Introduction to Lattice QCD in Hadronic Physics

Giannis Koutsou

Computational-based Science and Technology Research Center (CaSToRC), The Cyprus Institute

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Outline

- **Introduction to Lattice QCD**
  - Discretization - fermions and gluons
  - Simulation - the path integral formulation

- **Hadrons on the Lattice**
  - Hadron spectrum on the lattice
  - Hadron matrix elements on the lattice

- **Techniques for Hadron matrix elements**
  - Systematic effects
  - Noise reduction techniques
Lattice Quantum Chromodynamics

- **Numerical solution of QCD**
  - *Ab initio* simulation of QCD, i.e. of the underlying fundamental theory
  - Well-established method for non-perturbative region of QCD
  - Access non-perturbative phenomena (confinement, quark-gluon plasma)
Discretization

- **Lattice QCD allows direct simulation, from the QCD Lagrangian**
  - The QCD Lagrangian:
    \[
    \mathcal{L}_{\text{QCD}} = \bar{\psi}(i\slashed{D} - m)\psi - \frac{1}{4} F^a_{\mu\nu} F^{\mu\nu}_a,
    \]
    where:
    \[
    F^a_{\mu\nu} = \partial_\mu G^a_\nu - \partial_\nu G^a_\mu - g f^{abc}_{\mu\nu} G^b_\mu G^c_\nu
    \]
  - Define *link variables*
    \[
    U_\mu(x_1; x_0) \equiv e^{-ig \int^c dx G^c_\mu(x) T_c}
    \]
Discretization

- Discretizing the gluon action
  - 4D space-time lattice, with lattice spacing $a$
  - Gluon link variables "live" between sites

\[ U_\mu(x_n) \equiv e^{-iagG^c_\mu(x_n)T_c} \]

- Simplest choice for gluon action:

\[ S_G[U] = -\frac{1}{4} \int d^4xF^c_{\mu\nu}F^c_{\mu\nu} \rightarrow \beta \sum_n \sum_{\mu<\nu} \Re \left\{ \text{Tr} \frac{1}{3} [1 - P_{\mu\nu}(x_n)] \right\} \]

Plaquette: \( P_{\mu\nu}(x_n) = U_\mu(x_n)U_\nu(x_n + \hat{\mu})U^\dagger_\mu(x_n + \hat{\nu})U^\dagger_\nu(x_n) \)
Discretization

- Discretizing the fermion action
  - Fermion variables "live" on sites
  - Various ways to define the fermion action on the lattice
  - All choices recover the continuum fermion action as $a \to 0$

- Naive:

\[
S_F = a^4 \sum_{x, \mu} \frac{1}{2a} \gamma^\mu [\bar{\psi}(x) U_\mu(x) \psi(x + a\hat{\mu}) - \bar{\psi}(x) U_{-\mu}(x) \psi(x - a\hat{\mu})] + m\bar{\psi}(x)\psi(x)
\]

Introduces "fermion doublers"
Discretization

- Wilson fermions:
  - Add a Laplacian term which "lifts" the doubler's mass as $a \to 0$

$$S_F = -a^4 \sum_{x,\mu} \frac{1}{2a} [\bar{\psi}(x)U_\mu(x)(r - \gamma_\mu)\psi(x + a\hat{\mu}) + \bar{\psi}(x)(r + \gamma_\mu)U_{-\mu}(x)\psi(x - a\hat{\mu})] + a^4 \sum_x (m + \frac{4}{a} r)\bar{\psi}(x)\psi(x)$$

- Additive renormalization to quark mass ($am_{\text{crit}} \neq 0$)
- Local fermion action
  $\rightarrow$ nearest-neighbor coupling
Discretization

