Lattice QCD

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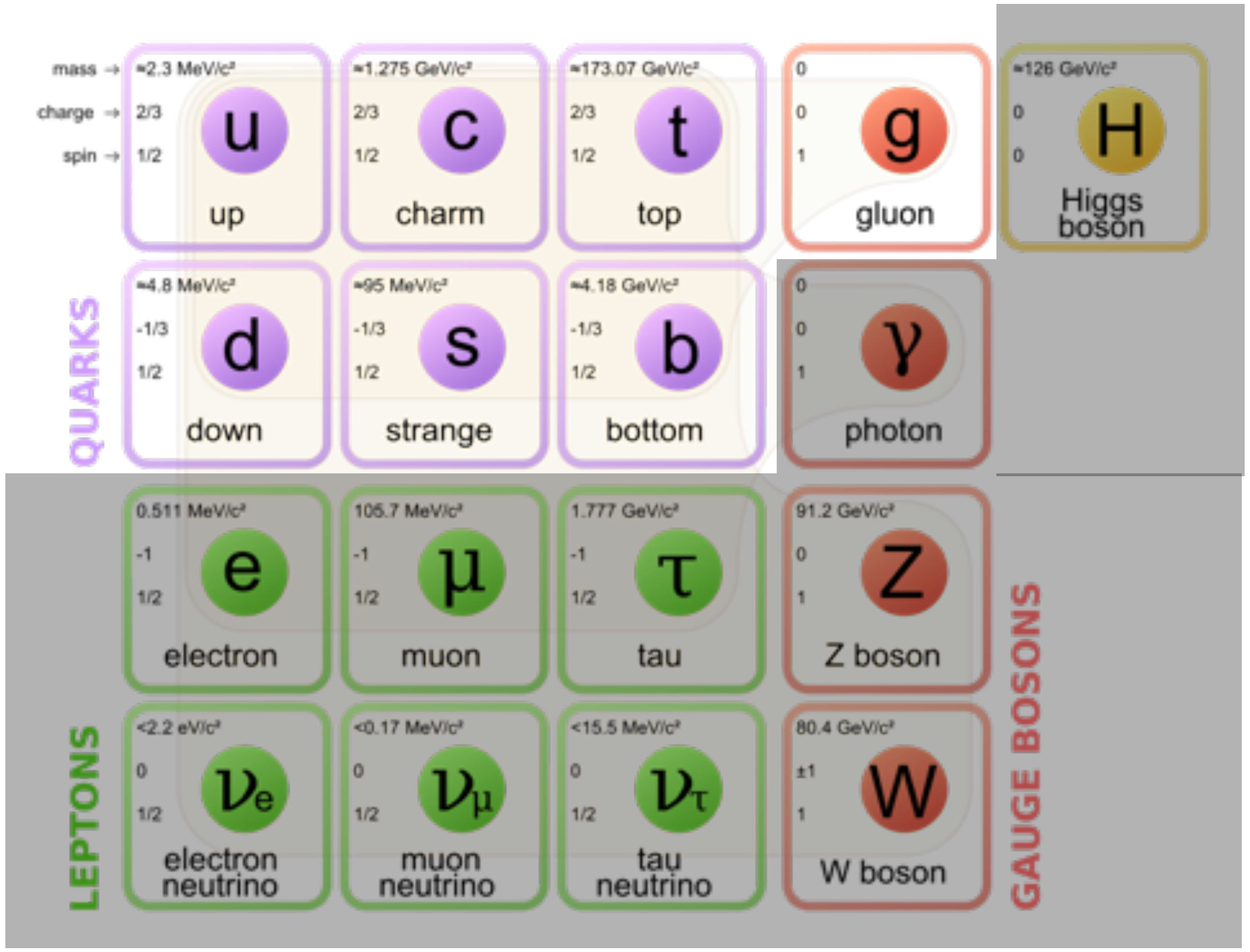
Outline

- Basic formalism — QCD on a space-time lattice
- Numerical computation — hardware, algorithms and analysis
- From lattice to physics — results and challenges

Basic formalism

Quantum chromodynamics

The Standard Model



http://en.wikipedia.org/wiki/Standard_Model

Lagrangian

$$\mathcal{L}_{QCD} = -\frac{1}{2g^2}\mathrm{Tr}F_{\mu\nu}F^{\mu\nu} + \bar{q}(i\gamma_\mu D_\mu - m)q$$

$$D_\mu = \partial_\mu + iA_\mu \qquad A_\mu = \sum_{a=1}^{N_c^2-1} T_\mu^a A_\mu^a \qquad m = \mathrm{diag}(m_u, m_d, m_s, \cdots)$$

$$F_{\mu\nu} = -i[D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu + i[A_\mu, A_\nu]$$

$$T^a = T^{a\dagger} \qquad [T^a, T^b] = if^{abc}T^c \qquad \mathrm{Tr}\left(T^a T^b\right) = \frac{1}{2}\delta_{ab}$$

- Lagrangian consists of 1+N_f free parameters:
  - bare coupling (g), bare quark masses (m_f)
  - once fixed, theory completely predictive

Lagrangian

$$\mathcal{L}_{QCD} = -\frac{1}{2g^2}\mathrm{Tr}F_{\mu\nu}F^{\mu\nu} + \bar{q}(i\gamma_\mu D_\mu - m)q$$

$$D_\mu = \partial_\mu + iA_\mu \qquad A_\mu = \sum_{a=1}^{N_c^2-1} T^a_\mu A^a_\mu \qquad m = \mathrm{diag}(m_u, m_d, m_s, \cdots)$$

$$F_{\mu\nu} = -i[D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu + i[A_\mu, A_\nu]$$

$$T^a = T^{a\dagger} \qquad [T^a, T^b] = if^{abc}T^c \qquad \mathrm{Tr}\left(T^aT^b\right) = \frac{1}{2}\delta_{ab}$$

$$q(x) \to \Omega(x)q(x) \qquad \Omega(x) \in SU(N_c)$$

$$A_\mu(x) \to \Omega(x)A_\mu(x)\Omega^\dagger(x) - i\Omega(x)\partial_\mu(x)\Omega^\dagger(x) \qquad D_\mu q(x) \to \Omega(x)D_\mu q(x)$$

Important properties

- **Chiral symmetry:** classical level, massless quark limit

$$U(N_f)_L \times U(N_f)_R \supset SU(N_f)_V \times U(1)_B \times U(1)_A$$

- **Anomalous U(1)$_A$:** at quantum level; important consequences for lattice discretization of fermions

- **Chiral symmetry breaking:**
  - $SU(N_f)_L \times SU(N_f)_R \times U(1)_B \to SU(N_f)_V \times U(1)_B$
  - pseudoscalar meson octet are pseudo-Goldstone bosons; ninth pseudoscalar meson is not
  - quark masses explicitly break chiral symmetry:

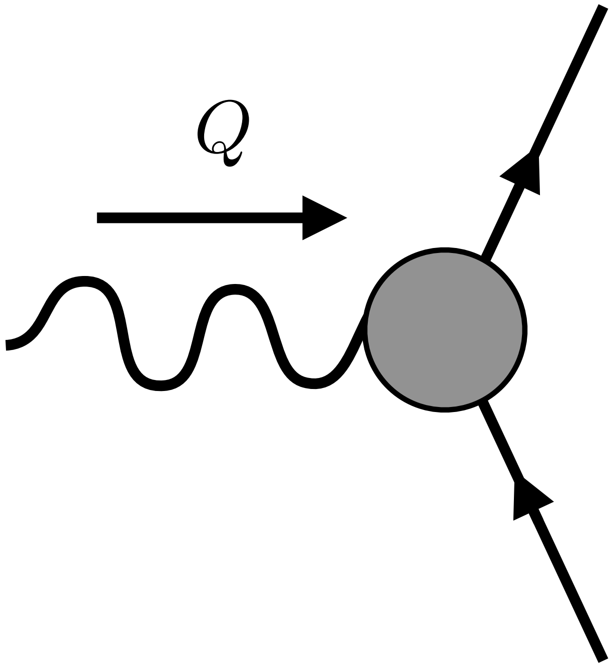
$$m_\pi^2 \propto (m_u + m_d) \qquad m_K^2 \propto (m_{u,d} + m_s) \qquad m_{\eta'} \sim \Lambda_{QCD}$$

Important properties

- **Asymptotic freedom:** strength of interaction decreases with increasing momentum transfer Q between quarks; conversely, at low energies, perturbation theory becomes unreliable

$$\alpha_s(Q) = \frac{\bar{g}^2(Q)}{4\pi} \approx \frac{1}{\beta_0 \ln(Q^2/\Lambda^2)}$$

D. Gross, D. Politzer, F. Wilczek



- **Confinement:** low-energy degrees of freedom are different from fundamental degrees of freedom

Lattice regularization

- Nonperturbative phenomena require a nonperturbative treatment (e.g., chiral symmetry breaking, confinement)
- Lattice regularization:
  - offers a gauge-invariant nonperturbative framework
  - is ideally suited for numerical simulation
  - typically defined in Euclidean space-time
  - powerful tool, yet has some fundamental limitations:
    - connecting Euclidean space observables to physics
    - numerical: sign problems, signal/noise

Lagrangian in Euclidean space-time

$$\mathcal{L}^E_{QCD} = \frac{1}{2g^2}\mathrm{Tr}F_{\mu\nu}F^{\mu\nu} + \bar{q}(\gamma_\mu D_\mu + m)q$$

$$\gamma_\mu = \gamma_\mu^\dagger = \gamma_\mu^{-1} \qquad \gamma_\mu^2 = 1 \qquad \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$$

$$\gamma_5 = -\gamma_1\gamma_2\gamma_3\gamma_4 \qquad \gamma_5^2 = 1 \qquad \{\gamma_5, \gamma_\mu\} = 0$$

- Gamma matrices are Hermitian
- Continuum Dirac operator: $D(m) = \gamma_\mu D_\mu + m$
  - satisfies γ_5-Hermiticity: $\gamma_5 D(m)\gamma_5 = -D(-m) = D^\dagger(m)$
  - has paired eigenvalues: $\pm i\lambda + m$

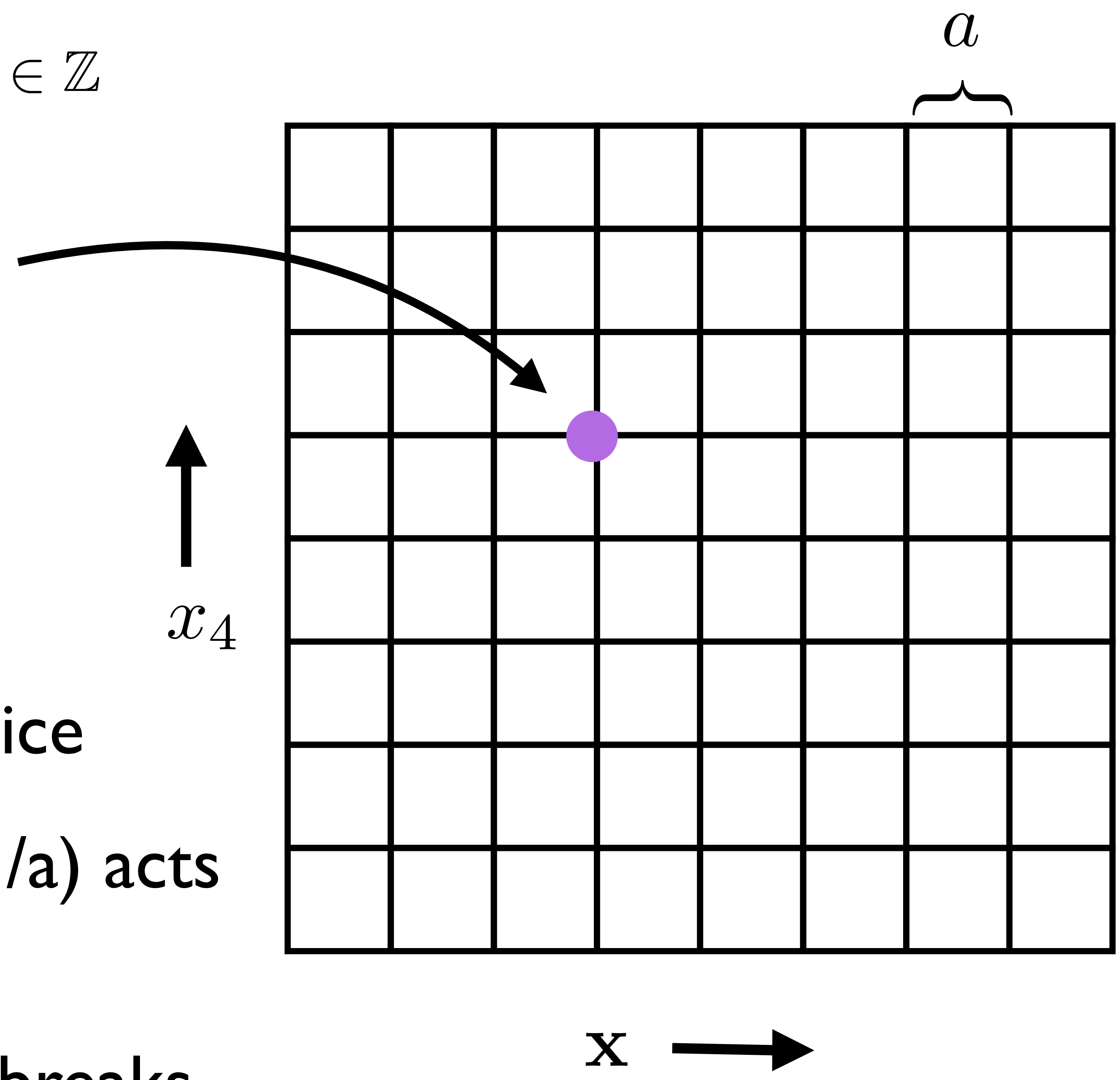
Discretization of space-time

$$x = a\{n_1, n_2, n_3, n_4\} \qquad n_\mu \in \mathbb{Z}$$

$$q(x) = \int_{-\pi/a}^{\pi/a} d^4p\, \tilde{q}(p) e^{ipx}$$

$$\tilde{q}(p) = \sum_x q(x) e^{-ipx}$$

- Usually a hypercubic lattice
- Inverse lattice spacing (1/a) acts as a UV cut-off
- Discretization explicitly breaks Poincare symmetry



Constructing lattice actions — guiding principles

In order to minimize fine-tuning of operators in the quantum theory, lattice discretization should preserve a maximal amount of symmetry

- Preserve gauge invariance
- Preserve maximum number of global symmetries as possible:
    - hypercubic symmetry (discrete rotations, reflections, etc)
    - discrete translational symmetries
    - chiral symmetry? (massless quark limit)

