Introduction to lattice QCD

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Lecture #1 :
- Why lattice QCD
- Euclidean, discretised path integrals
- Defining lattice actions

Lecture #2 :
- Observables in LQCD
- Building intuition: what is easy/hard and why.

1. Why lattice QCD

A: QCD is non-perturbative! Now define notation, discuss further....

QCD Lagrangian:

$$\mathcal{L}_{QCD} = -\frac{1}{4}\overset{\text{colour Tr}}{\mathrm{Tr}}\left[F^{\mu\nu}F_{\mu\nu}\right] + \sum_f \bar{\Psi}_f\left(i\overset{\not{D} = D_\mu\gamma^\mu}{\not{D}} - \underset{\text{quark masses}}{m_f}\right)\Psi_f + \overset{\text{CP-violating }\theta\text{-term}}{\theta}\, \varepsilon_{\mu\nu\rho\sigma}\mathrm{Tr}\left[F^{\mu\nu}F^{\rho\sigma}\right]$$

contains quark degrees of freedom:

$\Psi_{f,\alpha,c}(x)$ with f = flavour $\in \{\overbrace{u, d, s, c}^{\text{LQCD default}}, b, \overset{\text{does not hadronize}}{t}\}$

↑ [HQET, NRQCD action,....

tricky, discretisation errors $\propto am_q$... HISQ,....

α = dirac $\in \{1,2,3,4\}$

c = colour $\in \{1,2,3\}$

- Dirac matrices γ^μ in fermion Lagrangian are elements of a Clifford algebra

$$\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu} \quad (\to 2\delta_{\mu\nu} \text{ Euclidean}) \qquad \mu,\nu \in \{0,1,2,3\}$$

with the γ_μ being 4×4 matrices, can be written in many bases

and gluon degrees of freedom:

$A_{\mu,a}(x)$ with μ = Lorentz index $\in \{0,1,2,3\}$

a = colour $\in \{1,2,\ldots,8\}$

which we can write in terms of a matrix-valued field

$$A_\mu(x) = A_{\mu,a}(x)\, T_a$$

↖ generators of SU(3) ← e.g. $\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ .. etc.

$T_a = \lambda_a/2$

↑ Gell-Mann matrices

generators satisfy SU(3) algebra $[T^a, T^b] = i f^{abc} T^c$

↑ antisym structure constant

- Covariant derivative built from gauge field

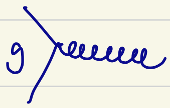
$$D^\mu = \partial^\mu - igA^\mu \qquad \text{(matrix notation)}$$

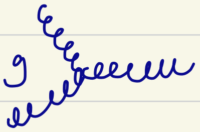
and gluon field strength tensor is

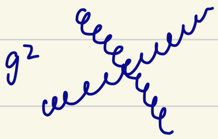
$$F^{\mu\nu} = \frac{2i}{g}[D^\mu, D^\nu] \equiv F^{\mu\nu}_a T_a \qquad \text{(matrix object)}$$

$$F^{\mu\nu}_a = \partial^\mu A^\nu_a - \partial^\nu A^\mu_a + g f_{abc} A^\mu_b A^\nu_c$$

- $\mathcal{L}_{QCD}$ contains interactions

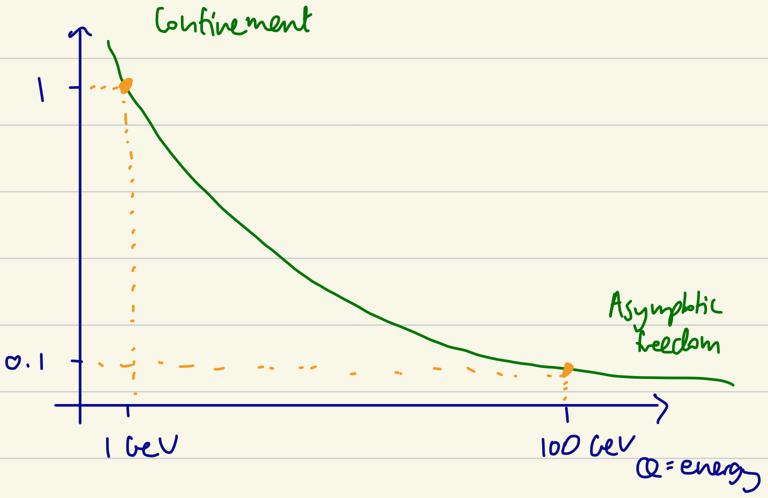






gluon self-interactions ⇒ QCD is fundamentally different from QED

Important features of QCD:
asymptotic freedom, confinement
occur through running of
QCD coupling $\alpha_s = \frac{g^2}{4\pi}$
with energy scale as a result of
quantum effects



i.e. low-energy QCD is non-perturbative.
Physical quantities are not analytic in the QCD coupling.

