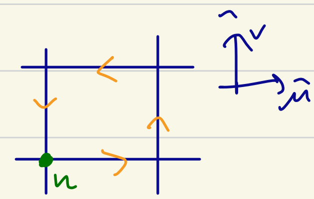
Gauge action:

- Closed paths of gauge links (Wilson loops) can be used to construct all gauge-invariant quantities involving only gauge fields
- As for fermions, precise construction of gauge action is irrelevant if it has the correct continuum limit (will have different discretisation artefacts, some better than others...)
- Simplest closed loop is the 1×1 plaquette:

$$P_{\mu\nu}(n) = \mathrm{Re}\,\mathrm{Tr}\left[U_\mu(n)\,U_\nu(n+\hat{\mu})\,U^\dagger_\mu(n+\hat{\nu})\,U_\nu^\dagger(n)\right]$$



Taylor-expand path-ordered expression for U_μ in terms of A_μ to identify

$$P_{\mu\nu}(n) = 1 - \tfrac{1}{2} g^2\,\mathrm{Tr}\left[F_{\mu\nu}(n)^2\right] + \mathcal{O}(g^2a^2,\, a^4,\, g^4a^2)$$

$\Rightarrow$ "Wilson" gauge action

$$S_G^W[U] = \frac{2}{g^2}\sum_{n\in\Lambda}\sum_{\mu<\nu}\left[1 - P_{\mu\nu}(n)\right] \xrightarrow[a\to0]{} \frac{1}{2g^2}\sum_{n\in\Lambda}\sum_{\mu<\nu}\mathrm{Tr}\left[F_{\mu\nu}(n)^2\right]$$

- Can "improve" the gauge action by including additional loops (e.g. 1×2 rectangles) coefficients tuned to remove leading discretisation artefacts, names like "Iwasaki gauge action", "tree-level improved" gauge action etc.

Now the total lattice action is $S_{QCD} = S_G[U] + S_F[U,\psi,\bar\psi]$ with some choice for each piece.

Check in about symmetries:

- SU(3) gauge – preserved by lattice actions
- Lorentz $\rightarrow$ broken down to hypercubic $H(4)$ $\Rightarrow$ induces operator mixing
- chiral – depends on action

4. Observables

What can be computed in LQCD are Euclidean n-point correlation functions

→ relate physics of interest to matrix elements of local (or non-local, see quasi/pseudo PDF/TMDs) operators.

Example #1 : Mass of the pion from 2pt correlation fn

Consider two equivalent expressions for hadron 2-point correlator

$$C_\pi(\vec{x},t) \equiv \langle \mathcal{O}_\pi(\vec{x},t)\, \mathcal{O}_\pi^\dagger(\vec{0},0)\rangle$$
$$= \frac{1}{Z}\, \mathrm{Tr}\left[e^{-\hat{H}(T-t)}\, \hat{\mathcal{O}}_\pi(\vec{x})\, e^{-\hat{H}t}\, \hat{\mathcal{O}}_\pi^\dagger(\vec{0})\right] \quad ① \text{ Trace in Hilbert space (transfer matrix)}$$
$$= \int \mathcal{D}U\, \mathcal{D}\psi\, \mathcal{D}\bar{\psi}\; e^{-S_{glue} + \int \bar{\psi} M \psi}\; \mathcal{O}_\pi(\vec{x},t)\, \mathcal{O}_\pi^\dagger(\vec{0},0) \quad ② \text{ Path integral}$$

The operator $\mathcal{O}_\pi[U,\psi,\bar{\psi}]$ is an "interpolating operator" with the quantum numbers of the state of interest

e.g. for pion $\quad \mathcal{O}_\pi(x) = \bar{u}(x)\gamma_5 d(x)$

[or e.g $\tilde{\mathcal{O}}_\pi(x) = \tilde{\bar{u}}(x)\gamma_4\gamma_5\tilde{d}(x)$ i.e. "smeared" quark field with some smearing function $f(x,y)$

with $\tilde{q}(x) = \sum_y f(x,y)\, q(y)$]