Lattice derivatives

Forward difference operator: $$\partial_\mu q(x) = \frac{1}{a}\left[q(x+ae_\mu) - q(x)\right]$$

Backward difference operator: $$\partial^\star_\mu q(x) = \frac{1}{a}\left[q(x) - q(x-ae_\mu)\right]$$

$$\partial_\mu \to \frac{e^{iap_\mu}-1}{a} \approx ip_\mu\left[1+\mathcal{O}(ap)\right] \qquad \partial^\star_\mu \to \frac{1-e^{-iap_\mu}}{a} \approx ip_\mu\left[1+\mathcal{O}(ap)\right]$$

Symmetric difference operator: $$\frac{1}{2}\left(\partial_\mu + \partial^\star_\mu\right) \to \frac{i}{a}\sin\left(ap_\mu\right) \equiv i\hat{p}_\mu$$

Lattice Laplacian: $$-\partial^\star_\mu\partial_\mu \to \frac{4}{a^2}\sin^2\left(\frac{ap_\mu}{2}\right) \equiv \Delta(p)$$

Naive fermions

Choice of derivative matters: individually, these lead to forward/backward propagation only

$$D_{naive}(m) = \frac{\gamma_\mu}{2}\left(\partial_\mu + \partial^\star_\mu\right) + m \qquad \tilde{D}^{-1}_{naive}(m) = \frac{-i\gamma_\mu \hat{p}_\mu + m}{\hat{p}^2 + m^2}$$

Propagator poles located at:

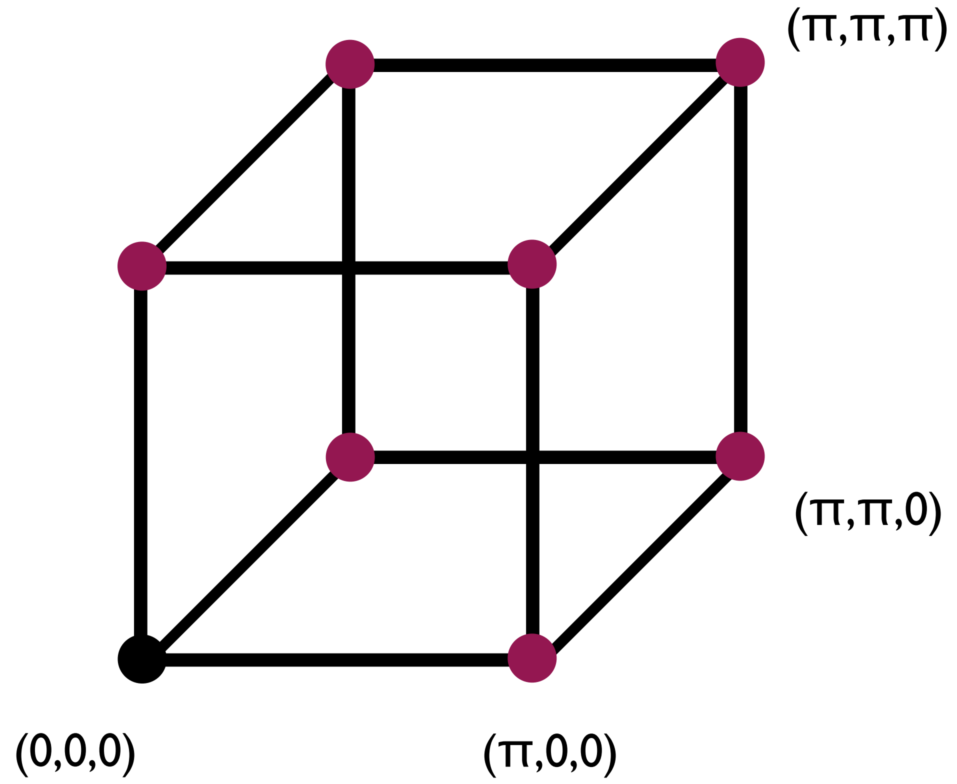
$$\omega = ip_4$$

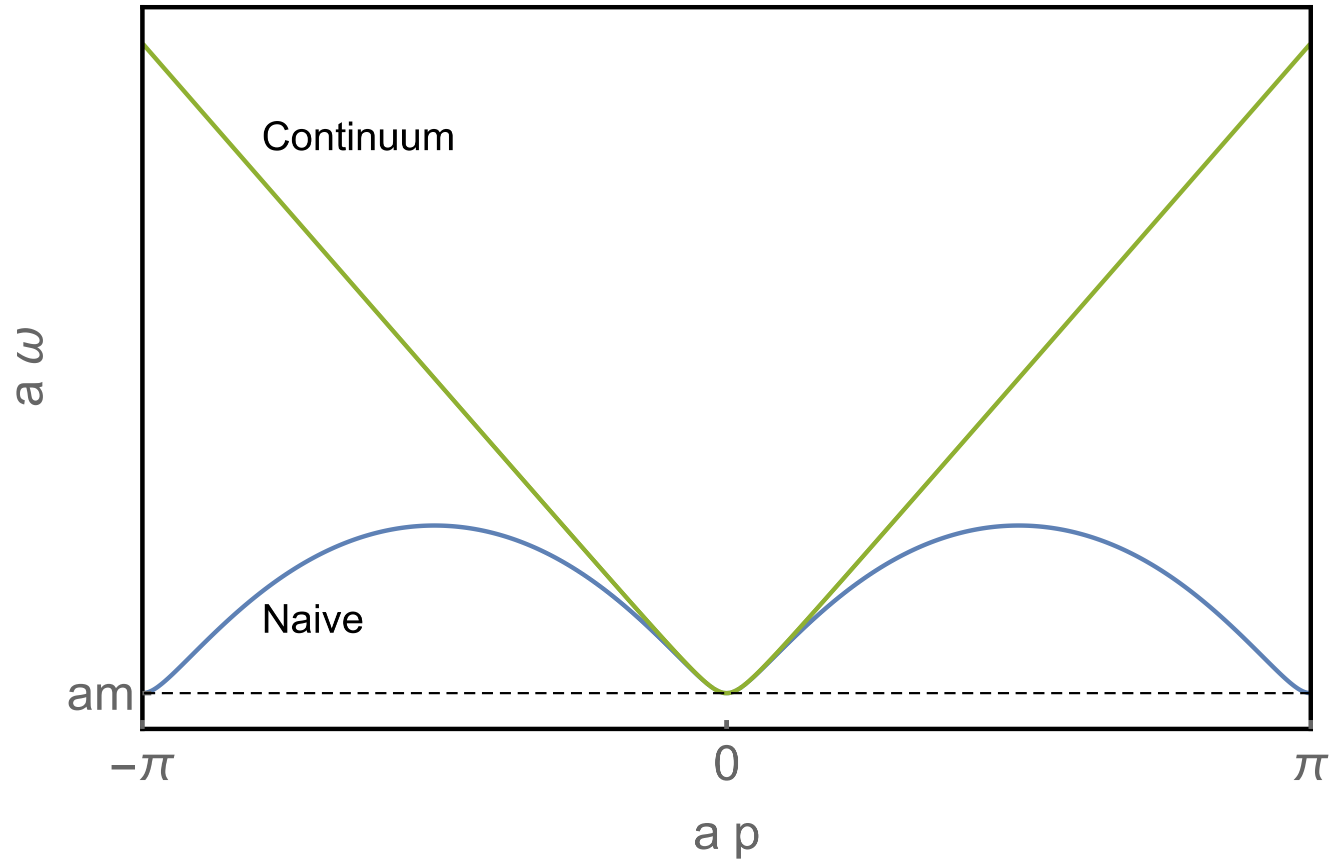
$$\omega(\mathbf{p}) = \frac{1}{a}\sinh^{-1}\sqrt{(a\hat{\mathbf{p}})^2 + (am)^2} \qquad \hat{p}_j = \frac{1}{a}\sin\left(ap_j\right)$$

$$\omega(\mathbf{p}) \to \sqrt{\mathbf{p}^2 + m^2} \qquad a\hat{\mathbf{p}} \to 0$$

Fermion doublers

Brillouin zone:





- Poles in propagator indicate 2^d-1 doubler modes, appearing at each corner of the Brillouin zone
- Doublers represent *physical* degrees of freedom in continuum; too many for QCD….

Nielsen-Ninomiya's no-go theorem

A fermion discretization cannot simultaneously satisfy the following conditions:

1. absence of doubler modes
2. invariance under continuum chiral symmetry
3. locality of the fermion operator D
4. correct continuum limit

Absence of chiral anomaly

- Doubler modes are a fundamental problem — intimately related to chiral symmetry and anomalies in gauge theories
  - lattice gauge theory constructions are finite and therefore must be free of anomalies
  - in a lattice chiral gauge theory, doubler modes are necessary to cancel off anomaly

Nielsen-Ninomiya's no-go theorem

- Must sacrifice one of the no-go theorem conditions — results in a wide variety of fermion actions
- Many fermion actions in use today
  - actions give the same continuum limit, up to flavor content
  - have different advantages/disadvantages in terms of chiral properties, renormalization requirements and computational cost

An abundance of fermion actions…

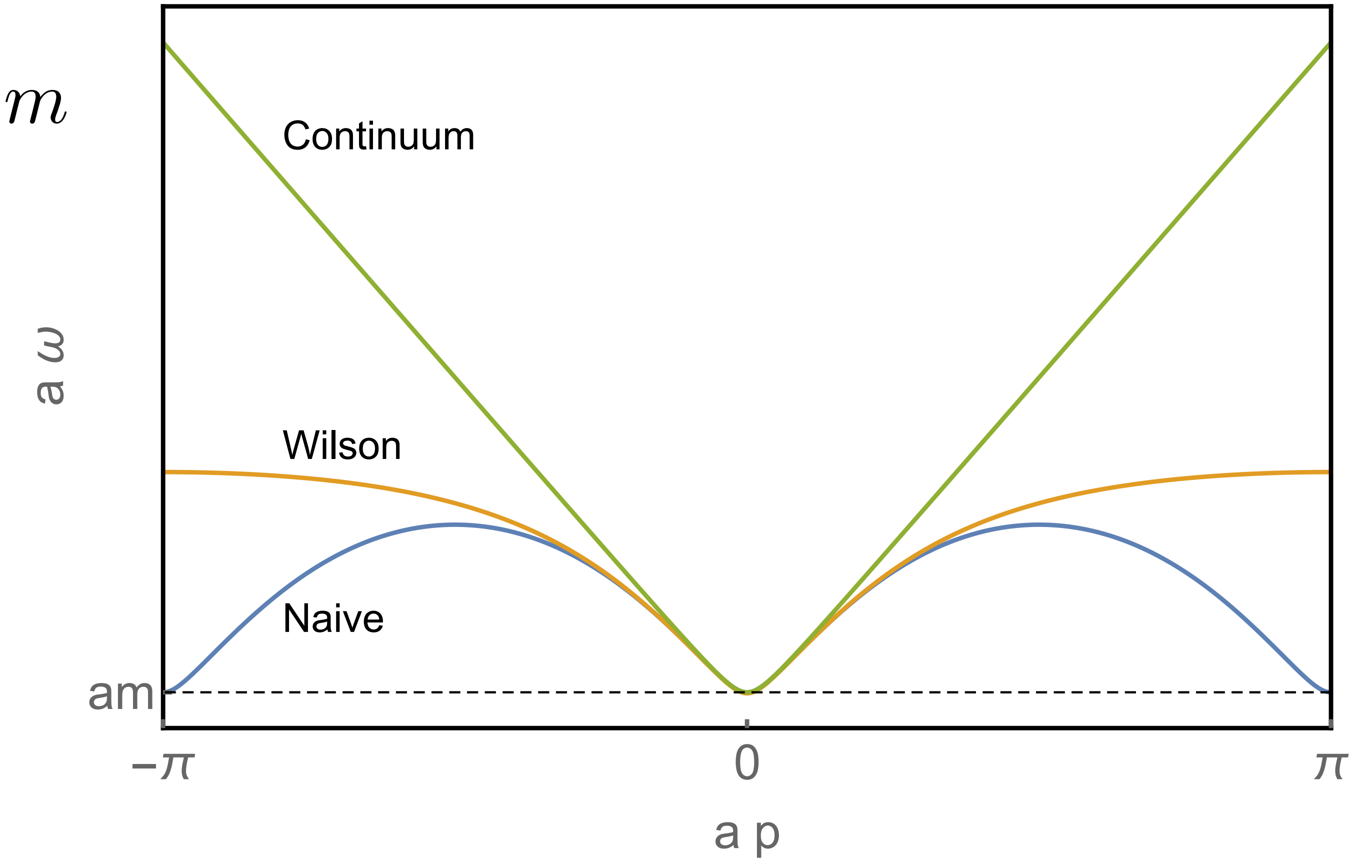
- **Wilson:** breaks chiral symmetry, O(a) lattice artifacts
- **Staggered:** fewer (but nonzero) doubler modes
- **Ginsparg-Wilson (overlap, domain-wall):** breaks continuum chiral symmetry, but preserves a modified chiral symmetry
- **Minimally doubled:** single doubler pole, breaks lattice rotational invariance
- **Many others:** twisted mass, reduced staggered, Dirac-Kaeler

Wilson fermions

$$D_W(m) = \frac{\gamma_\mu}{2}\left(\partial_\mu + \partial_\mu^\star\right) - \frac{a}{2}\partial_\mu^\star\partial_\mu + m$$

$$\tilde{D}_W^{-1}(m) = \frac{-i\gamma_\mu\hat{p}_\mu + M(p)}{\hat{p}^2 + M^2(p)}$$

$$M(p) = m + \frac{a}{2}\Delta(p)$$



- Doubler modes receive a mass ~ 1/a
- Wilson term is irrelevant in continuum limit
- Explicit breaking of chiral symmetry implies additive mass renormalization; additional tuning of operators

