce physical world in continuum limit

Each collaboration typically has a favorite action, different actions are nontrivial consistency checks



Uncertainties in LQCD

LQCD Statistics

Statistical uncertainties obtained from sampling on ${\bf gauge \ configurations}$

Can get a rough idea of signal quality based on Lepage scaling:

Signal	$Noise^2$
$\langle \mathcal{O} \rangle$	$\sigma_{\mathcal{O}}^{2} = \left \langle \mathcal{O} ^{2} \right \rangle - \left \left \langle \mathcal{O} \right \rangle \right ^{2} \leq \left \langle \mathcal{O} ^{2} \right \rangle$
$\langle = \rangle$	$\langle \left \begin{array}{c} \hline \\ \hline \\ \hline \\ \hline \\ \end{array} \right ^2 \rangle = \langle \begin{array}{c} \hline \\ \hline \\ \hline \\ \hline \\ \end{array} \rangle$
$\sim e^{-M_n t}$	$\sim e^{-3M_{\pi}t}$

Example baryon correlator $\langle \mathcal{O} \rangle = \langle [q(t)]^3 [q(0)]^3 \rangle \implies S/N \sim \exp\left[-(M_N - \frac{3}{2}M_\pi)t\right]$

Samples are usually **autocorrelated** because of Markov Chain gauge ensemble generation Correlation functions on the same ensemble also **highly correlated**:

- ▶ different Euclidean times with same correlation function
- ▶ correlation functions computed on same configurations with different operators

Approaching the "Physical Point"

At a minimum, a complete error budget includes:

- $\blacktriangleright a \rightarrow 0$ Continuum extrapolation $\blacktriangleright L \to \infty$ Finite volume (FV) extrapolation \blacktriangleright $M_{\pi} \rightarrow M_{\pi, \text{phys}}$ "Chiral" extra(inter)polation
- Every point in extrapolation is a *separate ensemble* \implies very expensive!

Incomplete results will get reported,

updated later with more ensembles

Always compare to extrapolated values or use due caution!



Physical result

Finite Volume Effects

Finite volume effects for hadrons via virtual particle exchange with themselves through periodic boundary

Like time dependence, falls off $\propto \exp[-EL]$

For typical ensembles, $M_{\pi}L \sim 4 \implies$ only π nonnegligible

No analogue using QFT definition of asymptotic separation particles in multiparticle states cannot be isolated

Presence of other nearby particles has large effects on spectrum

Strong spectrum modifications $\propto L^{\alpha}$





Resonances in Finite Volume



Toy example above: $\pi\pi$ scattering with ρ state

- ▶ (Left) Resonances, avoided level crossings:
- ▶ (Right) Single-particle states:

FV corrections $\propto L^{\alpha}$

- FV corrections $\propto \exp\{-M_{\pi}L\}$
- \implies Particle count is *not* a good quantum number

Continuum Limit

[Lepage Proceedings]

Reminder of the link definition:



Define a plaquette: $P_{\mu\nu}(x) = \frac{1}{3} \operatorname{Re} \left[\operatorname{Tr} \left[\frac{U_{\mu}(x)U_{\nu}(x+a\hat{\mu})U_{\mu}^{\dagger}(x+a\hat{\nu})U_{\nu}^{\dagger}(x) \right] \right]$ $= \frac{1}{3} \operatorname{Re} \left[\operatorname{Tr} \left[e^{-ig \oint_{\Box} A \cdot dx'} \right] \right] = \frac{1}{3} \operatorname{Re} \left[\operatorname{Tr} \left[\underbrace{\Box} \right] \right]$

Continuum Limit

[Lepage Proceedings]



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Taylor expand:
$$P_{\mu\nu}(x) = \frac{1}{3} \operatorname{Re} \left[\operatorname{Tr} \left[1 - ig \left(\oint_{\Box} A \cdot dx' \right) - \frac{1}{2} g^2 \left(\oint_{\Box} A \cdot dx' \right)^2 + \ldots \right] \right]$$