↑ locally given by convergent power series

Symmetries: [will need to think about when discretising the theory]

- SU(3) gauge symmetry i.e., local rotations in colour space

$$\psi(x) \to \psi'(x) = \Omega(\vec{\theta})\psi(x)$$

with $\Omega(\vec{\theta}) = \exp[\frac{-i}{2}\theta^a(x)T^a]$ $\theta^a(x)$ parameterise transform

also $A_\mu(x) \to A_\mu'(x) = \Omega(\theta)A_\mu(x)\Omega^{-1}(\theta) - \frac{2i}{g}[\partial_\mu\Omega(\theta)]\Omega^{-1}(\theta)$

$$D_\mu \to \Omega(\theta)D_\mu\Omega^{-1}(\theta)$$

$$F_{\mu\nu} \to \Omega(\theta)F_{\mu\nu}\Omega^{-1}(\theta)$$

- Lorentz, C, P, T
- U(1) global symmetry

$$\psi \to \exp[\tfrac{-i}{2}\alpha]\psi, \qquad \bar{\psi} \to \bar{\psi}\exp[\tfrac{i}{2}\alpha]$$

- In the chiral limit ($m_f = 0$), also chiral symmetry

i.e. global invariance under axial transformations $U(1)_A$

$$\psi \to \exp[\tfrac{-i}{2}\alpha\gamma_5]\psi, \qquad \bar{\psi} \to \bar{\psi}\exp[\tfrac{-i}{2}\alpha\gamma_5]$$

where $\gamma_5 = i\gamma_0\gamma_1\gamma_2\gamma_3$, $\gamma_5^2 = 1$, $\gamma_5^\dagger = \gamma_5$

and global flavour rotations

$$\psi \to \exp[\tfrac{-i}{2}\alpha^a\tau^a]\psi$$

$$\psi \to \exp[\tfrac{-i}{2}\alpha^a\tau^a\gamma_5]\psi$$

[τ^a generators of $SU(N_f)$ in fundamental rep.
e.g. $N_f = 2$, Pauli matrices]

i.e. $SU(N_f)_V \times SU(N_f)_A \times U(1)_V \times U(1)_A \leftarrow$ not manifest, broken by the axial anomaly

$\uparrow$ spontaneously broken by vacuum → Goldstone's theorem

- fermion mass breaks chiral symmetry explicitly

* Lattice regularisation gives us a way to describe non-perturbative QCD in systematically-improvable way
i.e. recover QCD when all limits are taken (much more later: lattice spacing $a \to 0$, lattice volume $V \to \infty$ etc.)

* Free parameters in LQCD will be same as in QCD itself: quark masses, strong coupling. Once fixed, everything else is QCD prediction.

Important application areas of LQCD:

- Thermodynamics → QCD phase diagram vs temp, density (chemical potential μ) shows existence of a crossover to quark-gluon plasma at $T_c \sim 150$ MeV. Experimental exploration of this is major goal of RHIC program at BNL

- Precision flavour physics - Constrain parameters of the SM that encode quark mixings (CKM matrix) → use to make SM predictions of other process + hence search for BSM physics.

- Hadron spectroscopy → can we understand spectrum of particle states from SM? e.g. mass of the proton (last 5 years - yes!) states that aren't quark-model-like?

- Hadron interactions + nuclei → how do hadrons interact?
  → how do nuclei emerge from QCD?
  → how do nuclei interact w/ electroweak or possibly BSM currents? etc.