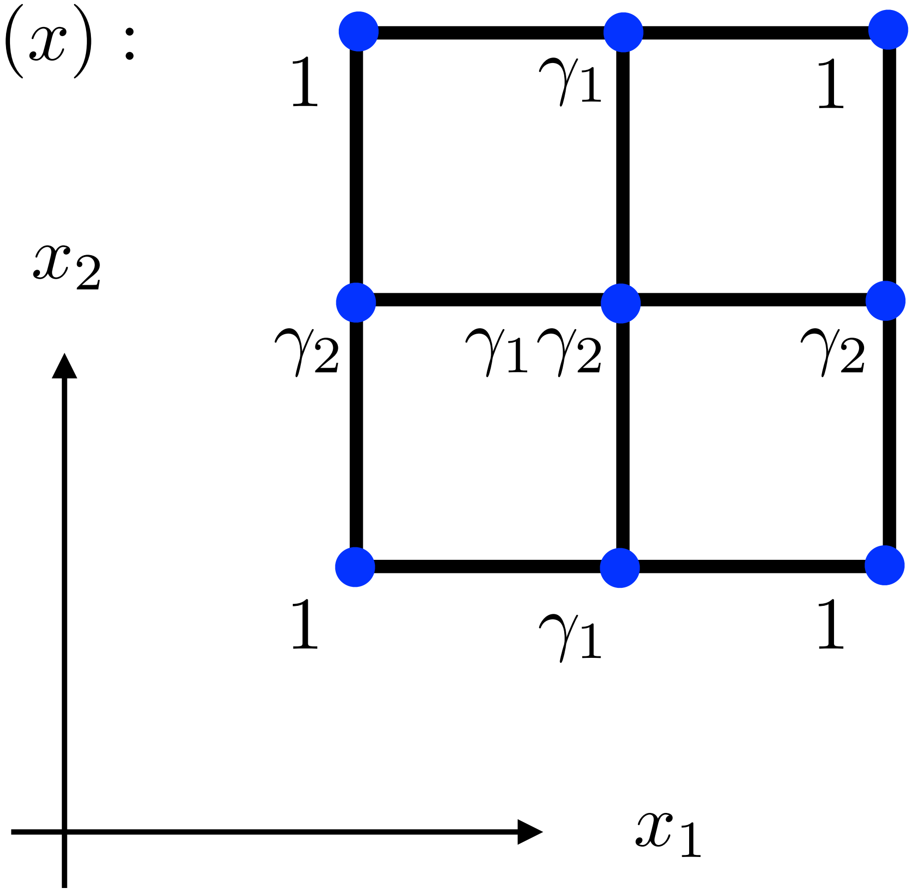
Staggered fermions

$$S(x) = \gamma_1^{x_1/a}\gamma_2^{x_2/a}\gamma_3^{x_3/a}\gamma_4^{x_4/a}$$

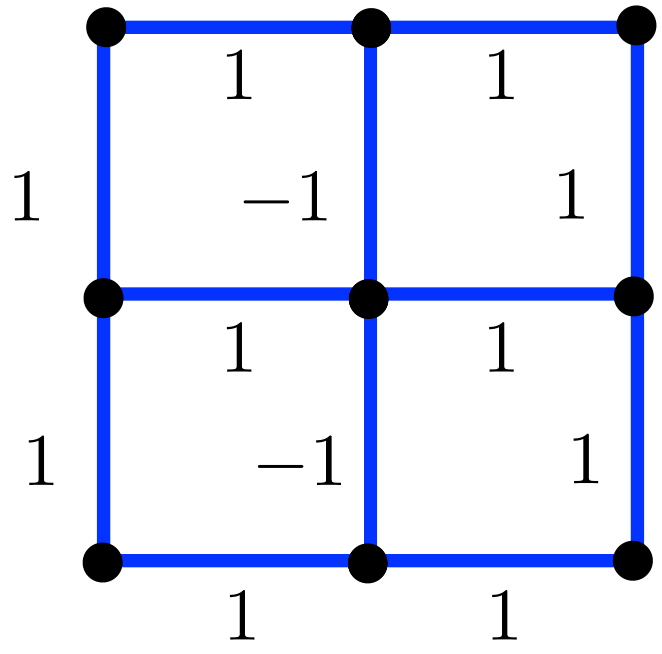
$$(\partial_\mu + \partial_\mu^\star)S = \eta_\mu\gamma_\mu S(\partial_\mu + \partial_\mu^\star)$$

$$\eta_\mu(x) = (-1)^{\sum_{\nu<\mu} x_\nu/a}$$

$S(x)$:



$\eta_\mu(x)$:



Staggered fermions

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$$(\partial_\mu + \partial_\mu^\star)S = \eta_\mu \gamma_\mu S(\partial_\mu + \partial_\mu^\star) \qquad \eta_\mu(x) = (-1)^{\sum_{\nu<\mu} x_\nu/a}$$

$$S^\dagger D_{naive}(m) S = S^\dagger \left[\frac{\gamma_\mu}{2}\left(\partial_\mu + \partial_\mu^\star\right) + m\right] S$$

$$= D_{st}(m) \times 1_{spinor} \qquad D_{st}(m) = \eta_\mu(x)\frac{\partial_\mu + \partial_\mu^\star}{2} + m$$

— 15 doublers reduced to 3 (“tastes”)

— Residual taste non-singlet chiral symmetry at m=0:

$$\eta_5(x) = (-1)^{x_1/a + x_2/a + x_3/a + x_4/a} \qquad \{\eta_5, \eta_\mu\} = 0 \qquad \{\eta_5, D_{st}(0)\} = 0$$

Staggered fermions

- Transformation exposes four-fold degeneracy in naive fermions
- Action defined by taking only one component of the four
- Fermion components are spread over the hypercube
- Computationally inexpensive
- Four remaining degrees of freedom (“tastes”)
- To achieve the proper number of continuum degrees of freedom, requires rooting trick; questions about validity due to non locality of rooted Dirac operator

Ginsparg-Wilson fermions

$$\gamma_5 D + D\gamma_5 = aD\gamma_5 D$$

$S_{GW} = \bar{q}Dq$ invariant under $q \to e^{i\theta\gamma_5(1-aD)}q \qquad \bar{q} \to \bar{q}e^{i\theta\gamma_5}$

Proof:
$$\begin{aligned} e^{-i\gamma_5\theta}De^{-i\gamma_5(1-aD)\theta} &= e^{-i\gamma_5\theta}e^{-iD\gamma_5(1-aD)D^{-1}\theta}D \\ &= e^{-i\gamma_5\theta}e^{-i(D\gamma_5-aD\gamma_5D)D^{-1}\theta}D \\ &= e^{-i\gamma_5\theta}e^{i\gamma_5\theta}D \end{aligned}$$

Manifestation of anomaly:

— symmetry transformation depends explicitly on the gauge field
— integration measure is not invariant under flavor-singlet transformation

Ginsparg-Wilson fermions

$$\gamma_5 D + D\gamma_5 = aD\gamma_5 D$$

$S_{GW} = \bar{q}Dq$ invariant under $q \to e^{i\theta\gamma_5(1-aD)}q$ $\bar{q} \to \bar{q}e^{i\theta\gamma_5}$

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One solution to the G-W relation is the overlap operator:

$$D_{ov} = \frac{1}{a}\left[1 + \frac{D_W(-1/a)}{\sqrt{D_W^\dagger(-1/a)D_W(-1/a)}}\right]$$

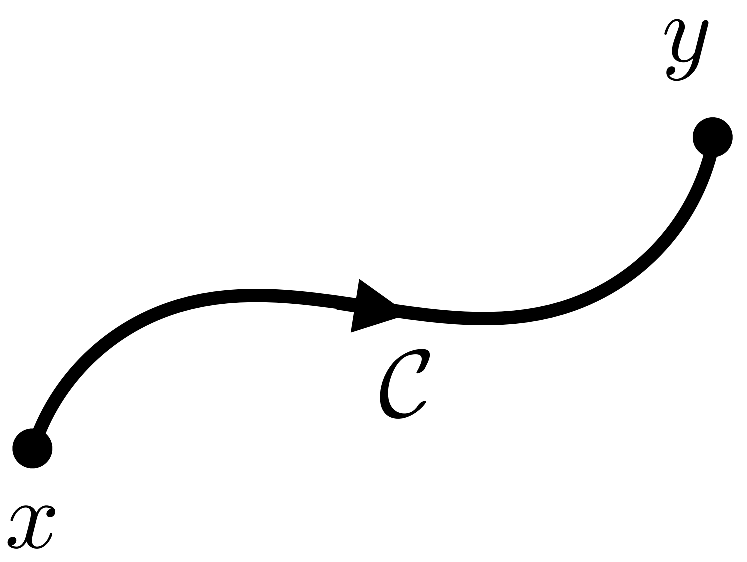
Ginsparg-Wilson fermions

- Continuum chiral symmetry restored in the continuum limit, but violated on the lattice
- Main disadvantage: computationally costly
- Other Dirac operators also satisfy the G-W relation, e.g.,
  - Domain-wall fermions: four-dimensional fermions arise as zero-modes of a five-dimensional theory with a mass defect in the fictitious fifth dimension of extent L_5
  - Overlap fermions are equivalent to domain-wall fermions in the limit of infinite L_5

Parallel transport

Wilson line:

$$L_{\mathcal{C}}(x,y) = \mathcal{P} e^{i\int_{\mathcal{C}_{x\to y}} dz_\mu A_\mu(z)}$$



Under a gauge transformation:

$$L_{\mathcal{C}}(x,y) \to \Omega(x) L_{\mathcal{C}}(x,y) \Omega^\dagger(y) \qquad \mathrm{Tr} L_{\mathcal{C}}(x,x) \to \mathrm{Tr} L_{\mathcal{C}}(x,x)$$

Parallel transport:

$L_{\mathcal{C}}(x,y) q(y)$ transforms like $q(x)$

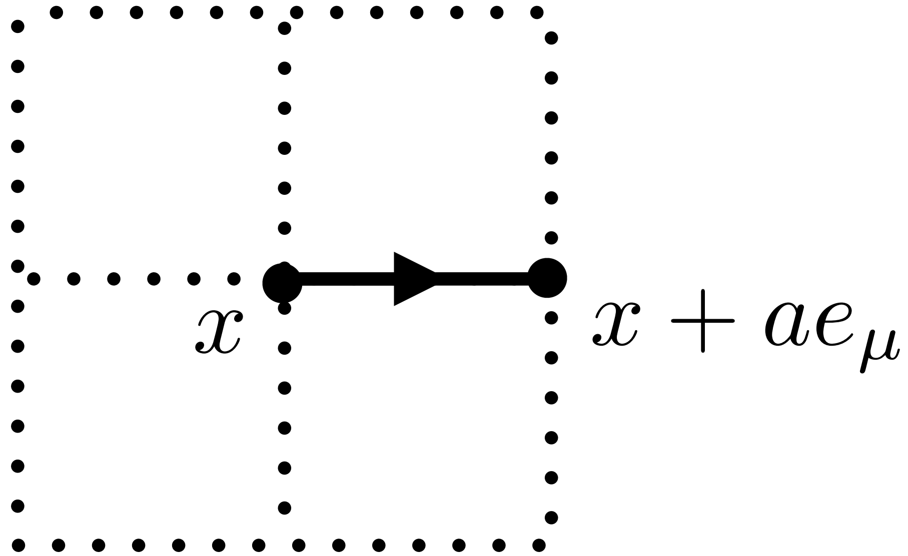
Gauge fields defined on the lattice

Introduce gauge link variables on the lattice:

$$U_\mu(x) = e^{iaA_\mu(x)} \approx L(x, x + ae_\mu) + \mathcal{O}(a)$$

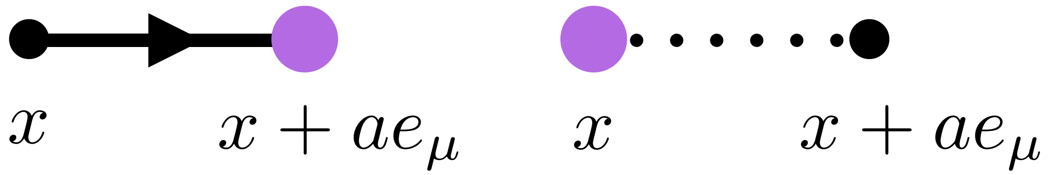
Under a gauge transformation:

$$U_\mu(x) \to \Omega(x) U_\mu(x) \Omega^\dagger(x + ae_\mu)$$



Covariant lattice derivatives

$$\nabla_\mu q(x) = \frac{1}{a}\left[U_\mu(x) q(x+ae_\mu) - q(x)\right] \qquad \nabla_\mu q(x) \to \Omega(x) \nabla_\mu q(x)$$



$$\nabla^\star_\mu q(x) = \frac{1}{a}\left[q(x) - U^\dagger_\mu(x-ae_\mu) q(x-ae_\mu)\right] \qquad \nabla^\star_\mu q(x) \to \Omega(x) \nabla^\star_\mu q(x)$$

$$\frac{1}{2}\left(\nabla_\mu + \nabla^\star_\mu\right) \approx D_\mu + \mathcal{O}(a^2) \qquad -\nabla^\star_\mu \nabla_\mu \approx -D_\mu D_\mu + \mathcal{O}(a^2)$$

Gauge-invariant fermion actions

Gauge-invariant fermion actions are defined by:

$$S_F[U,\bar{q},q] = a^4 \sum_x \bar{q} D[U] q \qquad D = D_{naive}, D_W, D_{st}, D_{ov}, \cdots$$

with the simple replacement:

$$\partial_\mu \to \nabla_\mu \qquad \partial^\star_\mu \to \nabla_\mu$$

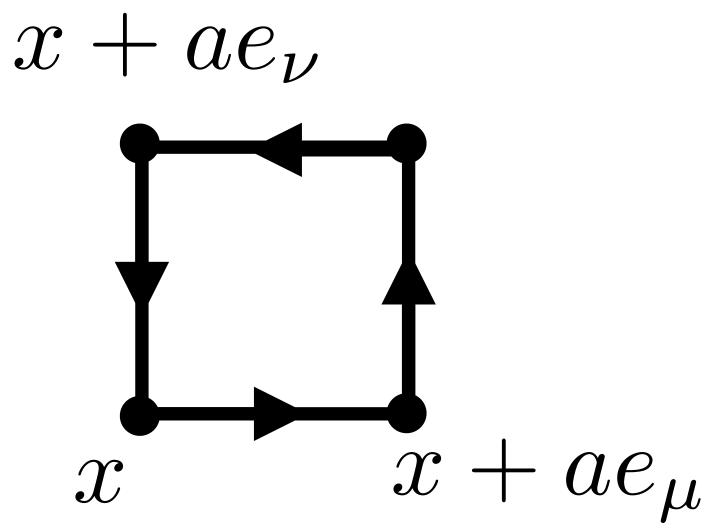
Example: Wilson gauge action

$$D_W(m) = \frac{1}{2}\gamma_\mu \left(\nabla_\mu + \nabla^*_\mu\right) - \frac{a}{2}\nabla^*_\mu \nabla_\mu + m$$