- $O(a)$-improvement for Wilson fermions
  - In today's calculations Wilson fermions are combined with a prescription for removing $O(a)$ discretization effects
    - Twisted Mass
      Change of variables: $\psi = \begin{bmatrix} u \\ d \end{bmatrix}$ to $\chi = \frac{1}{\sqrt{2}} (1 - i\gamma_5\tau_3)\psi$
      Tune bare mass to critical value and exchange for twisted-mass $\mu$: $(m_{\text{crit}} + i\gamma_5\mu\tau_3)\bar{\chi}\chi$
    - Clover fermions
      Adds an irrelevant: $c_{SW}\bar{\psi}\sigma_{\mu\nu}F^{\mu\nu}\psi$ term
      Tune $c_{SW}$ for $O(a)$-improvement
  - Recent simulations exist which combine both Clover improvement and twisted mass
Discretization

- **Chiral Symmetry is tricky**
  - No-go theorem (Nielsen and Ninomiya)
  - On the lattice, need to either
    - Break locality of operator
    - Introduce doublers

- **Actions which preserve Chiral symmetry**
  - Staggered (allows for doublers)
  - Domain Wall (introduce 5th dimension)
  - Overlap (non-local operator)
Simulation

- Lattice QCD simulations via the Feynmann path integral formulation:

\[ \langle O \rangle = \frac{\int \mathcal{D}[U] \mathcal{D}[\bar{\psi}] \mathcal{D}[\psi] O(U, \psi, \bar{\psi}) e^{iS[U, \psi, \bar{\psi}]} }{ \int \mathcal{D}[U] \mathcal{D}[\bar{\psi}] \mathcal{D}[\psi] e^{iS[U, \psi, \bar{\psi}]} } \]

\( \psi, \bar{\psi} \): Grassmann variables, no way to represent on computers

⇒ integrate over the fermion fields analytically:

\[ \langle O (\psi(x), \bar{\psi}(y), U_\mu(z)) \rangle = \frac{\int \mathcal{D}[U] O (M^{-1}, U_\mu(z)) \det(M) e^{iS[U]} }{ \int \mathcal{D}[U] \det(M) e^{iS[U]} } \]

where:

\[ M = i\not{\psi} - m \]
Simulation

- Wick Rotation to imaginary time:

\[
\langle O \rangle = \frac{1}{Z} \int \mathcal{D}[U] O e^{-S_G[U] + \ln(\det(M[U]))}
\]

- Introduce pseudo-fermion fields for the determinant calculation (e.g. for two degenerate flavors)

\[
\langle O \rangle = \frac{1}{Z} \int \mathcal{D}[U] \mathcal{D}[\phi] \mathcal{D}[\bar{\phi}] O e^{-S_G[U] - \bar{\phi}(M^+M)^{-1}\phi}
\]

- Compute quark correlation functions via Wick's theorem

\[
\langle \psi_{j_1} \psi_{j_2} \cdots \bar{\psi}_{i_1} \bar{\psi}_{i_2} \cdots \rangle_U = \langle (\pm)^p M_{i_1j_1}^{-1} M_{i_2j_2}^{-1} \cdots + \text{all permutations} \rangle_U
\]

\( p \): number of permutations
Simulation

- **Monte Carlo simulation**

\[
\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U, \bar{\phi}, \phi] \mathcal{O} e^{-S_G[U] - \bar{\phi}(M^\dagger M)^{-1}\phi}
\]

- Generate representative configurations of the gauge field \( U \) with weight \(-S_G[U] - \bar{\phi}(M^\dagger M)^{-1}\phi\)
- \( \mathcal{O} \) depends on \( M^{-1}[U] \)
- \( \bar{\phi} \) and \( \phi \) integrated out

- **Boils down to** \( Mx = b \)

- Need \( \bar{\phi}(M^\dagger M)^{-1}\phi \) for update
- Need \( M^{-1} \) for observables
- Repeated applications of \( M \)
- Iterative solvers employed for inversions: CG, GMRES, BiCG, etc.
Simulation