- Beyond - SM → many intersting field theory q's beyond perturbative regime e.g. technicolour (strong dynamics at EW scale)

2. Euclidean, discretised path integrals

- Path integral approach to field theory:

  generating functional contains all information about the theory

$$Z[J,\eta,\bar{\eta}] = \int DA\, D\bar{\psi}\, D\psi \; \exp\left[i \int d^4x \left(\mathcal{L}_{QCD} + J_\mu^a A^{\mu a} + \bar{\eta}\psi + \bar{\psi}\eta \right)\right]$$

$\uparrow\uparrow\uparrow$ external sources

↑ integral over all possible gauge and fermion fields

  Expectation values / Greens functions / correlation functions expressed as functional derivatives

$$\langle 0 | A_\mu(x)\, \bar{\psi}(y) \dots \psi(z) | 0 \rangle = \frac{1}{Z[0]} \frac{\delta}{\delta J_\mu(x)} \cdots \frac{\delta}{\delta \bar{\eta}(z)} Z[J,\eta,\bar{\eta}] \Big|_{J=\eta=\bar{\eta}=0}$$

- Fermion fields are anticommuting (Grassman-number-valued)

- To compute: need to define / interpret the measure (and regularise mtm integrals)
- Perturbation theory: expand Z / correlators in powers of couplings
- Instead: define Z directly through lattice regulator, valid beyond perturbation theory, provides numerical evaluation approach.

- Oscillatory integrand from $e^{-iS_{QCD}}$ → cancellations between different regions of phase space, numerical difficulties

$\Rightarrow$ Wick rotation ($t \to -it_E$) from Minkowski to Euclidean space-time gives probabalistic interpretation to functional integral i.e. $e^{-iS_{QCD}} \to e^{-S_{QCD}}$

(exponential is exactly the Boltzmann weighting of a statistical ensemble)

- Discretise theory onto e.g. 4D cubic lattice

$$\Lambda = \{ x \in \mathbb{R}^4 \mid x = an, \; n \in \mathbb{Z}^4 \}$$

↑ "lattice spacing"

[In practice, finite extent, boundary conditions (e.g. (anti)-periodic)]

Quark fields on sites: $\psi(x) \to \psi(\vec{n})$, $\vec{n} \in \Lambda$

$$\int d^4x \to \sum_{\vec{n}\in\Lambda} \;, \qquad \int D\psi \to \prod_{\vec{n}\in\Lambda} d\psi(\vec{n}) \qquad \text{etc.}$$

↑ probably how path int. was <u>defined</u> in your field theory class.

- we will see (soon) that to maintain gauge symmetry in the discretised action, it is convenient to define gauge link variables (parallel transporters between neighbouring sites)

  so $A_\mu(x) \rightarrow U_\mu(\vec{n}) = e^{-iagA_\mu(\vec{n})}$

Then, basic idea of LQCD: [details soon]

$$\underset{\substack{\uparrow\\ \text{operator of}\\ \text{interest}}}{\langle O \rangle} = \frac{1}{Z}\int DU\, D\psi\, D\bar{\psi}\; e^{-S_{QCD}[U,\psi,\bar{\psi}]}\, O[U,\psi,\bar{\psi}] \qquad S_{QCD} = \underset{\substack{\uparrow\\ -\frac{1}{4}F_{\mu\nu}F^{\mu\nu}}}{S_{glue}} + \int \bar{\psi}\, \overset{\substack{\text{Dirac operator}\\ \downarrow}}{M}\, \psi$$

$$= \frac{1}{Z}\int DU\, \det M[U]\, e^{-S_{glue}[U]}\, O[U, M^{-1}[U]]$$

→ first integrate out fermions to arrive at a numerical integral

→ discretise and compactify (focus on some finite volume w/ some BCs)

$$DU \rightarrow \underset{\substack{\mu\\ \uparrow\\ \text{direction}}}{\prod}\; \underset{\substack{a\\ \uparrow\\ \text{colour}}}{\prod}\; \underset{\substack{\vec{n}\in\Lambda\\ \uparrow\\ \text{discrete volume}}}{\prod} dU^a_\mu(\vec{n}) \qquad \text{large but finite-dim integral}$$

→ integrand has a weight factor: $e^{-S_{glue}[U]} \det \underset{\substack{\uparrow\\ O(\text{volume}) \times O(\text{volume}) \text{ matrix on discrete system}}}{M}[U]$

→ sample space of Us according to this weight = probability measure

→ do this via Markov chain process $U^{[0]} \rightarrow U^{[1]} \rightarrow \dots$ with transitions required to satisfy certain conditions s.t desired prob. distribution emerges as equilib. dist of the process

→ once a representative set of configurations is available, observables can be computed as simple averages w/ uncertainties falling w/ the number of samples taken

$$\langle O \rangle = \sum_i^{n_{cfg}} \tilde{O}[U_i] + O(1/\sqrt{N_{cfg}})$$

→ complete calculation requires dealing w/

statistical uncertainties: $N_{cfg} \rightarrow \infty$

systematic uncertainties: multiple lattice spacings, couplings, box sizes, etc.