Plaquettes, rectangles, and the likes

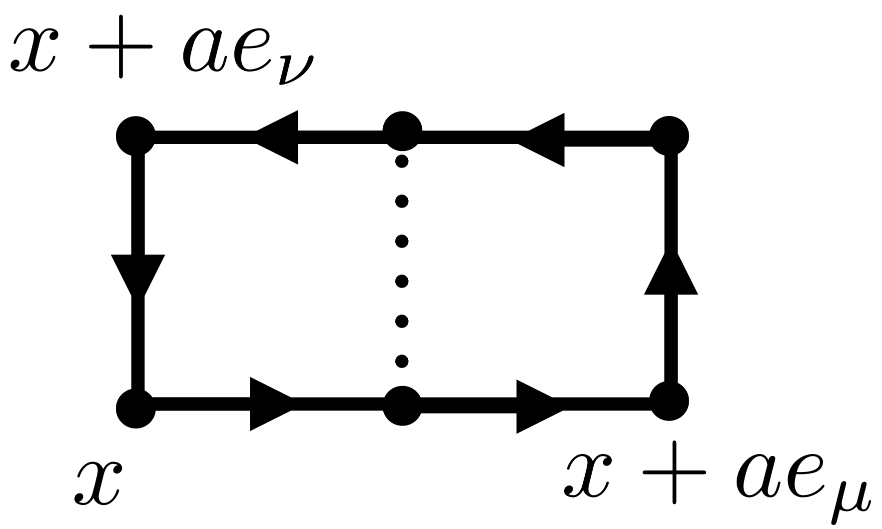
$$P_{\mu\nu} = \mathrm{Tr}\, U_\mu(x) U_\nu(x+ae_\mu) U_\mu^\dagger(x+ae_\nu) U_\nu^\dagger(x)$$

$$P_{\mu\nu} \to \mathrm{Tr}\, e^{ia^2 F_{\mu\nu}[1+\mathcal{O}(a)]}$$



$$R_{\mu\nu} = \mathrm{Tr}\, U_\mu(x) U_\mu(x+ae_\mu) U_\nu(x+2ae_\mu) U_\mu^\dagger(x+ae_\nu+ae_\mu) U_\mu^\dagger(x+ae_\nu) U_\nu^\dagger(x)$$

$$R_{\mu\nu} \to \mathrm{Tr}\, e^{i2a^2 F_{\mu\nu}[1+\mathcal{O}(a)]}$$



Gauge actions

$$S_G[U] = -\frac{1}{g^2}\sum_x \sum_{\mu\nu} \Re\left[c_P P_{\mu\nu} + c_R R_{\mu\nu}\right]$$

$$S_G[U] \approx \mathrm{const} + (c_P + 4c_R)\frac{a^4}{2g^2}\sum_x \sum_{\mu\nu} F_{\mu\nu}^2 \left[1 + \mathcal{O}(a)\right]$$

- Naive continuum limit requires: $C_P + 4C_R = 1$
- Tune C_R to remove higher order lattice artifacts
  - Wilson gauge action: $C_R=0$
  - tree-level $O(a^2)$ improved Luscher-Weiz action: $C_R=1/12$

Quantization of lattice QCD — partition function

Path-integral representation:

$$Z = \int [dU][d\bar{q}][dq]\, e^{-S_G[U] - \bar{q}D[U]q}$$

$$[dU] = \prod_{x,\mu} dU_\mu(x) \qquad\qquad D = D_{naive}, D_W, D_{st}, D_{ov}, \cdots$$

Gauge-invariant integration measure:

$$\int dU\, f(U) = \int dU\, f(U\Omega) = \int dU\, f(\Omega U) \qquad \int dU = 1$$

Quantization of lattice QCD — partition function

Path-integral representation:

$$Z = \int [dU][d\bar{q}][dq]\, e^{-S_G[U] - \bar{q} D[U] q}$$

$$= \int [dU]\, e^{-S_G[U]} \det D[U]$$

gauge integration volume is finite; no need to gauge fix

Quantization of lattice QCD — observables

A general observable can be written as:

$$\mathcal{O}(U,\bar{q},q) = \mathcal{O}^{[U]}_{i_1,\cdots,i_N;j_N,\cdots,j_1} q_{i_1}\cdots q_{i_N}\bar{q}_{j_N}\cdots\bar{q}_{j_1}$$

generalized index: color, flavor, spin, subset of space-time coordinates

Quantization of lattice QCD — observables

$$\langle \mathcal{O}(U,\bar{q},q)\rangle = \frac{1}{Z}\int [dU][d\bar{q}][dq]\, e^{-S_G[U]-\bar{q}D[U]q}\mathcal{O}(U,\bar{q},q)$$

$$\langle \mathcal{O}(U,\bar{q},q)\rangle = \frac{1}{Z}\int [dU]\, e^{-S_G[U]}\det D[U]\mathcal{O}^{[U]}_{i_1,\cdots,i_N;j_N,\cdots,j_1}\Delta^{[U]}_{i_1,\cdots,i_N;j_N,\cdots,j_1}$$

Wick contractions $\rightarrow$ Slater determinant

$$\boxed{\Delta^{[U]}_{i_1,\cdots,i_N;j_N,\cdots,j_1} = \det\begin{pmatrix} D^{-1}_{i_1,j_1}[U] & \cdots & D^{-1}_{i_1,j_N}[U] \\ \vdots & \ddots & \vdots \\ D^{-1}_{i_N,j_1}[U] & \cdots & D^{-1}_{i_N,j_N}[U] \end{pmatrix}}$$

Quantization of lattice QCD — observables

$$\langle \mathcal{O}(U,\bar{q},q)\rangle = \frac{1}{Z}\int [dU][d\bar{q}][dq]\, e^{-S_G[U]-\bar{q}D[U]q}\mathcal{O}(U,\bar{q},q)$$

$$= \frac{1}{Z}\int [dU]\, e^{-S_G[U]}\det D[U]\underline{\mathcal{O}^{[U]}_{i_1,\cdots,i_N;j_N,\cdots,j_1}\Delta^{[U]}_{i_1,\cdots,i_N;j_N,\cdots,j_1}}$$

$$= \frac{1}{Z}\int [dU]\, e^{-S_G[U]}\det D[U]\underline{\tilde{\mathcal{O}}(U)}$$

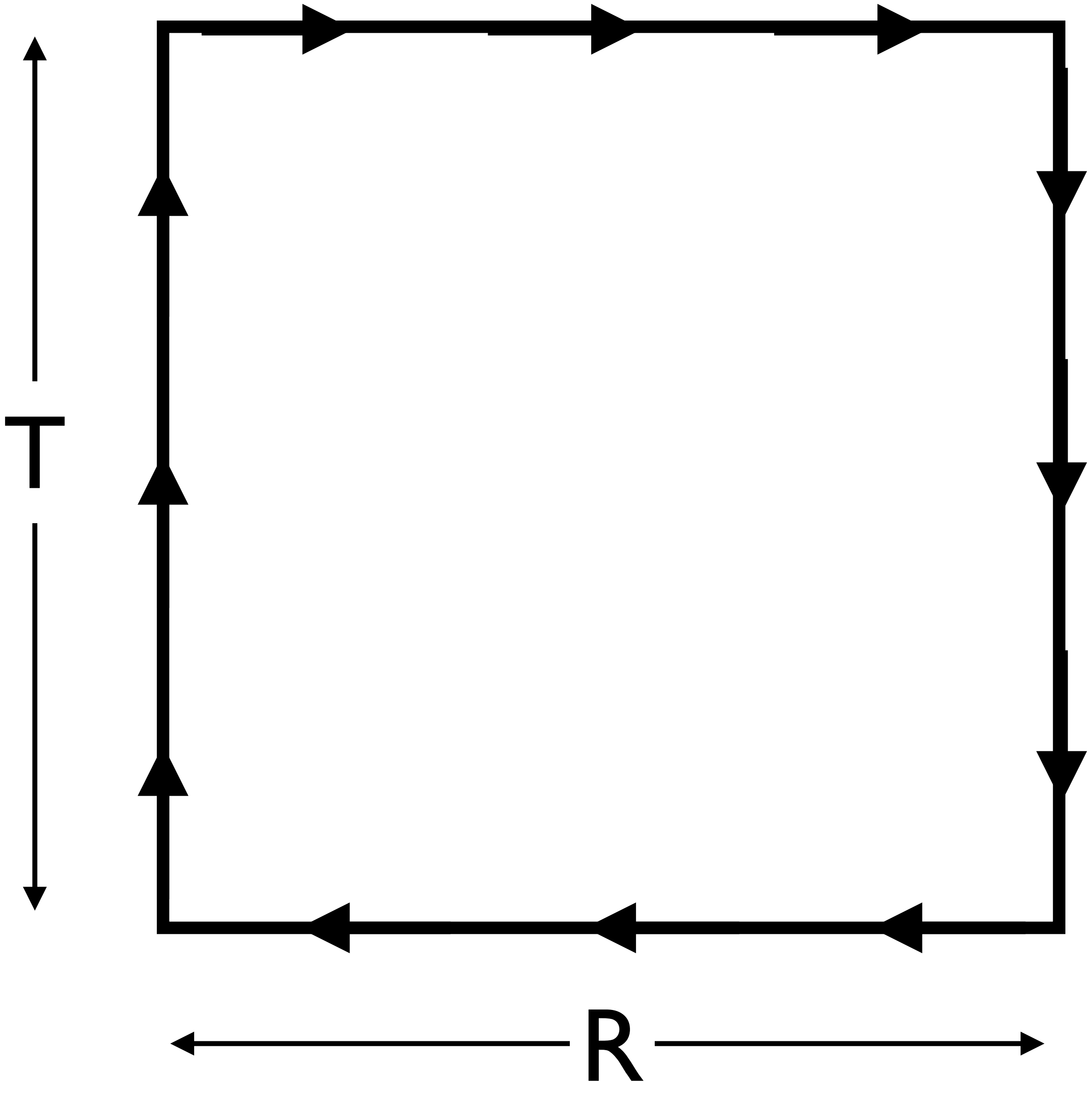
$$= \langle \tilde{\mathcal{O}}(U)\rangle_U$$

Observables — Wilson loop

$$W(R,T) = \langle \text{product of link variables, } U\text{, along an } R \times T \text{ rectangle } \rangle$$

$$\rightarrow e^{-TV(R)}\,, \qquad T \rightarrow \infty$$

- Wilson loop represents space-time path taken by a static quark/anti-quark pair
- Confining potential— WL exhibits area-law behavior
  - easily verified in strong-coupling expansion



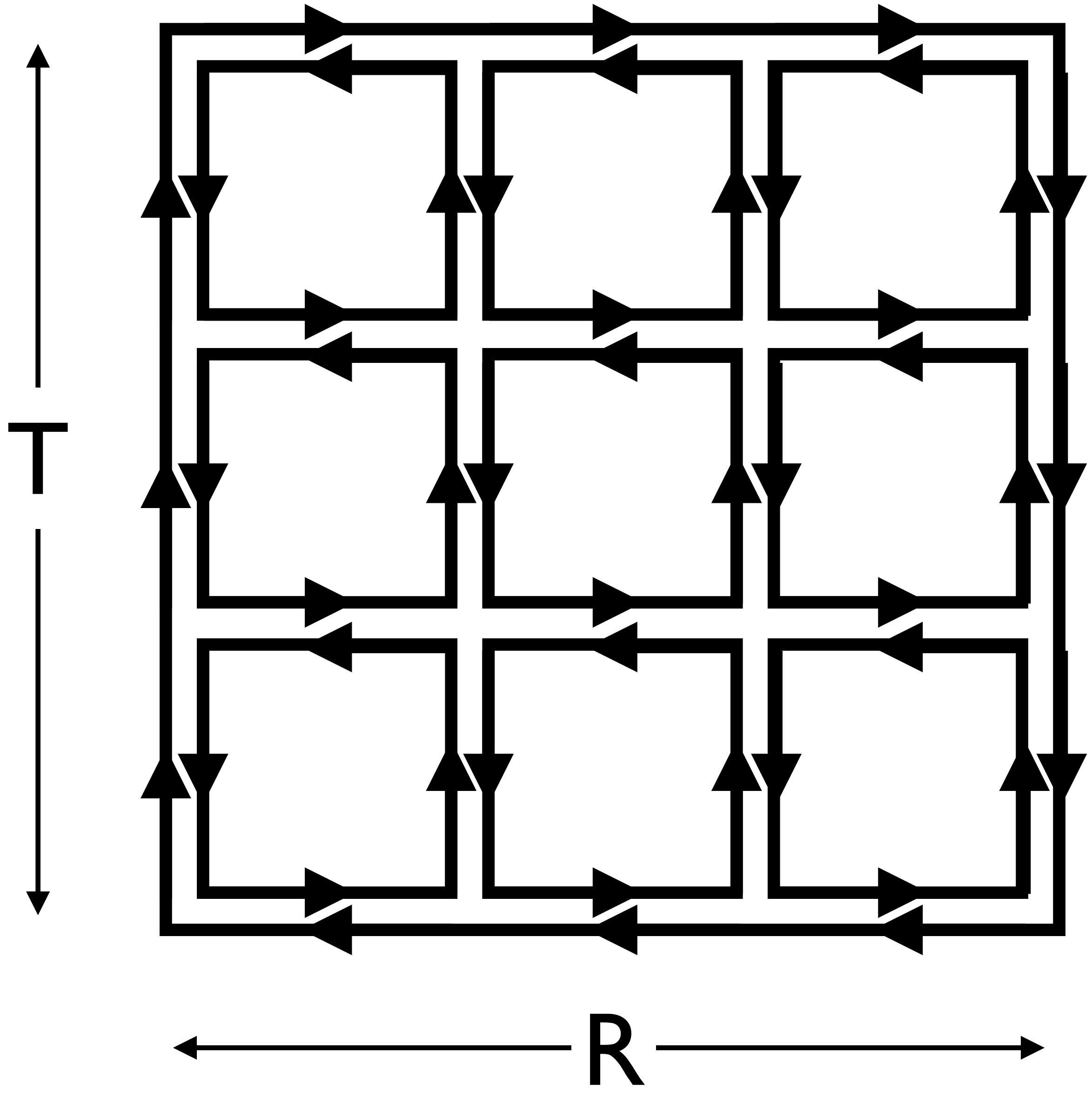
Observables — Wilson loop

Example: pure YM, Wilson action

$$\int dU U_{ij} U^\dagger_{kl} = \frac{1}{N_c}\delta_{jk}\delta_{il}$$

$$W(R,T) = \frac{1}{Z}\int [dU]\, e^{-S_G[U]}[R \times T \text{ loop}]$$

- Expand integrand in powers of $1/g^2$
- Integrate term by term
- Leading contribution corresponds to a single tiling of plaquettes



Observables — Wilson loop

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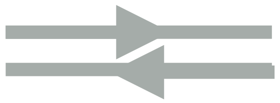
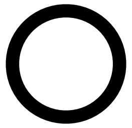