Stokes' theorem

$$\oint_{\Box} A \cdot dx' = \int_{x}^{x+a\hat{\mu}} \int_{x}^{x+a\hat{\nu}} dx'_{\mu} dx'_{\nu} \left(\partial_{\mu} A_{\nu}(x') - \partial_{\nu} A_{\mu}(x') \right)$$
$$= a^{2} F_{\mu\nu}(\bar{x}) + \frac{a^{4}}{24} \left(D_{\mu}^{2} + D_{\nu}^{2} \right) F_{\mu\nu}(\bar{x}) + \dots \qquad \bar{x} = x + \frac{a}{2} \left(\hat{\mu} + \hat{\nu} \right)$$

Continuum Limit

[Lepage Proceedings]

$$a_{\mu}(x) = e^{-ig \int_{x}^{x+a\hat{\mu}} A_{\mu}(x')dx'} =$$

Define a plaquette:
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 U_{L}

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The Wilson action:
$$S_W = \beta \sum_{x,\mu>\nu} (1 - P_{\mu\nu}(x))$$

= $\int d^4x \sum_{\mu\nu} \left\{ \frac{1}{2} \text{Tr} F_{\mu\nu}^2 + \frac{a^2}{24} \text{Tr} F_{\mu\nu} (D_{\mu}^2 + D_{\nu}^2) F_{\mu\nu} + \dots \right\}$

Lattice action same as physical continuum action up to order a^2 corrections...

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Continuum Limit Universality



Different actions can have different approach $a \to 0$

Usually $O(a^2)$, some improved to e.g. $O(a^2\alpha_s)$ \implies additional terms added to action

All actions should give same result in continuum

Chiral Extra(Inter)polation

"Why is extrapolation in masses needed at all? Just compute directly at physical masses."



There was a time when we couldn't (the "Berlin Wall") [A. Ukawa (2002)]

Cheaper to simulate at large M_{π} , then extrapolate as long as extrapolation is controlled

Physical M_{π} ensembles relatively new (10 years)

Most modern computations include ≥ 1 physical M_{π} ensemble

Chiral Perturbation Theory (χPT)

Build effective theory, treat hadrons as degrees of freedom

Lagrangian constructed assuming chiral symmetry as a guiding principle

$$\begin{split} \mathcal{L}_{\pi N}^{(1)} &= \bar{\Psi} \left(i \ \overline{\mathcal{V}} - m + \frac{\dot{g}_A}{2} \ \# \gamma_5 \right) \Psi \\ \mathcal{L}_{\pi N}^{(2)} &= \overline{\Psi} \left\{ c_1 \langle \chi_+ \rangle - \frac{c_2}{4m^2} \left(\langle u_\mu u_\nu \rangle \nabla^\mu \nabla^\nu + \text{h.c.} \right) + \frac{c_3}{2} \ \langle u \cdot u \rangle + \frac{c_4}{4} i \sigma^{\mu\nu} \left[u_\mu, u_\nu \right] \right\} \Psi \\ \mathcal{L}_{\pi N}^{(3)} &= \frac{b}{(4\pi F)^2} \overline{\Psi}_2^1 \langle \chi_+ \rangle \ \# \gamma_5 \Psi \\ \mathcal{L}_{\pi N}^{(4)} &= \frac{d}{m(4\pi F)^2} \overline{\Psi} \langle \chi_+ \rangle^2 \Psi , \end{split}$$

Some uses:

- 1. get parametric dependence of LQCD results on M_{π} , FV corrections use to understand extrapolation to physical!
- 2. understand hadronic mechanisms driving physics behavior
- 3. applying LQCD results to make predictions of other observables



Example — χPT and $N\pi$ in Excited States





Excited state uncertainties are another critical systematic (Opinion: most challenging in nucleon computations)

 $\chi {\rm PT}:$ Contamination in $F_A(Q^2)$ primarily from enhanced $N\pi,$ mostly from induced pseudoscalar