3. Defining lattice actions

- In continuum field theory, demanding gauge symmetry → existence of gauge field to construct gauge covariant derivative (e.g. scalar QED)
  same in lattice formulation.

- Consider the Euclidean Dirac action for a free fermion

$$\int d^4x\, \bar\psi(x)[\not{\partial}+m]\psi(x)$$

→ discretize derivative with e.g. symmetric finite difference

but $\bar\psi(n)\gamma_\mu\psi(n+\hat\mu) - \bar\psi(n)\gamma_\mu\psi(n-\hat\mu)$ is not gauge invariant.

Recall: $\psi(n) \to \Omega(n)\psi(n)$, $\bar\psi(n) \to \bar\psi(n)\Omega^\dagger(n)$, $\Omega(n) \in SU(3)$

Introduce "gauge links" as parallel transporters:

$$U_\mu(n) \to \Omega(n)U_\mu(n)\Omega^\dagger(n+\hat\mu)$$

and replace

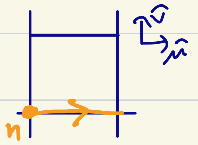
$\bar\psi(n)\gamma_\mu\psi(n+\hat\mu)$ in naive finite-diff with $\bar\psi(n)\gamma_\mu U_\mu(n)\psi(n+\hat\mu)$

- Gauge links are special case of parallel transporters that map coordinates in internal symmetry space from one point to another:

$$U_\mu(n) = P\exp i\int_0^a A_\mu(n+\lambda\hat\mu)\,d\lambda \quad = \exp(iaA_\mu)$$

$$\to 1 + iaA_\mu(n) + \mathcal{O}(a^2) \quad \text{for small } a$$

- Identify gauge links on "edges" of lattice



$U^\dagger_\mu(n) = U_{-\mu}(n+\hat\mu)$

So, "naive" fermion action

$$S_F^N[U,\psi,\bar\psi] \underset{\substack{\uparrow\\ \text{factors of a}}}{\sim} \sum_{n\in\Lambda} \bar\psi(n)\Big(\sum_{\mu=1}^{4}\gamma_\mu\big[U_\mu(n)\psi(n+\hat\mu) - U^\dagger_\mu(n-\hat\mu)\psi(n-\hat\mu) + m\psi(n)\Big)$$

$$= \sum_{n,m\in\Lambda} \bar\psi(n)\underset{\substack{\uparrow\\ \text{naive interaction matrix}}}{M^N_{nm}[U]}\psi(m)$$

- Taylor-expand U_μ, ψ in a → has $O(a^2)$ errors.
  BUT "doubling problem": 1st order derivative only couples sites separated by 2a → in the continuum limit there are $2^d = 16$ quark flavours instead of one

[See this: look at poles of inverse free two-pt function (fermion propagator) $\tilde{D}^{-1}(k)$:
for $m=0$ poles not only at $k^\mu = (0,0,0,0)$ but $k^\mu = (0,0,0,\pi/a), \ldots, (\pi/a, \pi/a, \pi/a, \pi/a)$]

Nilsen - Ninomiya no-go theorem:

It is not possible to construct a lattice fermion action that is (ultra)-local, chirally-symmetric, undoubled, with correct continuum limit

Choices:

- Wilson fermions: break chiral sym explicitly (even when $m=0$) by adding a second derivative term that acts as a large mass (of order of the cutoff) at the doubler poles but is irrelevant at zero mtm i.e. drive doublers to higher energies with extra term that vanishes as $a \to 0$
  [introduces $O(a)$ discretisation errors, can improve "Symanzik improvement" by adding e.g. "clover" term tuned to remove $O(a)$ artefacts]
- Staggered fermions: distribute the 4 components of the Dirac spinor to different lattice sites → 4 species or "tastes", break taste symmetry
- Ginsparg-Wilson fermions: Preserve "lattice chiral symmetry" i.e. Ginsparg-Wilson relation, that reduces to usual sym. in the chiral limit
  e.g.
  - Domain-wall fermions (Kaplan + Shamir)
  - Overlap fermions (Narayanan + Neuberger)
  - Perfect actions / fixed-point fermions (Hasenfratz et al)

  BUT computationally more expensive.

* Which fermion action is best can depend on the particular application. *