$\sim N_c^{-1}$

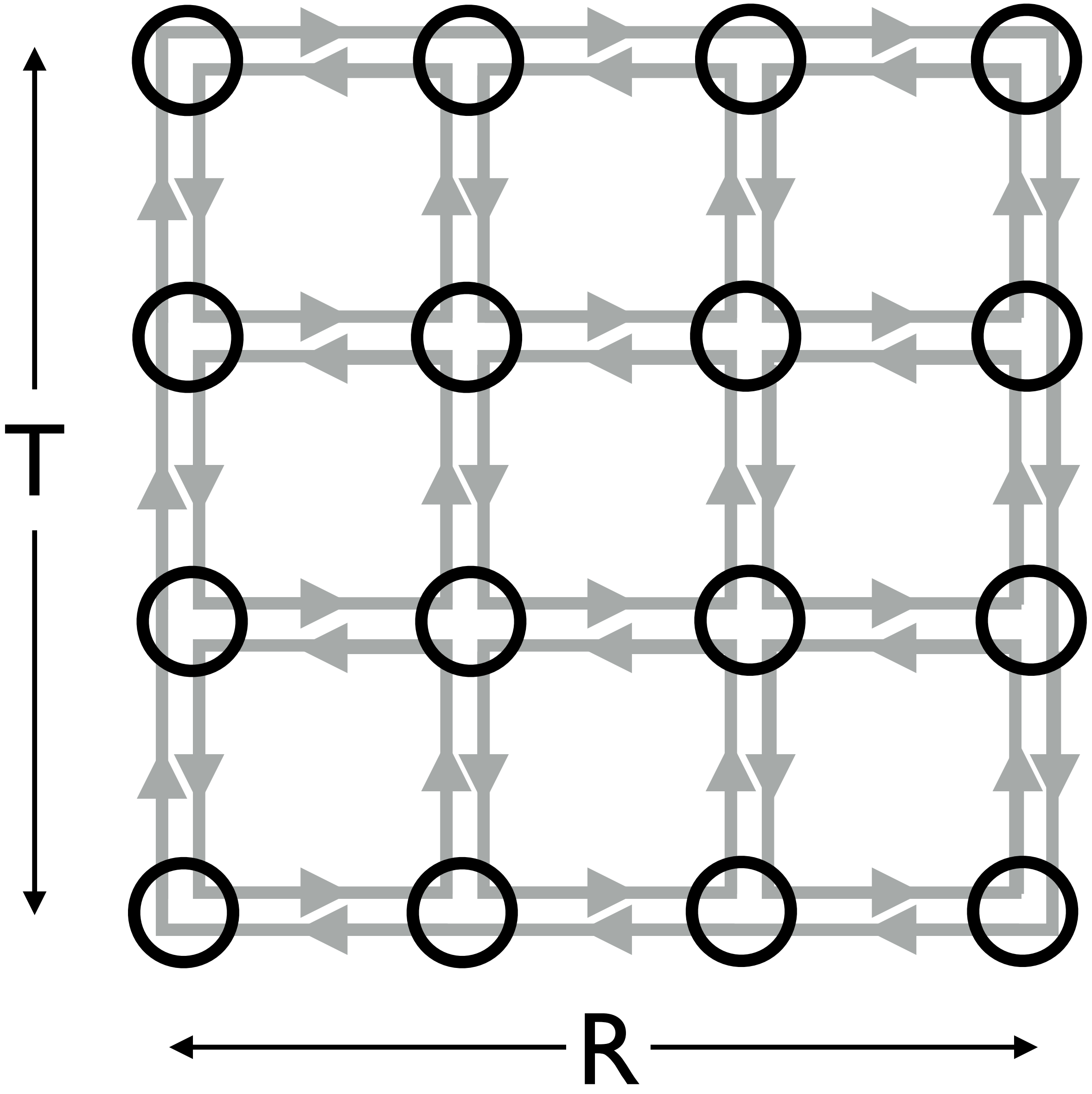


$\sim N_c$

$$W(R,T) \sim \left(\frac{1}{N_c g^2} \right)^{RT/a^2}$$

$$\sim e^{-TRa^{-2} \log(N_c g^2)}$$

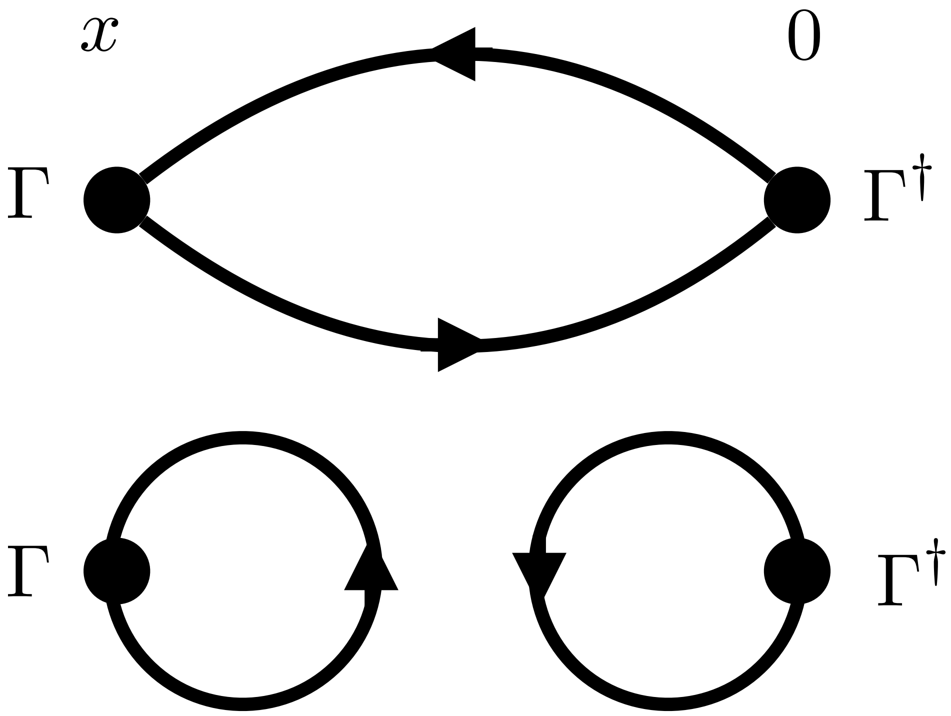
$$\boxed{V(R) = \frac{R}{a^2} \log(N_c g^2)}$$



Observables — meson correlation functions

$$\mathcal{M}(x) = \bar{q}_f(x)\Gamma q_g(x)$$

flavor indices



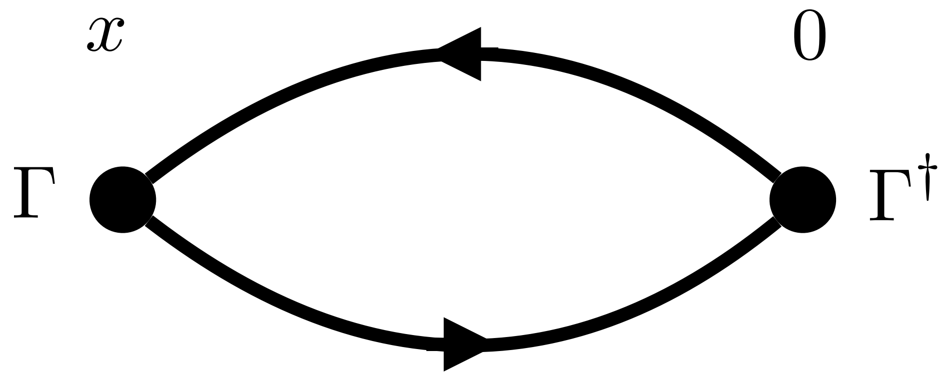
$$C_{\mathcal{M}}(x) \ = \langle \mathcal{M}(x)\mathcal{M}^\dagger(0)\rangle_{U,\bar{q},q}$$

$$\begin{aligned}\langle C_{\mathcal{M}}(x)\rangle \quad &= \quad -\left\langle \mathrm{Tr}\left[D_f^{-1}(0,x)\Gamma D_g^{-1}(x,0)\Gamma^\dagger\right]\right\rangle_U \\ &+ \quad \left\langle \mathrm{Tr}\left[D_f^{-1}(x,x)\Gamma\right]\mathrm{Tr}\left[D_g^{-1}(0,0)\Gamma^\dagger\right]\right\rangle_U \delta_{fg}\end{aligned}$$

trace over color and spin

flavor singlet correlator gets “disconnected” contribution

Observables — meson correlation functions



$$\mathcal{M}(x) = \bar{q}_f(x)\Gamma q_g(x)$$

flavor indices

$$C_{\mathcal{M}}(x) \; = \langle \mathcal{M}(x)\mathcal{M}^\dagger(0)\rangle_{U,\bar{q},q}$$

$$C_{\mathcal{M}}(x) \quad = \quad -\left\langle \mathrm{Tr}\left[D_f^{-1}(0,x)\Gamma D_g^{-1}(x,0)\Gamma^\dagger\right]\right\rangle_U$$

$$\mathcal{M} = \pi^+ : f = d, g = u, \Gamma = \gamma_5$$

$$\rightarrow -\left\langle \mathrm{Tr}\left[D_d^{-1\dagger}(x,0)D_u^{-1}(x,0)\right]\right\rangle_U \qquad \gamma_5 D^{-1}(0,x)\gamma_5 = D^{-1\dagger}(x,0)$$

Continuum limit

- Lattice action depends explicitly on the bare parameters and lattice spacing
- Lattice spacing is a redundant parameter, can be absorbed by redefinition of the fields and bare parameters:

$$a^{3/2}q \qquad a^{3/2}\bar{q} \qquad am_f \qquad g$$

- Lattice spacing set by the choice of bare coupling (g)
- In lattice QCD, it is convenient to work with dimensionless bare parameters (that's what goes into the computer)

Continuum limit — Pure YM

$$aM_{phys} = M_{lat}(g(a))$$

$$\boxed{a\frac{d}{da}} \longrightarrow \quad \beta(g)\frac{d}{dg}M_{lat}(g) = M_{lat}(g)$$

$$\beta(g) \equiv -a\frac{dg}{da} = \quad -b_0 g^3 - b_1 g^5 + \mathcal{O}(g^7)$$

$$b_0 = \frac{1}{(4\pi)^2}\left(\frac{11}{3}N_c - \frac{2}{3}N_f\right) > 0$$

$$b_1 = \frac{1}{(4\pi)^4}\left(\frac{34}{3}N_c^2 - \frac{N_c^2-1}{N_c}N_f - \frac{10}{3}N_cN_f\right)$$

b_0, b_1 are universal

Continuum limit — Pure YM

$$aM_{phys} = M_{lat}(g(a))$$

$$\boxed{a\frac{d}{da}} \longrightarrow$$

$$\beta(g)\frac{d}{dg}M_{lat}(g) = M_{lat}(g)$$

$$\beta(g) \equiv -a\frac{dg}{da} = \ -b_0 g^3 - b_1 g^5 + \mathcal{O}(g^7)$$

$$\boxed{\int}$$

In asymptotic scaling region:

$$M_{lat}(g) = aM_{phys} \propto e^{-\frac{1}{2\beta_0 g^2}}\, g^{\frac{-\beta_1}{\beta_0}}$$

$$a(g) = \frac{1}{\Lambda}e^{-\frac{1}{2\beta_0 g^2}}\, g^{\frac{-\beta_1}{\beta_0}}$$

Continuum limit — Pure YM

- Scale setting:

$$a = \frac{M_{lat}(g)}{M_{phys}}$$

measured at bare coupling g

input from experiment

- Continuum limit: $aM_{phys} \to 0 \Leftrightarrow g \to 0$
  - corresponds to tuning bare coupling to a critical point
  - g=0 corresponds to a gaussian fixed point
- All dimensionless ratios of dimensionful quantities are predictions and have a finite continuum limit

Continuum limit — 2+1 flavor QCD

Three bare parameters: $g, m_l = m_u = m_d, m_s$

Three physical scales:
(any choice will do, in princple)

$$aM_{p,phys} = M_{p,lat}(g, am_l, am_s)$$

$$aM_{\pi,phys} = M_{\pi,lat}(g, am_l, am_s)$$

$$aM_{K,phys} = M_{K,lat}(g, am_l, am_s)$$

$$\frac{M_{K,lat}}{M_{p,lat}} = \text{physical value}$$

$$\frac{M_{\pi,lat}}{M_{p,lat}} = \text{physical value}$$

defines

$$am_s(g) \quad am_l(g)$$

Continuum limit — 2+1 flavor QCD

Along the curve of constant physics: $\{am_l(g), am_s(g)\}$

The lattice spacing is given by:

measured at bare coupling g

$$a = \frac{M_{p,lat}(g)}{M_{p,phys}}$$

$M_{p,phys} = 938\mathrm{MeV}$

- Lattice spacing a[fm] is convention dependent
- The continuum limit corresponds to taking g to zero, and is independent of conventions