- **Typical parameter space requirements**
  - Need at least 3 lattice spacings to take $a \to 0$ limit
  - Need several $m_q$ to take $m_q \to 0$ limit
  - Need at least two volumes sizes to check for finite volume effects
  - Need $O(1000)$ configurations per ensemble

- **However, simulations with quark masses at the physical point have become possible**
Computational requirements

- **Typical problem sizes**
  - Box length $L \sim 5$ fm
  - Lattice spacing $a \sim 0.1$ fm

- **Typical lattice size $> 48^3 \times 96 = \mathcal{O}(10^7)$ sites**
  - Link variables are color matrices $U_\mu(x)$: $3 \times 3$ complex matrix, 1 per 4 directions $\Rightarrow$ 36 complex numbers per grid-point
  - Resulting quark propagators are color-spinors $M^{-1}b$: $3 \times 4$ complex vector $\Rightarrow$ 12 complex numbers per grid-point

  **Data-sets of typically several GBytes per gauge-field configuration**

- **Cost of 1000 gauge configurations at physical quark mass is currently of $\mathcal{O}(10)$ TFlop $\times$ year**
Computational requirements

- One of the most computationally demanding problems on today's supercomputers
  - 4D grid means problem scales with $L^4$ where $L$ the box-length
  - Depending on the quantity under investigation, the required statistics vary from $\mathcal{O}(10^3)$ to $\mathcal{O}(10^6)$

- However it is also an extremely "computer friendly" problem
  - Regular, nearest-neighbor communications allow for perfect scaling
  - Simple, deterministic compute kernels mean code optimization is more effective

- Advances in algorithms and numerical techniques, have opened the way for precision lattice QCD calculations of hadronic matrix elements
Computational requirements

- Precision single-hadron measurements require petaflops sustained resources
Computational requirements

- Precision single-hadron measurements require petaflops sustained resources
- Multi-nucleon physics require escallops sustained
Hadron spectrum

- Hadron masses are computed by calculating an appropriate two-point correlation function
  - An interpolating operator with the quantum numbers of the required hadronic state serves as the trial state, e.g.:
    - A pion interpolating operator: \( \chi^{\pi^+}(x) = \bar{d}(x)\gamma_5 u(x) \)
    - A proton interpolating operator: \( \chi^p(x) = \epsilon^{abc} u^a(x)[u^b(x)\gamma_5 d^c(x)] \)
  - The hadronic two-point correlation function is expressed in terms of quark propagators after the appropriate Wick contractions, e.g. for the \( \pi^+ \):
    \[
    \langle \chi^{\pi^+}(x)\bar{\chi}^{\pi^+}(0) \rangle = \langle \Omega|\gamma_5 G_u(x; 0)\gamma_5 G_d(0; x)|\Omega \rangle
    \]
    where \( G_u \) (\( G_d \)) is the up- (down-) quark propagator:
    \[
    G^{ab}_{\mu\nu}(y; x) = q^a_\mu(y)\bar{q}^b_\nu(x), \quad q = u, d
    \]
Hadron spectrum

- Hadron masses are computed by calculating an appropriate two-point correlation function
  - The quark propagator is computed as the inverse of the descretized Dirac matrix
    - It is computationally unfeasible to compute the complete inverse (from all elements to all elements) due to computational cost as well as storage requirements
  - Rather, the propagator multiplying an appropriately defined spinor is computed:
    $$ G(y; x) = \sum_{x'} M^{-1}(y; x') b_x(x'), $$
    where $b$ the source vector
    - E.g. when $b_x(x') = \delta(x - x')$ (a point source) then $G$ is a column of the propagator (a point-to-all lattice-sites propagator)
  - The lattice Dirac matrix obeys $\gamma_5$-hermiticity allowing the reversal of the propagator coordinates without extra inversions, e.g.:
    - For Wilson: $G_q(y; x) = \gamma_5 G_q^\dagger(x; y)\gamma_5$
    - For Twisted Mass: $G_u(y; x) = \gamma_5 G_d^\dagger(x; y)\gamma_5$
Hadron spectrum