Empirical: two $N\pi$ states dominate contamination at nonzero Q^2

Future Prospects

State of the Art

									P. Boyle
Location	System	Interconnect (GB/s) per node (X+R)	Floating point performance (GF/s) per node	Memory Bandwidth (GB/s) per node	Year	System peak (PF/s)	FP / Interconnect	FP / Memory	Memory / Interconnect
LLNL	BlueGene/L	2.1	5.6	5.5	2004	0.58	2.7	1.0	2.6
ANL	BlueGene/P	5.1	13.6	13.6	2008	0.56	2.7	1.0	2.7
ANL	BlueGene/Q	40	205	42.6	2012	20	5.1	4.8	1.1
ORNL	Titan	9.6	1445	250	2012	27	150.5	5.8	26.0
NERSC	Edison	32	460	100	2013	2	14.4	4.6	3.1
NERSC	Cori/KNL	32	3050	450	2016	28	95.3	6.8	14.1
ORNL	Summit	50	42000	5400	2018	194	840.0	7.8	108.0
RIKEN	Fugaku	70	3072	1024	2021	488	43.9	3.0	14.6
NERSC	Perlmutter/GPU	200	38800	6220	2022	58	194.0	6.2	31.1
ORNL	Frontier	200	181200	12800	2022	>1630	906.0	14.2	64.0

Systems with exaflop peak performance



State of the Art

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β	a [fm]	$T \times L$	#conf		
3.7000	0.1315	64×48	904		
3.7500	0.1191	96×56	2072		
3.7753	0.1116	84×56	1907		
3.8400	0.0952	96×64	3139		
3.9200	0.0787	128×80	4296		
4.0126	0.0640	144×96	6980		
[L. Lellouch]					

 $96^3 \times 144 \implies > 10^9$ sites 8.5 GB/config, 154 GB/propagator

Systems with exaflop peak performance



Energy Regimes



LQCD Target Calculations





QE Axial FF - $N\pi$ Interpolating Operators



Excited state contamination largely dominated by $N\pi$ states

Empirical: need $N\pi$ -like operators (must include $qqq \cdot q\bar{q}$ operators) to isolate states [Phys.Rev.D 92 (2015)]

Several groups working on better multiparticle analyses, more expensive than only qqq operators

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Resonance Production - $N \to \Delta$



 1π cross section known to 30% [Phys.Rev.C 88 (2013)] DUNE error budget $\lesssim 10\%$ precision [2002.03005 [hep-ex]]

Unconstrained axial form factors in $J^P = 3/2^-$ channels $\implies 100\%$ uncertainties from V - A, A - A interference terms [Phys.Rev.D 74 (2006)]

Large overlap of tasks with $N\pi$ in QE form factors

Some previous work by ETM: [Phys.Rev.D 83 (2011)] [Phys.Rev.Lett. 98 (2007)]

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 π

N'

Resonance Production - $N \rightarrow N^*$





Calculable in Euclidean time Ill-posed inverse problem Euclidean→Minkowski

Hadronic tensor methods for addressing SIS (1.4 GeV $\leq W \leq 2.0$ GeV)

Like optical theorem: 4-point function, \boldsymbol{X} state in middle

 $\langle \mathcal{O}(t_3)\mathcal{J}_4(t_2)\mathcal{J}_4(t_1)\bar{\mathcal{O}}(0) \rangle$

Challenging for LQCD, some techniques being developed

Currently no practical $Q^2 \neq 0$ experimental data in this region [S.Nakamura - NuSTEC S&DIS]

Conclusions

Outlook



- LQCD is a computational tool useful for obtaining weak matrix elements in neutrino physics in most cases, it is complementary to experiment
- LQCD is in general **inclusive**

get all of QCD, whether it was asked for or not

 LQCD can be used to isolate some quantities that are not separable in experiment e.g. strangeness content of neutral current Homework will be a hands-on lattice computation of the 1 + 1-dimensional Schwinger model.

It will be included as a separate packet on the Indico page.

If you do not see it, please check back tomorrow!