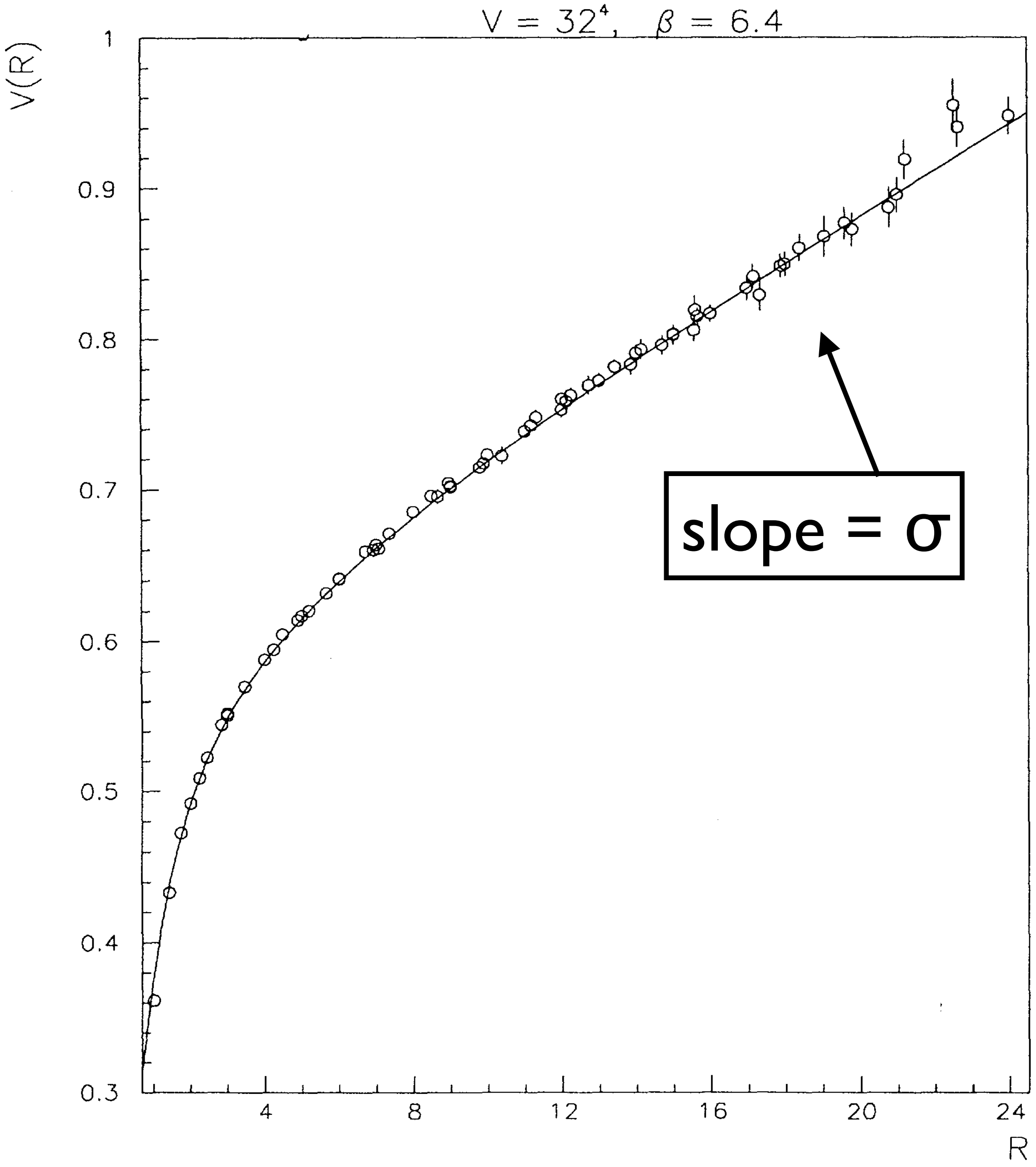
Scale setting: string tension

$$V(r) = V_0 - \frac{c}{r} + \sigma r$$

$$\sigma = \lim_{r\to\infty} \frac{\partial}{\partial r} V(r)$$

- string tension extracted from asymptotic behavior of the static quark potential
- phenomenological value: $\sigma^{1/2} \sim 440$ MeV

hep-lat/9208028

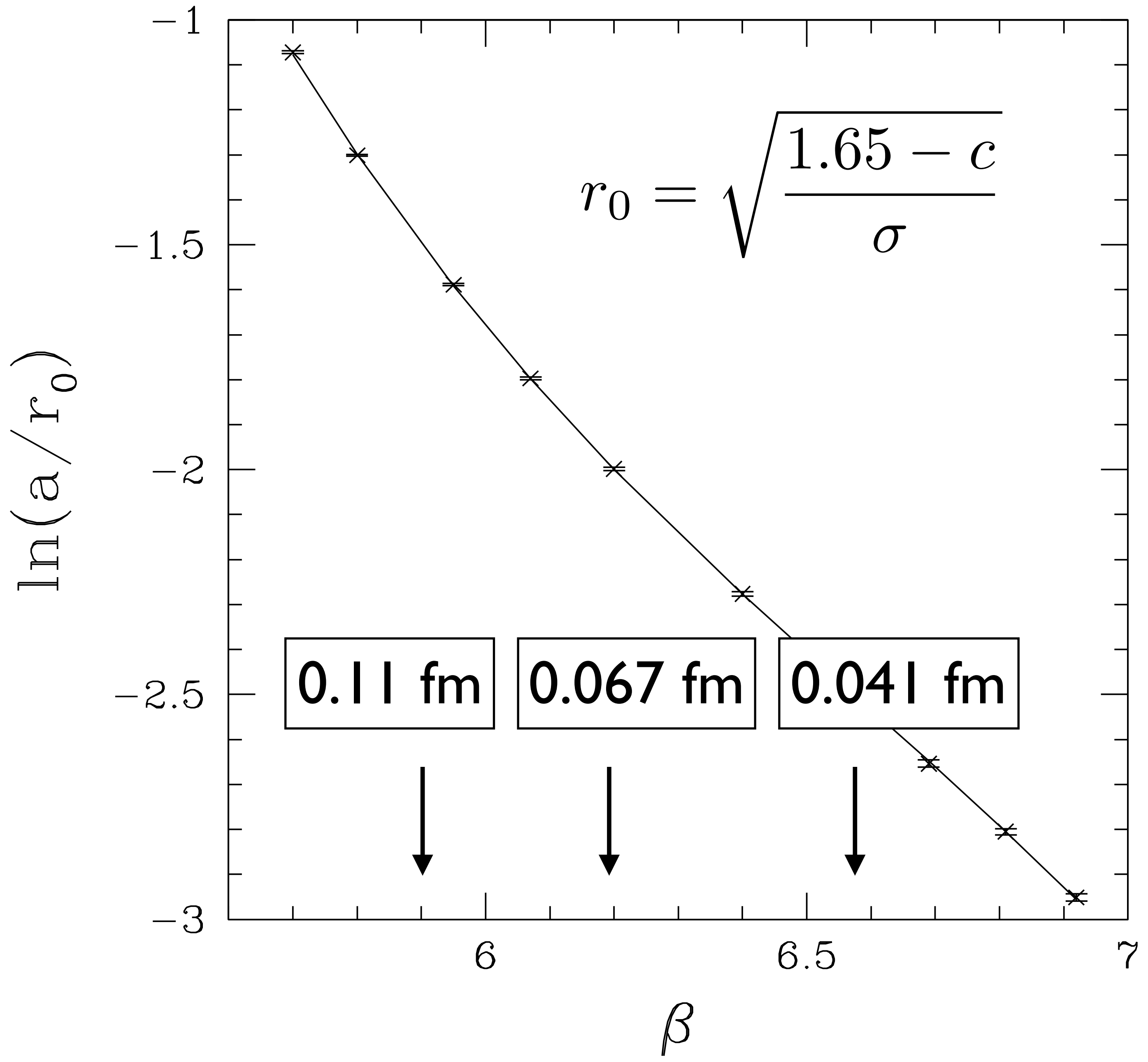


Scale setting: Sommer scale (r_0)

$$r^2 \frac{\partial}{\partial r} V(r)\bigg|_{r=r_0} = 1.65$$

- r_0 defined in terms of force between static quarks at intermediate distances r
- r_0 ~0.5 fm based on phenomenological potential models

Alpha collaboration: hep-lat/0108008



Scale setting: gradient flow (t_0)

- Computation of string tension and Sommer scale requires numerical computation of static quark potential:
  - computation of Wilson loops of all sizes TxL — computationally costly
  - large T extrapolation, estimates get noisy in this regime
  - fits to V(R)
- State-of-the-art scale setting based on Gradient flow (t_0); numerically simple computation

arXiv:1006.4518

Scale setting: gradient flow (t_0)

- Evolution of gauge fields in fictitious fifth time dimension according to a gauge-covariant diffusion equation
- Flow has a smoothing effect on field configurations
- **Key property:** gauge fields at flow time t>0 are smooth, renormalized fields; observables constructed from them contain physical properties of the system
- Scale t_0 defined as:

defined in terms of “flowed” gauge field

$$t^2 \langle E \rangle \Big|_{t=t_0} = 0.3 \qquad E = \frac{1}{2} \mathrm{Tr} F_{\mu\nu} F_{\mu\nu}$$

- Many other uses (e.g., defining stress-energy tensor on he lattice, measuring topological charge,…)

Universality and improvement

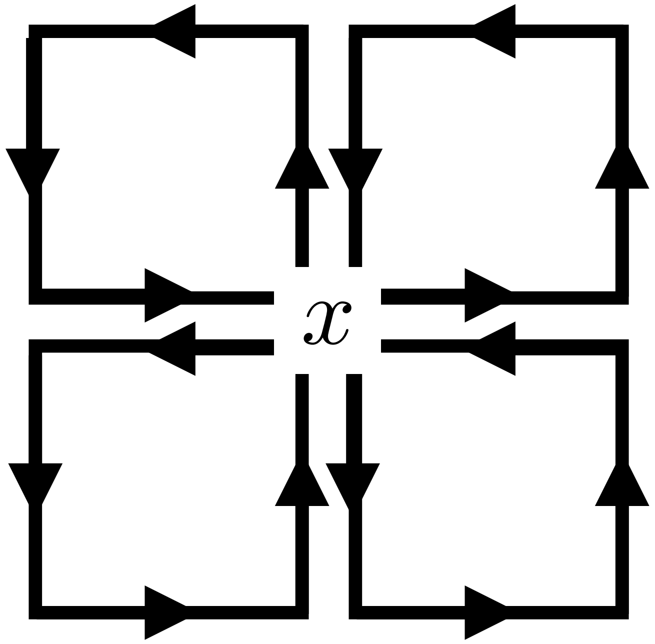
- Continuum limit is independent of the choice of lattice action, however, the rate at which the continuum limit is reached **will** depend on the choice of action

- Can improve actions, by adding irrelevant lattice operators, which are tuned in some way to remove lattice artifacts at the quantum level (i.e., Symanzik improvement)

Example: $S_{imp}[U,\bar{q},q] = S[U,\bar{q},q] + \frac{i}{4}c_{sw}a^5 \sum_x \bar{q}(x)\sigma_{\mu\nu}G_{\mu\nu}(x)q(x)$

$$\sigma_{\mu\nu} = -\frac{i}{2}[\gamma_\mu,\gamma_\nu]$$

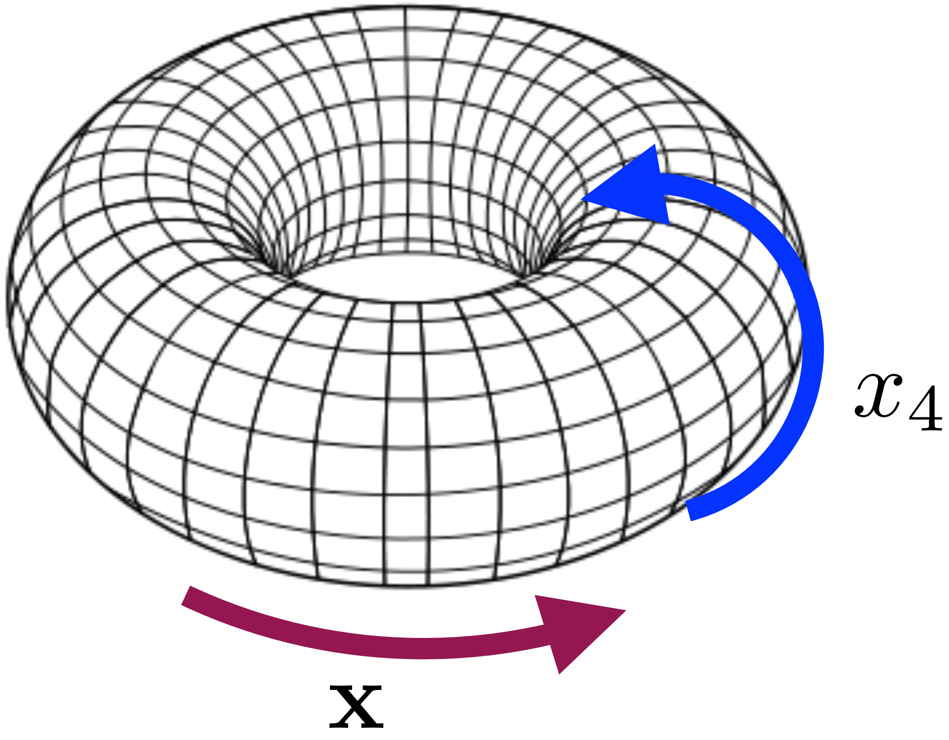
$$G_{\mu\nu}(x) =$$



Finite volume and temperature effects

- Finite memory — finite number of grid points
  - finite temperature effects, controlled by T
  - finite volume effects, controlled by L
  - choice of boundary conditions are arbitrary, but some choices are sometimes better for addressing specific physics questions