- Hadron masses are computed by calculating an appropriate two-point correlation function

\[
\langle \chi^{\pi^+}(x) \bar{\chi}^{\pi^+}(0) \rangle = \langle \Omega | \chi^{\pi^+} e^{-\hat{H}t} e^{i\vec{p}\vec{x}} \bar{\chi}^{\pi^+} | \Omega \rangle = \sum_{\vec{p}, n} | \langle \Omega | \chi^{\pi^+} | \vec{p}, n \rangle |^2 e^{-E_n(\vec{p})t} e^{i\vec{p}\vec{x}}
\]

after inserting a complete set of states

\[
1 = \sum_{\vec{p}, n} | \vec{p}, n \rangle \langle \vec{p}, n |, \quad \hat{H} | \vec{p}, n \rangle = E_n(\vec{p}) | \vec{p}, n \rangle
\]
Hadron spectrum

- Hadron masses are computed by calculating an appropriate two-point correlation function

  At large time separations, the smallest energy exponential dominates, such that the ground state mass can be extracted

  \[
  \langle \chi^{\pi^+}(x) \bar{\chi}^{\pi^+}(0) \rangle \xrightarrow{t \gg} \sum_{\vec{p}} |\langle \Omega | \chi^{\pi^+} | \pi^+ (\vec{p}) \rangle|^2 e^{-E(\vec{p})t} e^{i\vec{p} \cdot \vec{x}}
  \]

- Project to any momentum via a discreet Fourier Transform

  \[
  \sum_{\vec{x}} e^{-i\vec{q} \cdot \vec{x}} \langle \chi^{\pi^+}(x) \bar{\chi}^{\pi^+}(0) \rangle \xrightarrow{t \gg} |\langle \Omega | \chi^{\pi^+} | \pi^+ (\vec{q}) \rangle|^2 e^{-E(\vec{q})t} e^{i\vec{q} \cdot \vec{x}}
  \]
Hadron spectrum

- Nucleon and pion two-point correlation functions

- Signal drops exponentially with mass while statistical errors constant
- Heavier hadrons get "lost in noise" at smaller time-separations
- Effective mass: \( a m_{\text{eff}}(t) = \frac{1}{2} \log\left[\frac{C(t-1)}{C(t+1)}\right] \) becomes constant when ground state dominates (plateau region)
Hadron spectrum

- **Setting the scale**
  - Obtaining masses in physical units requires *setting the scale*, i.e. determining the lattice spacing
  - This can only be done after calculating an observable on the lattice of which the physical value is known
  - Examples of quantities typically used are the pion decay constant $f_\pi$ and the nucleon mass $m_N$

- From eight ensembles of Twisted Mass gauge-field configurations
- Four lattice spacings are let to vary such that the curve passes through the physical point
- Curve is drawn from HB$\chi$PT
Hadron spectrum

- **What about excited states?**
  - As opposed to low-lying states, calculation of excited states remains a challenge in lattice QCD.
  - This is usually done using a variational method where different interpolating fields are used as a basis.
  - A Generalized Eigenvalue Problem (GEVP) is then solved:

\[
C(t)\nu_n(t, t_0) = \lambda_n(t, t_0)C(t_0)\nu_n(t, t_0), \quad n = 1, \ldots, N, \quad t > t_0
\]

where \(C\) is now an \(N \times N\) matrix of two-point correlation functions.