Starting from ①, rearrange to solve for t-dep of $C_\pi(\vec{x},t)$

$$C_\pi(\vec{x},t) = \frac{1}{Z}\, \mathrm{Tr}\left[e^{-\hat{H}(T-t)}\, \hat{\mathcal{O}}_\pi(\vec{x})\, e^{-\hat{H}t}\, \hat{\mathcal{O}}_\pi^\dagger(\vec{0})\right]$$
$$= \frac{1}{Z}\sum_\rho \langle \rho|\, e^{-\hat{H}(T-t)}\, \hat{\mathcal{O}}_\pi(\vec{x})\, e^{-\hat{H}t}\, \hat{\mathcal{O}}_\pi^\dagger(\vec{0})\,|\rho\rangle \quad \text{(sum over all states in Hilbert space)}$$
$$= \frac{1}{Z}\sum_{\rho,\sigma} \langle \rho|\, e^{-\hat{H}(T-t)}\, \hat{\mathcal{O}}_\pi(\vec{x})\,|\sigma\rangle\langle\sigma|\, e^{-\hat{H}t}\, \hat{\mathcal{O}}_\pi^\dagger(\vec{0})\,|\rho\rangle \quad \text{(insert complete set of states)}$$
$$= \frac{1}{Z}\sum_{\rho,\sigma} e^{-E_\rho(T-t)}\, e^{-E_\sigma t}\, \langle \rho|\,\hat{\mathcal{O}}_\pi(\vec{x})\,|\sigma\rangle\langle\sigma|\,\hat{\mathcal{O}}_\pi^\dagger(\vec{0})\,|\rho\rangle \quad (*)$$

Similarly $\mathcal{Z} = \sum_p \langle p | e^{-\hat{H}T} | p \rangle = \sum_p e^{-E_p T} = e^{-E_0 T}(1 + e^{-\Delta E_1 T} + e^{-\Delta E_2 T} + \cdots)$

where $\Delta E_n = E_n - E_0$, E_0 the vacuum energy

Taking T large, only $|p\rangle = |\sigma\rangle$ contributes to (*)

$$\Rightarrow \quad C_\pi(\vec{x},t) \xrightarrow[T\to\infty]{} \sum_\sigma \langle 0 | \hat{O}_\pi | \sigma \rangle \langle \sigma | \hat{O}_\pi^\dagger | 0 \rangle e^{-\Delta E_\sigma t}$$

Project to zero three-momentum by taking $\sum_{\vec{x}}$

$$\Rightarrow \quad C_\pi(t) = \sum_{\vec{x}} C_\pi(\vec{x},t) = \sum_{\sigma(\vec{p}=0)} |Z_\sigma|^2 e^{-M_\sigma t} \qquad (\#)$$

i.e. depends on energies of all states for which $Z_\sigma \neq 0$ i.e. those that can be created from the vacuum by the creation op $O^+(x,t)$

In general, a creation operator creates a state that is a linear combination of all possible e-states of H that have the same quantum #s as the pion e.g., pion, excitations of the pion, three pions in $J=0$ state, etc, but a particular interpolator will have "stronger" overlap onto some states than others

Starting from (2) we see how to compute $C_\pi(t)$ in LQCD:

$$C_\pi(\vec{x},t) = \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi}\, e^{-S_{glue} + \int \bar{\psi} M \psi}\, \bar{\psi}_u(\vec{x},t)\gamma_5 \psi_d(\vec{x},t)\bar{\psi}_d(\vec{0},0)\gamma_5\psi_u(\vec{0},0)$$

$$= \int \mathcal{D}U \det M_u \det M_d\, e^{-S_{glue}}\, \mathrm{Tr}\left[M_u^{-1}(\vec{x},\vec{0})\gamma_5 M_d^{-1}(\vec{0},\vec{x})\gamma_5\right]$$

$$\to \frac{1}{N_{cfg}} \sum_{i=1}^{N_{cfg}} \mathrm{Tr}\left[M_u^{-1}[U_i]\gamma_5 M_d^{-1}[U_i]\gamma_5\right]$$

where the ensemble is $\{U_1, \ldots, U_{N_{cfg}}\}$

quark propagators computed by matrix inversion

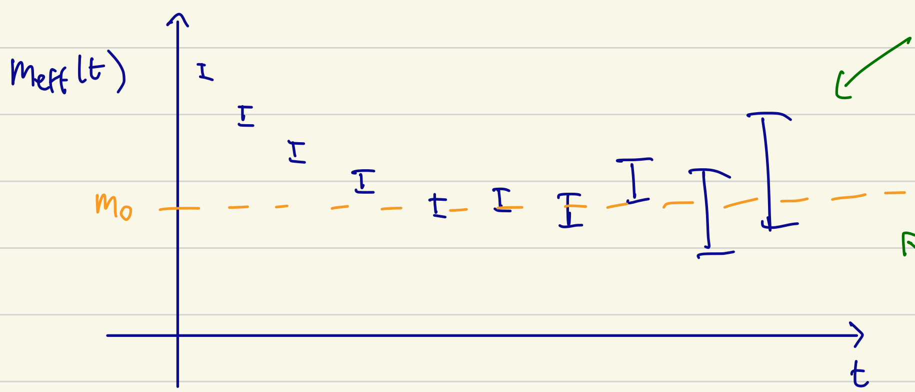
→ sum over positions $\vec{x}$ to compute $C_\pi(t)$

- Having computed $C_\pi(t)$ numerically, fit to functional form (#) to determine mass of lightest state with the given quantum #s