box size: L^3xT

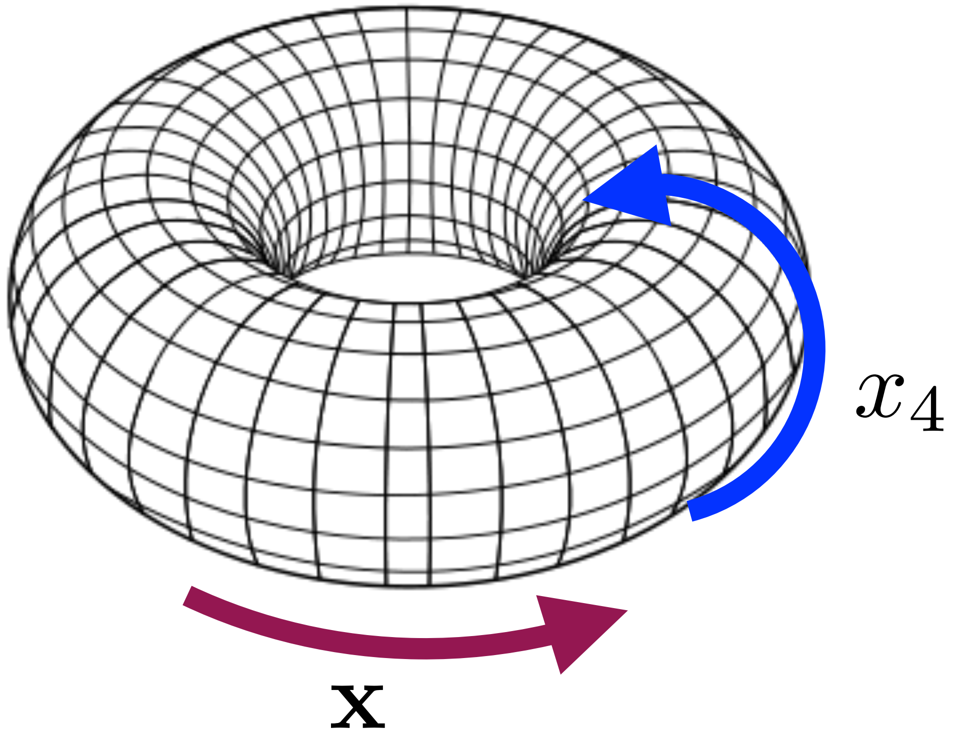


Typical Spatial Boundary conditions

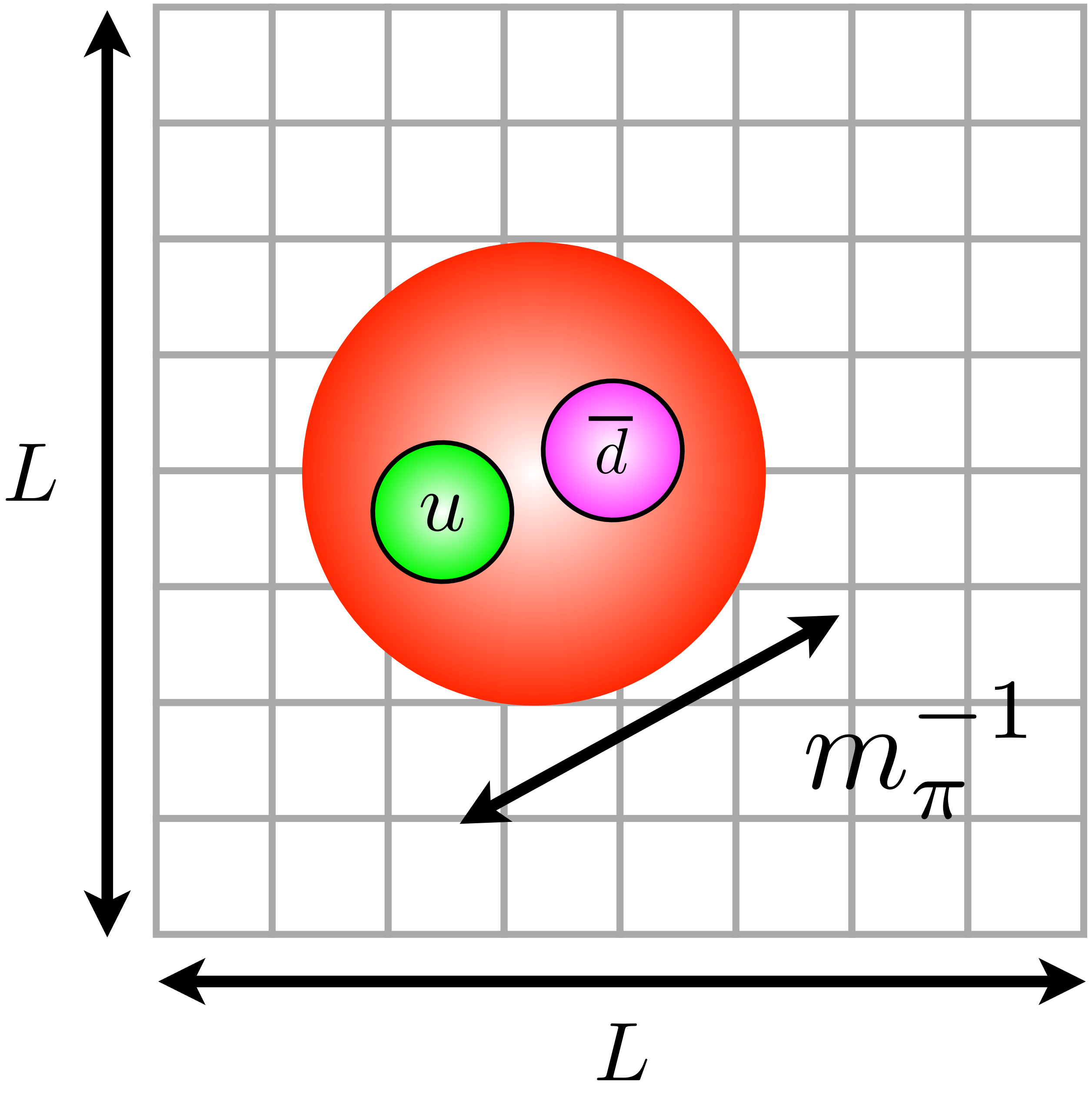
- Periodic/anti-periodic: $f(x+L) = \pm f(x)$
- Twisted: $f(x+L) = e^{i\phi} f(x)$

useful for interpolating between lattice momenta

box size: L^3xT



Finite volume

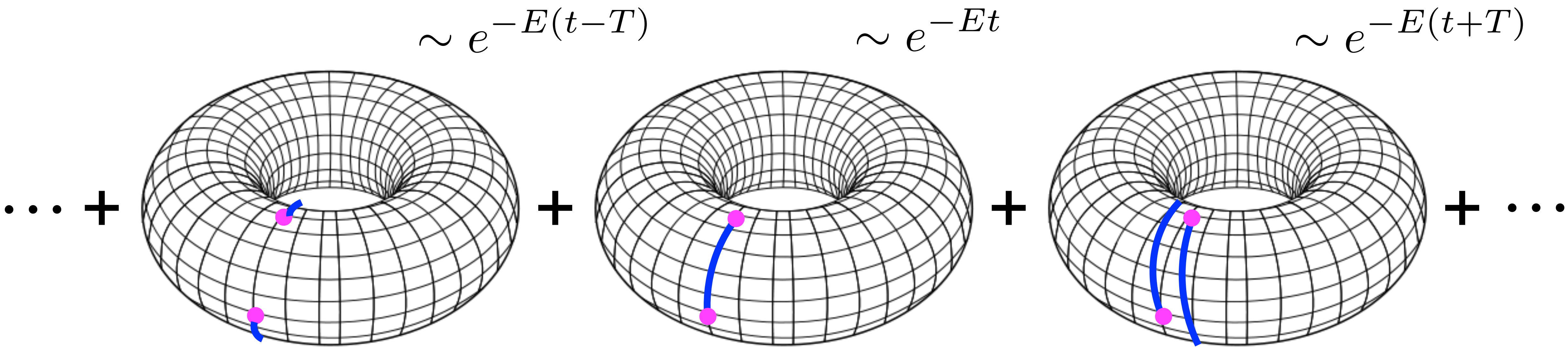


- Spatial extent should be larger than the Compton wave-length of lightest state (i.e., pions)
- Periodic lattice: states can interact with their images
- Typical finite volume corrections from around-the-world pion propagation:

$$\sim e^{-m_\pi L} \qquad m_\pi L \gtrsim 4$$

Finite temperature

- States can propagate “around the world”
  - correlation functions will pick up backward propagating states at large time separations
  - asymptotic “thermal effects”
- For correlation functions, around the world contributions can be summed



Basic formalism — summary

- Lattice QCD degrees of freedom
- Fermion and gauge actions
- Continuum limit/scale setting
- Computation of observables
- Finite volume/temporal extent effects

Outline

- ✓ Basic formalism — QCD on a space-time lattice
- Numerical computation — hardware, algorithms and analysis
- From lattice to physics — results and challenges

Numerical computation

Evaluation of the path integral

Goal is to *reliably* compute:

$$\langle \tilde{\mathcal{O}}(U) \rangle_U = \frac{1}{Z} \int [dU] \, e^{-S_G[U]} \det D[U] \tilde{\mathcal{O}}(U)$$

$$Z = \int [dU] \, e^{-S_G[U]} \det D[U]$$

- Gauge integration involves N_cxL^3xT degrees of freedom
- Fermion operator sparse but enormous: N_cxN_sxL^3xTxdx2
- Direct numerical integration is impractical
- Problem ideally suited for Monte Carlo

Evaluation of the path integral

General strategy:

$$\langle \tilde{\mathcal{O}}(U) \rangle_U = \frac{1}{Z} \int [dU]\, e^{-S_G[U]} \det D[U] \tilde{\mathcal{O}}(U)$$

- Generate uncorrelated field configurations: $\{U^1, U^2, \cdots, U^{N_{conf}}\}$
- Distributed according to the probability measure:

$$W(U) = e^{-S_G[U]} \det D[U]$$

- Stochastically estimate observables via:

$$\langle \tilde{\mathcal{O}}(U) \rangle_U \approx \frac{1}{N_{conf}} \sum_{n=1}^{N_{conf}} \tilde{\mathcal{O}}(U^n) + \mathcal{O}\left(N_{conf}^{-1/2}\right)$$

Configuration generation

- Generation of ensembles is performed using Markov Chain Monte Carlo methods (e.g., Metropolis Method)
  - Metropolis updating — requires ergodicity, detailed balance
  - autocorrelations — future configurations depend on past configurations $U^1 \to U^2 \to U^3 \to \dots$
- Dealing with fermion determinants is an added complication
  - naive computational cost ~ rank(D)^3
  - past strategy: quenched approximation (uncontrolled)
  - Current state-of-the-art: *Hybrid Monte Carlo*

Hybrid Monte Carlo in a Nutshell

$$Z = \int [dU]\, e^{-S_G[U]} \det D[U]$$

“integrate in” pseudo-fermions

$$= \int [dU][d\phi^\dagger][d\phi]\, e^{-S_G[U]-\phi^\dagger D[U]^{-1}\phi}$$

“integrate in” conj. momenta P

$$= \int [dP][dU][d\phi^\dagger][d\phi]\, e^{\underline{-S_K[P]}-S_G[U]-\phi^\dagger D[U]^{-1}\phi}$$

$$S_K[P] = \frac{1}{2}\sum_{x\mu} \mathrm{Tr} P_\mu(x) P_\mu(x) \qquad P_\mu(x) = \sum_{a=1}^{N_c^2-1} T^a P_\mu^a(x)$$

Hybrid Monte Carlo in a Nutshell

$$Z = \int [dU]\, e^{-S_G[U]} \det D[U]$$

“integrate in”
pseudo-fermions

$$= \int [dU][d\phi^\dagger][d\phi]\, e^{-S_G[U] - \phi^\dagger D[U]^{-1}\phi}$$

“integrate in”
conj. momenta P

$$= \int [dP][dU][d\phi^\dagger][d\phi]\, e^{-S_K[P] - S_G[U] - \phi^\dagger D[U]^{-1}\phi}$$

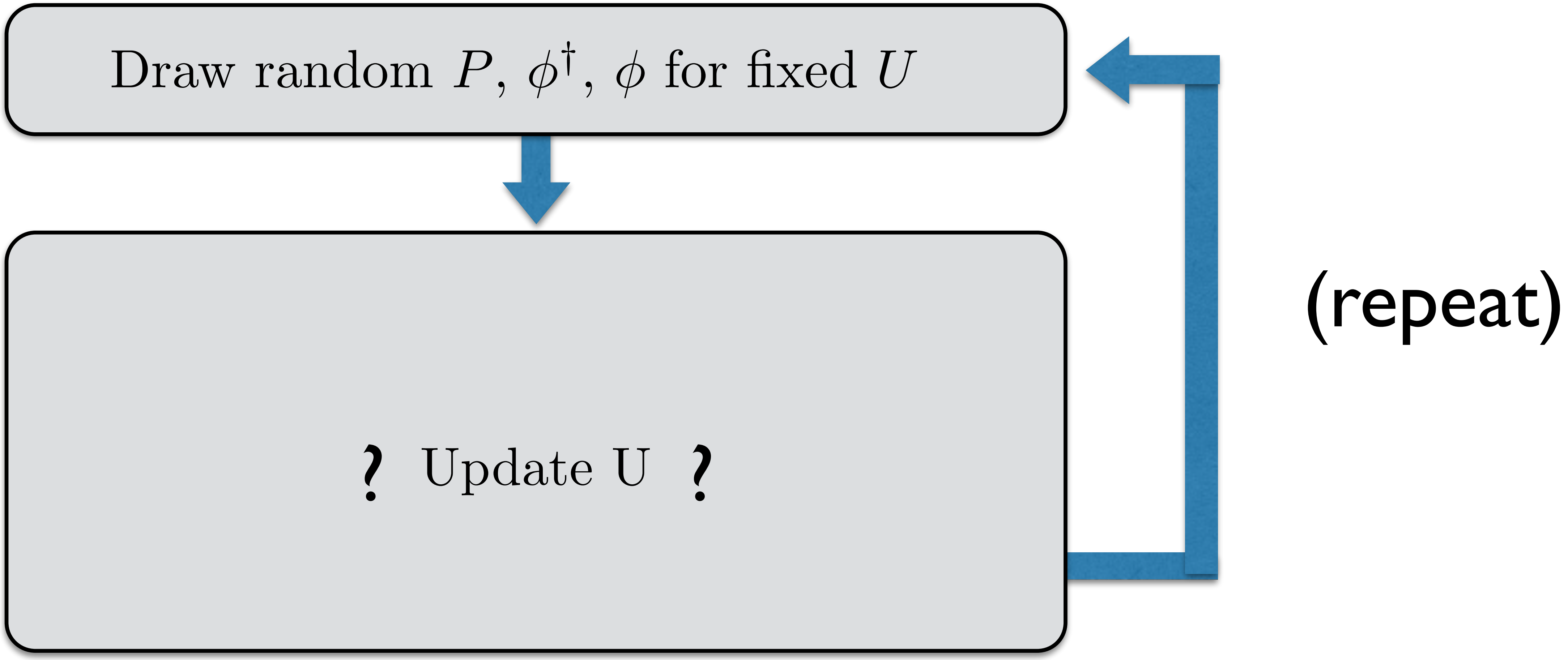
$$= \int [dP][dU][d\phi^\dagger][d\phi]\, e^{-H[P,U,\phi^\dagger,\phi]}$$

$$H[P,U,\phi^\dagger,\phi] = S_K[P] + S_G[U] + \phi^\dagger D[U]^{-1}\phi$$

Hybrid Monte Carlo in a Nutshell

$$Z = \int [dP][dU][d\phi^\dagger][d\phi]\, e^{-S_K[P]-S_G[U]-\phi^\dagger D[U]^{-1}\phi}$$

Gaussian distributed



Hybrid Monte Carlo in a Nutshell

Performing updating of gauge links U

- View partition function as a classical system with Hamiltonian:

$$H[P, U, \phi^\dagger, \phi] = S_K[P] + S_G[U] + \phi^\dagger D[U]^{-1}\phi \qquad U \equiv e^{iQ}$$

- Regard Q and P as conjugate variables
- Introduce fictitious time τ (i.e., a fifth dimension)
- For a fixed background field φ, define evolution in time τ according to Hamilton's equations:

$$\frac{d}{d\tau}Q_\mu(x) = P_\mu(x) \qquad \frac{d}{d\tau}P_\mu(x) = -\frac{\partial}{\partial Q_\mu(x)}H[P, U, \phi^\dagger, \phi]$$

Hybrid Monte Carlo in a Nutshell

$$H[P,U,\phi^\dagger,\phi] = S_K[P] + S_G[U] + \phi^\dagger D[U]^{-1}\phi \qquad U \equiv e^{iQ}$$