- The effective energy of the \(n^{th}\) state is given by the \(n^{th}\) eigenvalue \(\lambda_n\):

\[
E_n = \lim_{t \to \infty} -\partial_t \log \lambda_n(t, t_0)
\]
Hadron spectrum

- **What about excited states?**
  - A basis of initial/final states can also be built-up by *smearing* the source vectors
  - Gauge-invariant Gaussian smearing of the quark sources
    
    \[ q^{sm} = (1 + \alpha H)^{ns} q \]
    
    with:
    
    \[ H(\vec{x}, \vec{y}; U) = \sum_{i=1}^{3} \left[ U_i(\vec{x}, t) \delta_{\vec{x}, \vec{y} - a\hat{i}} + U_{-i}(\vec{x}, t) \delta_{\vec{x}, \vec{y} + a\hat{i}} \right] \]
    
    allows for the creation of Gaussian sources with different widths, altering the overlap of the trial state with the physical state.
Hadron spectrum

- What about excited states?
  - An example for the nucleon

  ![Graph showing the hadron spectrum with excited states]

  - Increased statistical noise for higher states
  - Identification of multi-particle states non-trivial
    - Multiple volumes are required to identify between resonance states and multi-particle states
Hadron matrix elements

- Hadron matrix elements require the calculation of an appropriate three-point function

\[ \langle H | J | H' \rangle \rightarrow \langle \chi_H(x_2) | J(x_1) | \bar{\chi}_{H'}(0) \rangle \]

- Access to
  - Charge radii, magnetic moments, axial charges
  - Form factors
  - Parton properties (momentum fraction, spin fraction)
  - Access to new physics (coupling to scalars)
  - Decay widths
Hadron matrix elements

Of interest is the matrix element at a given momentum transfer

The sink and insertion positions are Fourier transformed

\[
\langle H'(\vec{p}') | J(\vec{q}) | H(\vec{p}) \rangle \propto \sum_{\vec{x}_1, \vec{x}_2} \Gamma_{\beta\alpha} \langle \chi_H^\alpha(x_2) | J(x_1) | \bar{\chi}_{H'}^\beta(0) \rangle e^{ix_1\vec{q}} e^{-ix_2\vec{p}'}
\]

with \( \vec{p}' \) the momentum of the final state, \( \vec{q} \) the momentum of the current insertion and \( \vec{p} = \vec{p}' - \vec{q} \) the initial state momentum from momentum conservation
Hadron matrix elements

Expanding in terms of quark propagators:

\[
\sum_{x_1,x_2} \text{Tr} \left[ G(x_2; x_1) \mathcal{O}^I G(x_1; 0)[...G(x_2; 0)...] \right], \quad \text{with } J(x) = \bar{q}(x) \mathcal{O}^I q(x)
\]

- \(G(x_2; x_1)\) is being summed on both ends ⇒ requires knowledge of the all-to-all propagator
Hadron matrix elements

- **Sequential (or extended) propagator techniques**
  - Observe that during an inversion, the propagator is being summed over one coordinate
    \[
    G(y; x) = \sum_{x'} M^{-1}(y; x') b_x(x')
    \]
  - By defining an appropriate source: \( b_{\vec{q}, 0}(\vec{x}, t) = \mathcal{O}^J G(x; 0) e^{i\vec{x}\vec{q}} \delta_{t, t_1} \) with support only on \( t_1 \), the inversion yields the quark-line with the insertion current in:
    \[
    F(\mathcal{O}^J; \vec{q}; x_2; 0) \equiv \sum_x M^{-1}(x_2; x) b_{\vec{q}, 0}(x) = \sum_{\vec{x}_1} G(x_2; x_1) \mathcal{O}^J G(x_1; 0)
    \]
  - So-called **sequential inversion through insertion** or **fixed insertion** method
Hadron matrix elements

- Fixed insertion
  - Fix insertion current momentum
  - Fix insertion current time
  - Free final state
  - Free final state time

- Fixed sink
  - Fix final state
  - Fix final state time
  - Free insertion current momentum
  - Free insertion current time