To be concrete about fits:

$$C_\pi(t) = |Z_0|^2 e^{-m_0 t} + |Z_1|^2 e^{-m_1 t} + \dots$$

Effective mass: $m_{eff}(t) = \frac{1}{d} \ln\left(\frac{C_\pi(t)}{C_\pi(t+d)}\right) = m_0 + \underset{\text{constant}}{A} e^{-\underset{\text{energy gap.}}{\Delta m}\, t} + \dots$



typically computed with bootstrap or jackknife resampling

Growth of noise is exponential with t - come back to this later

- estimate m_0 as the average of points in the "plateau" region
- More sophisticated: fit to (multi)-exponential functional form (χ^2-min) (must take care to take correlations into account)

- Can determine excited states by fitting multi-exponential form to $C_\pi(t)$, but it is difficult. More typical: choose set of interpolating ops with same quantum #s $\{\mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_N\}$ and form $N\times N$ matrix of correlators, $C_{ij}(t) = \frac{1}{Z}\mathrm{Tr}\left[e^{-\hat{H}(T-t)}\hat{\mathcal{O}}_i e^{-Ht}\hat{\mathcal{O}}_j^\dagger\right] \xrightarrow[T\to\infty]{} \sum_\sigma Z_{ij}^{(\sigma)} e^{-E_\sigma t}$

  i.e. same energies but different overlaps → solve eigenvalue problem for E_σ

<u>Example #2:</u> Matrix elements : g_A

Isovector axial coupling of the nucleon is defined by the matrix element

$$\underset{\substack{\text{nucleon state}\\ \text{with } \vec{p}}}{\langle N(\vec{p})|}\, \underbrace{\bar{\psi}\gamma_\mu\gamma_5 \underset{\substack{\tau_3 = \left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)\\ \text{flavour}}}{\tau_3} \psi}_{J^3_{\mu 5}} |N(\vec{p})\rangle = g_A\, \underset{\text{spinor}}{\bar{u}_p(\vec{p})}\, \gamma_\mu\gamma_5\, u_p(\vec{p})$$

e.g $O_{N\alpha} \sim \varepsilon^{abc}(u^a C\gamma_5 d^b)\, u^c_\alpha$ ← colour ← spin

Relate desired matrix element to 3pt function

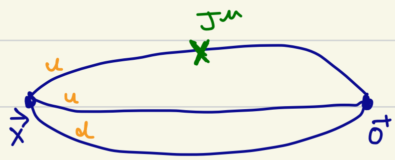
$$C_5^{\mu}(t,\tau) = \frac{1}{Z}\overset{\text{mtm-0}}{\sum_{x,y}} \mathrm{Tr}\left[e^{-\hat H(T-t)}\, O_N(\vec x)\, e^{-\hat H(t-\tau)}\, J^3_{\mu5}(\vec y)\, e^{-\hat H\tau}\, O_N^{\dagger}(\vec 0)\right]$$

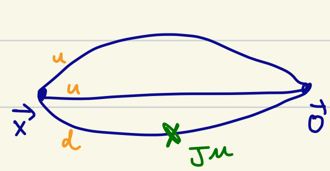
$$\xrightarrow[T\to\infty]{} \sum_{x,y}\sum_{n,m} \langle 0|\hat O_N|n\rangle\langle n|\, e^{-\hat H(t-\tau)}\, J^3_{\mu5}\, e^{-\hat H\tau}\,|m\rangle\langle m|\hat O_N^{\dagger}|0\rangle$$

$$= \sum_{x,y}\sum_{n,m} Z_n Z_m^{\dagger}\, e^{-E_n(t-\tau)}\, e^{-E_m\tau}\, \langle n| J^3_{\mu5}|m\rangle$$

- Use 2pt function with same O_N to determine Z_n, E_n (often useful to use ratios of 3pt / 2pt to eliminate leading time-dep before fitting)

Compute 3pt function in terms of quark propagators: "Skeleton diagram"

2 

− 

illustrate different contractions

What kinds of correlation functions are calculated?

2pt functions: Spectroscopy ...

3pt functions – matrix elements of local operators

- g_A, nucleon electromagnetic form factors, moments of parton distribution f^ns,
  B-π decay form factors to constrain CKM matrix elements....

3pt functions - matrix elements of non-local operators

- quasi / pseudo PDFs, TMDs...

4pt functions

- double-β decay matrix elements, K-$\bar{K}$ mass difference....

...