- Choice depends on the problem at hand
Hadron matrix elements

- **Hadronic level**
  - After inserting two sets of energy/momentum states:
    \[
    \sum_{\vec{x}_1,\vec{x}_2} \langle \chi^\alpha_H(\vec{x}_2) | J(\vec{x}_1) | \bar{\chi}^\beta_{H'}(0) \rangle e^{i\vec{x}_1 \vec{q}} e^{-i\vec{x}_2 \vec{p}'} = \\
    \sum_{n,n'} \langle \chi_H | \vec{p}', n' \rangle \langle \vec{p}, n | \bar{\chi}^\beta_{H'} \rangle e^{-(t_2-t_1)E_{n'}(\vec{p}')} e^{-t_1 E_n(\vec{p})} \langle \vec{p}', n' | J | \vec{p}, n \rangle
    \]
  - Need to take large time separations for ground state domination
    \[
    \frac{t_2-t_1}{t_1} \gg \langle \chi_H | H(\vec{p}') \rangle \langle H' (\vec{p}) | \bar{\chi}^\beta_{H'} \rangle e^{-(t_2-t_1)E_{H}(\vec{p}')} e^{-t_1 E_{H'} (\vec{p})} \langle H(\vec{p}') | J | H' (\vec{p}) \rangle
    \]
Hadron matrix elements

- **Hadronic level**

\[
\langle \chi_H | H(p') \rangle \langle H'(|p|) | \chi_{H'} \rangle e^{-(t_2-t_1)E_H(p')} e^{-t_1E_{H'}(p')} \langle H(p') | J | H'(p) \rangle
\]

- Cancel unknown overlaps and exponentials need to isolate matrix element
- Use two-point functions, optimally with as short separations as possible
- Optimum ratio:

\[
\frac{C^{HJH'}(p, p'; t_2, t_1)}{C^{HH}(t_2, p')} \sqrt{\frac{C^{H'H'}(t_2-t_1, p)C^{HH}(t_1, p')C^{HH}(t_2, p')}{C^{HH}(t_2-t_1, p')C^{H'H'}(t_1, p)C^{H'H'}(t, p)}}
\]

\[
\frac{t_2-t_1 \gg 1}{t_1 \gg 1} \Rightarrow \Pi(p, p'; J) \propto \langle H(p') | J | H'(p) \rangle
\]

Plateau region
Hadron matrix elements

- **Example: the momentum fraction**

  - Fixed sink method: new inversion for every $t_s$
  - Vary $t_{\text{ins}}$ for plateau identification
  - $a \simeq 0.087$ fm, plateau around 1.2 fm
  - Lattice matrix elements need to be renormalized
    - Renormalization constants typically evaluated in separate calculations
    - Various methods for calculation (perturbative, non-perturbative)
Hadron matrix elements

- Nucleon electromagnetic form factors

- Various sources for Electric and Magnetic form factors
- Current calculations are running at physical $m_\pi$
- Discreet values of momentum transfer
- No direct calculation of magnetic FF at $Q^2 = 0$
Hadron matrix elements

- **Disconnected diagrams**

  \[ \mathcal{C}^{2pt}(x_2) \text{Tr}[G(x_1; x_1) \mathcal{O}^I] \]

- Fermion quark loops arise as contributions to three-point functions
- Sum over diagonal of a all-to-all propagator
- In certain cases they can be omitted based on symmetry
  - E.g. in isovector current combinations: \( \bar{u}\mathcal{O}^I u - \bar{d}\mathcal{O}^I d \) they cancel assuming degenerate \( u \)- and \( d \)-quarks
- In other cases they are the only contributions
  - E.g. strange-quark content of a nucleon where no connected contributions arise
Hadron matrix elements

- **Disconnected diagrams**

\[
C^{2\text{pt}}(x_2) \text{Tr}[G(x_1; x_1) \mathcal{O}^I]
\]

- Crucial for evaluating key hadronic quantities, e.g.:
  - Individual quark spin contributions to nucleon spin
  - Individual quark angular momentum contributions to nucleon spin
  - Individual proton and neutron form factors

- Very challenging to evaluate; have only lately started to be included in lattice QCD calculations
Hadron matrix elements

- **Disconnected diagrams**
  \[ \chi_{H'}(\bar{x}_2, t_2) \xrightarrow{J(\bar{x}_1, t_1)} \chi_{H}(\bar{0}, 0) \]