Workflow of LQCD calculation

1 Generate ensemble of field configurations by Hamiltonian/Hybrid Monte Carlo
~100k cores or 1000 GPUs

② Compute propagators : $\det(M)$, M^{-1} expensive - use iterative method
e.g. conjugate gradient ~ few 100s GPUs, but many per config

③ Contract into correlation functions
~ few GPUs / CPUs

④ Fits, analysis ~ local cluster scale

5. Building intuition

Uncertainties

- Statistical ~ $1/\sqrt{N_{meas}}$ scaling
- fits to correlation functions - systematics on fit forms, range, ..
- $a \to 0$ } calculations on several ensembles → extrapolate
- $V \to \infty$
- m_π, CSV, QED, chiral sym, ... } Possibly neglected...
- For sub-1% precision, become important

What is hard / expensive

- light quark masses

  computing propagators is more expensive for lighter masses:
  requires inverting (Dirac) matrices which get closer to singular
  [instead of conjugate gradient, algorithms such as adaptive multigrid]
  Also, finite-volume effects set by longest correlation length (i.e. π)
  → lighter quark masses ⇒ larger lattice volumes needed

- large lattice volumes

  Large number of degrees of freedom for each configuration / propagator etc
  → just computationally expensive! [Also: Dirac op has more low modes...]

- fine lattice spacings

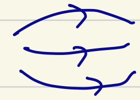
  Hybrid Monte Carlo (HMC) algorithm used to generate gauge fields
  involves close-to-local updates → more steps needed to update at scale of relevant
  correlation length as $a \to 0$ i.e "critical slowing-down" and cost of
  ensemble generation increases as $a \to 0$

- large Euclidean times

Euclidean time-evolution dampens excited states, but signal/noise degrades with t:

2pt function for proton:

$$C(t) \underset{t\to\infty}{=} \langle \Sigma_{\vec{x}}\, qqq\,(\vec{x},t)\ \bar{q}\bar{q}\bar{q}\,(\vec{0},0)\rangle \xrightarrow[\text{out quarks}]{\text{integrate}}$$

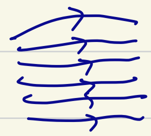


$$\to Z e^{-m_N t}$$

variance given by $\mathrm{var}(C) = \langle |C|^2\rangle - |\langle C\rangle|^2$

and $\langle |C|^2\rangle = \langle \Sigma_{\vec{x}}\, qqq(\vec{x})\, \Sigma_{\vec{y}}\, \bar{q}\bar{q}\bar{q}(\vec{y})\, qqq(\vec{0})\bar{q}\bar{q}\bar{q}(0)\rangle$

$\to$



[Note $q(x)$ does not contract with $\bar{q}(y)$, since quarks integrated out before $|\ |^2$]

States that propagate are $N+\bar{N}$ but also 3π:

$\langle |C|^2\rangle \sim \tilde{Z} e^{-3m_\pi t} + \hat{Z} e^{-2m_N t} + \cdots \qquad 3m_\pi < 2m_N \to 1^{st}$ term dominant.

$\Rightarrow$ signal/noise $\sim \langle C\rangle / \sqrt{\mathrm{var}(C)} \sim \exp(-(m_N - 3/2\, m_\pi))\,t$

- excited states

Damped out exponentially by Euclidean time-evolution

Variational method is expensive - need whole matrix of correlators

[Also, need interpolating ops with good overlap onto states - perhaps less intuitive than for ground states]

- large momenta

For non-zero hadron momenta, signal $\sim \exp(-E(p)\,t)$

but in variance the quark/antiquark have opposite momenta: $p+(-p)=0$

$\Rightarrow$ variance is still $\exp(-3m_\pi t)$

$\Rightarrow$ signal/noise $\sim \exp\left(-(E(p) - 3/2\, m_\pi)\right)t$ i.e. worse with increasing p.

[Also, a more dense excited state spectrum]

- nuclei

Signal-to-noise issues like for large momenta, but also factorial growth in # contractions with atomic number A.

"Typical" scales:

- lattice spacing — $a \sim 0.04 - 0.12$ fm
- lattice volume — $L^3 \times T \sim 24^3 \times 48 - 128^3 \times 256$

  [i.e. $128^3 \times 256 \times 4 \times N_c^2 \times \overset{\text{re/im}}{2} \sim 4 \times 10^{10}$ i.e. 320 GB per sample]
- Number of configs — 100 - 10,000
- Number of measurements — 100 - 100k
- quark masses — $m_\pi \sim 140$ MeV $-$ 800 MeV, sometimes lighter
- N_f — $N_f = 0, 2, 2+1, 3, 2+1+1, 2+1+1+1$
- computing resources — small calculations ~few M core-hours

  state-of-the-art ~ multi-year, 100s M core-hours

Useful references

Creutz: Quarks, gluons and lattices

Montvay + Münster: Quantum fields on the lattice

DeGrand + DeTar: Lattice methods for quantum chromodynamics

Gattringer + Lang: Quantum Chromodynamics on the lattice

Luscher: Computational strategies in LQCD arXiv: 1002.4232.