- **Hopping parameter expansion**
  - Another way is to expand the inverse around the inverse quark mass
    \[ M \propto (1 - \kappa H) \Rightarrow M^{-1} \propto 1 + \kappa H + \kappa^2 H^2 + \ldots \]
    where \( \kappa \) is a proxy for the bare quark mass \( \kappa = 1/(8 + 2am) \)
  - In the sum over diagonal elements only even powers of the hopping term contribute
  - Usually used in combination with stochastic method

\[ C^{2\text{pt}}(x_2) \text{Tr}[G(x_1; x_1) \mathcal{O}^I] \]
Hadron matrix elements

- **Disconnected diagrams**

\[
\begin{array}{c}
\chi_{H}(\vec{x}_{2}, t_{2}) \\
J(\vec{x}_{1}, t_{1}) \\
\chi_{H}(\vec{0}, 0)
\end{array}
\]

\[
C^{2pt}(\chi_{2}) \text{Tr}[G(\chi_{1}; \chi_{1}) \mathcal{O}^{J}]
\]

- **Stochastic evaluation**

  - Define a set of \( N_{r} \) source vectors \( \eta^{a}_{\mu}(x)_{r} \) which obey:

  \[
  \langle \eta^{a}_{\mu}(x) \eta^{b}_{\nu}(y) \rangle_{r} = \delta_{ab} \delta_{\mu\nu} \delta(x-y) + \mathcal{O}(1/\sqrt{N_{r}}) \quad \text{and} \quad \langle \eta^{a}_{\mu}(x) \rangle_{r} = \mathcal{O}(1/\sqrt{N_{r}})
  \]

  - A stochastic estimate of the all to all can be evaluated via:

  \[
  G^{ab}_{\mu\nu}(y; x) = \langle \phi^{a}_{\mu}(y) \eta^{b\dagger}_{\nu}(x) \rangle_{r} + \mathcal{O}(\frac{1}{N_{r}}) \quad \text{with} \quad \phi^{a}_{\mu}(y) = \sum_{x'} (M^{-1})^{ab'}_{\mu\nu'}(y; x') \eta^{b'}_{\nu'}(x')
  \]
Hadron matrix elements

- **Disconnected diagrams**

\[ C^{2pt}(x_2) \text{Tr}[G(x_1; x_1)O^J] \]

- **Stochastic evaluation**
  - Notoriously difficult to evaluate due to increased computational cost
  - \( N_r \) strongly depends on matrix element under study
  - Furthermore, statistical errors are usually large for disconnected quark loops
  - Need at least \( \mathcal{O}(10^4) \) measurements as opposed to \( \mathcal{O}(10^3) \) for connected
Hadron matrix elements

- An example: the nucleon axial charge $g_A$ (isoscalar)

- Connected diagram

- Disconnected diagram

- 1,200 statistics
- $\sim$3% relative error

- 150,000 statistics
- $\sim$13% relative error
Hadron matrix elements

- An example: quark intrinsic spin contributions to the nucleon

![Graph](image)

- Pion mass dependence of quark contributions to nucleon spin
- Linear combinations of isovector and isoscalar
- Disconnected fermion loops included in one measurement
Advanced methods for hadron matrix elements
Deflating the lattice Dirac Matrix

- It is common to require multiple inversions for the same gauge-field configuration
  - Propagators are computed as point-to-all
  - Better use of lattice gauge configurations can be used by computing multiple two- or three-point functions from different positions
  - Knowledge of the eigenvalues of the Dirac matrix can accelerate propagator calculations on the same configuration
  - These techniques are known as deflation
Deflating the lattice Dirac Matrix

- **Approximate deflation**
  - Iterative methods for the solution of $Mx = b$ require an initial guess $x_0$ and iterate for $x$ such that the residual $r = Mx - b$ reaches the desired threshold.
  - The number of iterations is a power of the ratio of largest to smallest eigenvalue.
  - With knowledge of approximate eigenvectors of the smallest eigenvalues of $M$, form a guess for the initial vector $x_0 = Vd$
    - $V = (v_1, v_2, ... v_n)$ the matrix of eigenvectors
    - $d = (V^\dagger MV)^{-1}V^\dagger b$
  - Projects-out the smallest eigenvalues, reducing the number of iterations required to solution.
Deflating the lattice Dirac Matrix

- **Incremental deflation**
  - Incrementally construct $V$ during the solver iteration
  - Most efficient when large number of inversions per configuration are required

- Improvement of $\times 3$ in computer time
Summation method

- In matrix element calculations, it is important to ensure excited state effects are under control
  - In either fixed-sink or fixed insertion methods, one source-sink separation is fixed
  - For multiple source-sink separations with the fixed-sink method, all data can be combined via the summation method
**Summation method**

- **Excited state effects in three-point functions**
  - After optimum ratio has been taken

\[
R(t_2; t_1) = \mathcal{M}[1 + e^{-\Delta(\vec{p})t_1} + e^{-\Delta(\vec{p}')(t_2-t_1)} + \ldots]
\]

- $\mathcal{M}$ ground state matrix element of interest
- $\Delta(\vec{p}) = E_1(\vec{p}) - E_0(\vec{p})$

- Sum over insertion

\[
\sum_{t_1} R(t_2; t_1) = \text{Const.} + \mathcal{M}[t_2 + \mathcal{O}(e^{-\Delta(\vec{p})t_2}) + \mathcal{O}(e^{-\Delta(\vec{p}')t_2}) + \ldots]
\]

- Elimination of powers of $t_1 \Rightarrow$ larger suppression of excited states
Summation method

- **Example of matrix element with large excited state contamination:** Nucleon $\sigma$-term (connected)

- Check for agreement between summation method and plateau
- Calculation of multiple source-sink separations can be accelerated with deflation
Mixed precision techniques

- Accuracy to which propagator is required is dependant on matrix element
  - Define an approximate correlation function which fluctuates closely with exact
    \[ r = \text{Corr}[C^{\text{appx}}(t), C(t)] \]
  - Then define transformations \( g \) on correlation function which are statistically equivalent, e.g. changing the position of the source
  - Approximation can be relaxed solver precision
  - Improved estimator:
    \[ C^{\text{imp}}(t) = C(t) - C^{\text{appx}}(t) + \frac{1}{N_g} \sum_g C_g^{\text{appx}}(t) \]
  - Error scales with \( N_g \):
    \[ \sqrt{2(1 - r)} + \frac{1}{N_g} \text{ assuming } r \approx 1 \]
**Mixed precision techniques**

- **Covariant approximation averaging**
  - Need a small number $\mathcal{O}(1)$ high-precision (HP) correlators
  - Need to choose low-precision (LP) such that
    - LP correlators are precise enough to correlate strongly with HP ($r \approx 1$)
    - LP correlator precision is relaxed enough to be much cheaper than HP
  - Nucleon two-point correlation function
  - Correlation between LP and HP largest at smaller time-separations
  - Can use deflation to speed up further inversion of consecutive LP propagators on same gauge-field configuration
Mixed precision techniques

- Covariant approximation averaging

- Test for statistical error on nucleon effective mass
- LP more than $\times 10$ faster to compute when also using deflation
- Error scales with $1/\sqrt{N_{LP}}$
Conclusions and summary

- Low-lying hadron masses at the percent level

- Milestone calculation in lattice QCD

- Confirmation of hadron masses from (lattice) QCD

  BMW collaboration, Science 322 (2008)
Conclusions and summary

- Hadron matrix elements: new era for lattice QCD

- New simulations at the physical quark mass
- New methods for efficient increase of statistical accuracy
- Techniques for assessing excited state effects and disconnected diagrams
Thank you, questions?