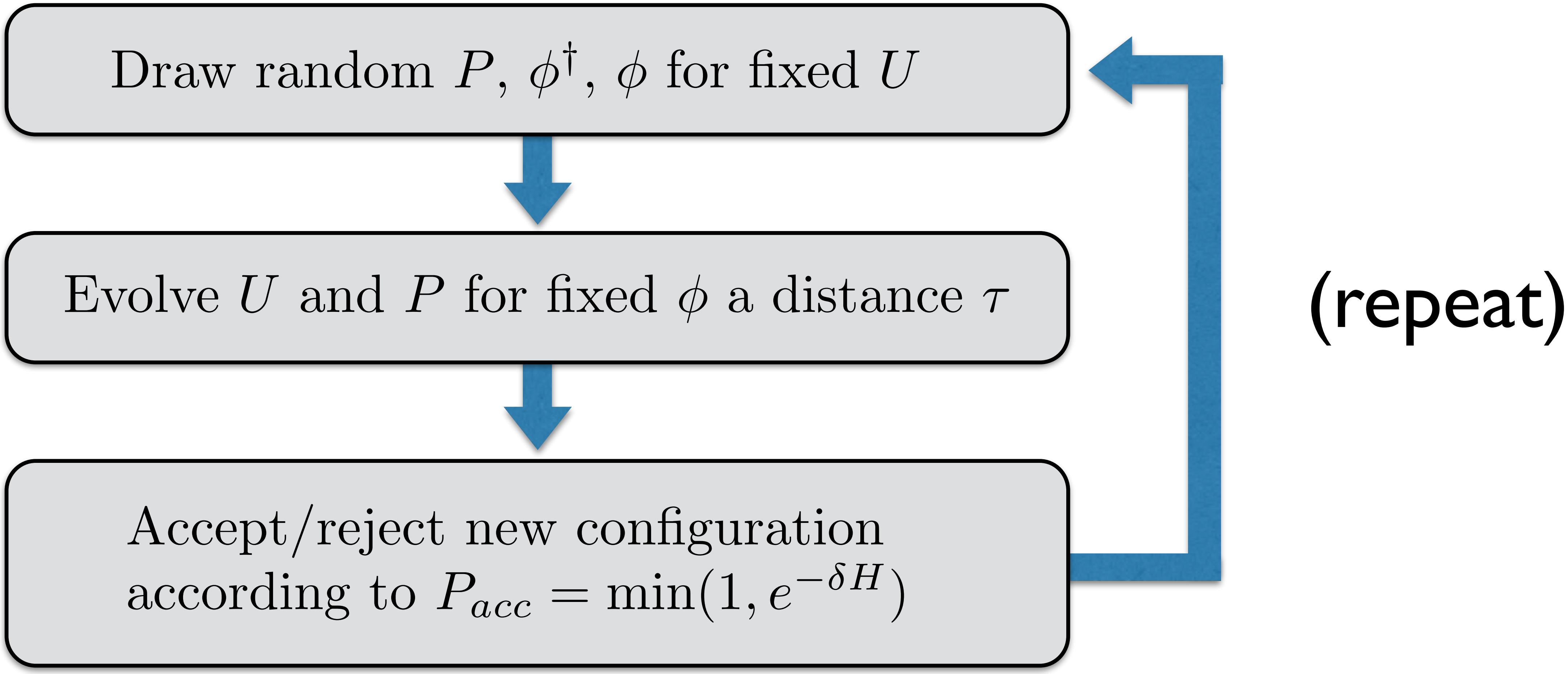
$$\frac{d}{d\tau}Q_\mu(x) = P_\mu(x) \qquad \frac{d}{d\tau}P_\mu(x) = -\frac{\partial}{\partial Q_\mu(x)}H[P,U,\phi^\dagger,\phi]$$

- **Erogodicy/ergodic hypothesis:** time average of observables along an evolution trajectory is equal to its phase-space average
- Classical Hamiltonian H is conserved along the trajectory
- Finite integration steps, results in small nonconservation of H
- Evaluation of fermion force term requires D-inversions

Hybrid Monte Carlo in a Nutshell

$$Z = \int [dP][dU][d\phi^\dagger][d\phi]\, e^{-S_K[P]-S_G[U]-\phi^\dagger D[U]^{-1}\phi}$$

Gaussian distributed



Draw random P, $\phi^\dagger$, ϕ for fixed U

Evolve U and P for fixed ϕ a distance τ

Accept/reject new configuration according to $P_{acc} = \min(1, e^{-\delta H})$

(repeat)

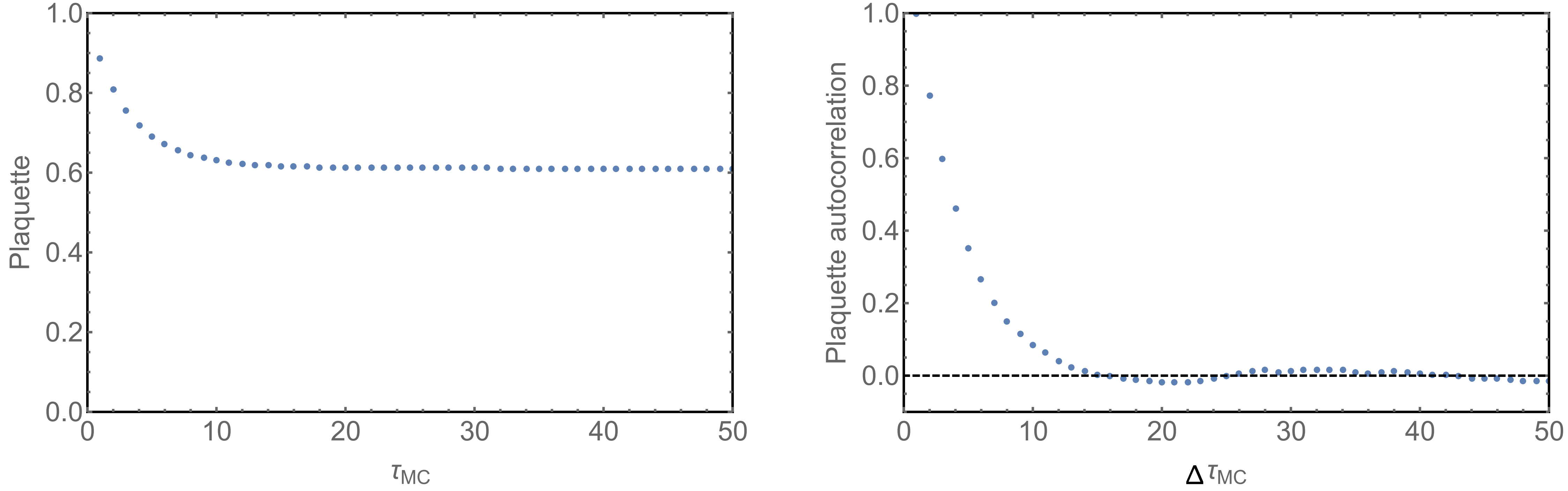
Hybrid Monte Carlo in a Nutshell

- HMC evolution requires many linear solves of form: $Dx = y$
    - can be solved cheaply, iteratively
    - but inversion cost grows as chiral limit approached
- Method is exact
    - errors in numerical integration of Hamilton's equations takes system away from constant energy surface
    - such errors removed with Metropolis accept/reject step
- Acceptance rate is controllable by integration step size Δτ
- Many algorithmic improvements

Thermalization and autocorrelations

- Deficiency of MCMC: future configs depend on the past
- Autocorrelation times are algorithm dependent
- Long distance quantities typically have longer autocorrelation times (e.g., topological charge, large Wilson loops)
- Critical slowing down in continuum/chiral limits

Example: Pure SU(3) gauge theory on an 32^3x72 lattice; β=6.17 (heat bath)

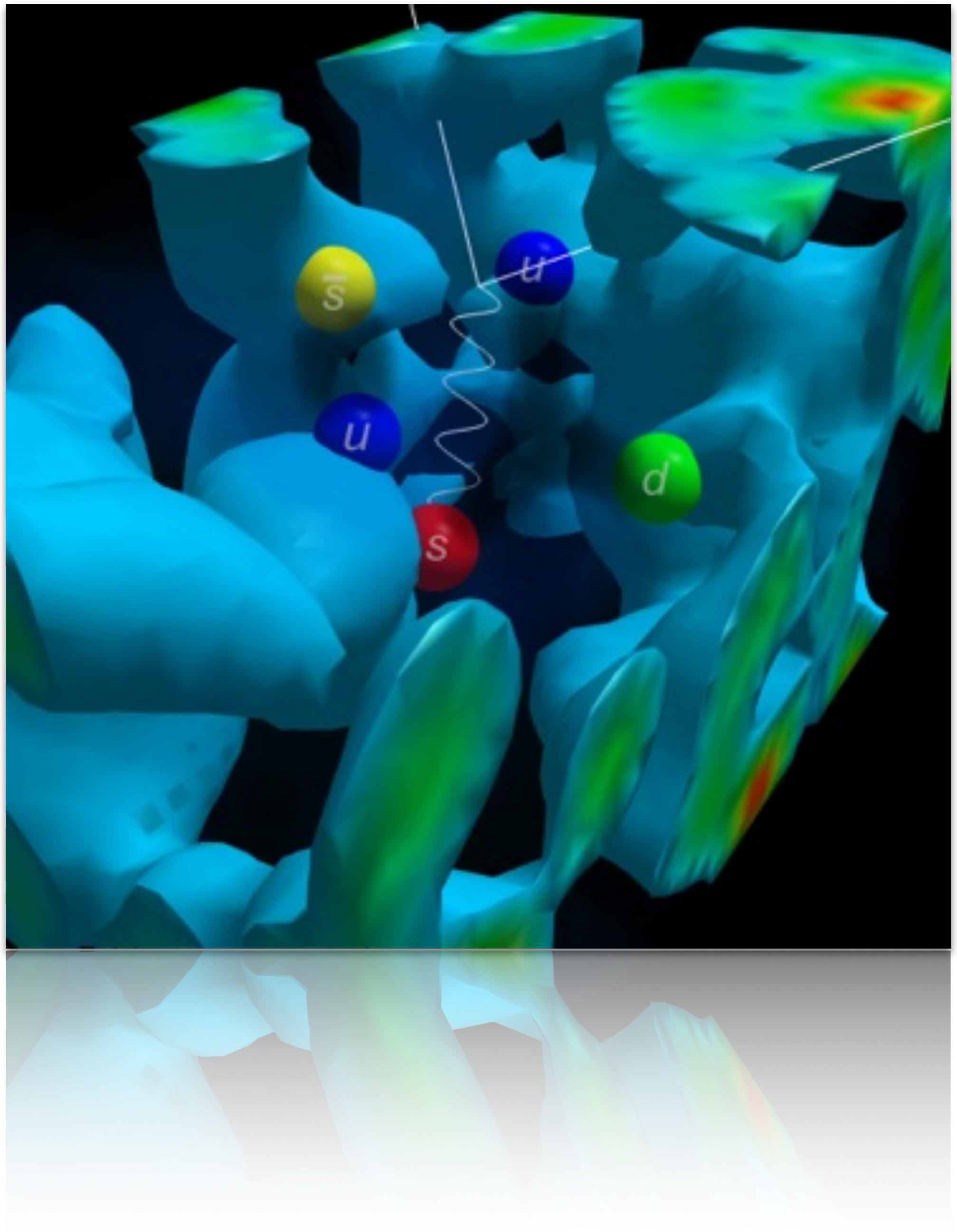


Lattice field configurations

Gauge fields configurations can be studies on an individual basis:

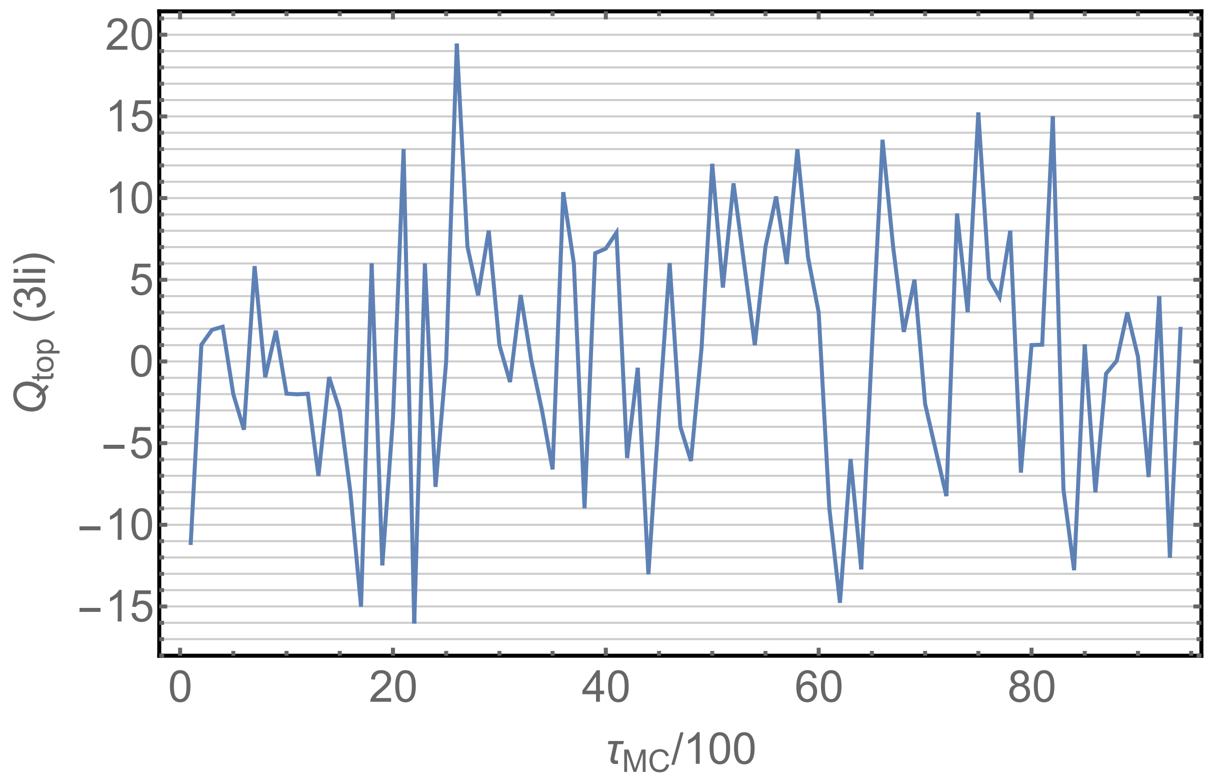
- action density
- configuration topology, topological charge density, topological charge
- spectrum of the Dirac operator; zero modes

D. Leinweber, http://www.physics.adelaide.edu.au

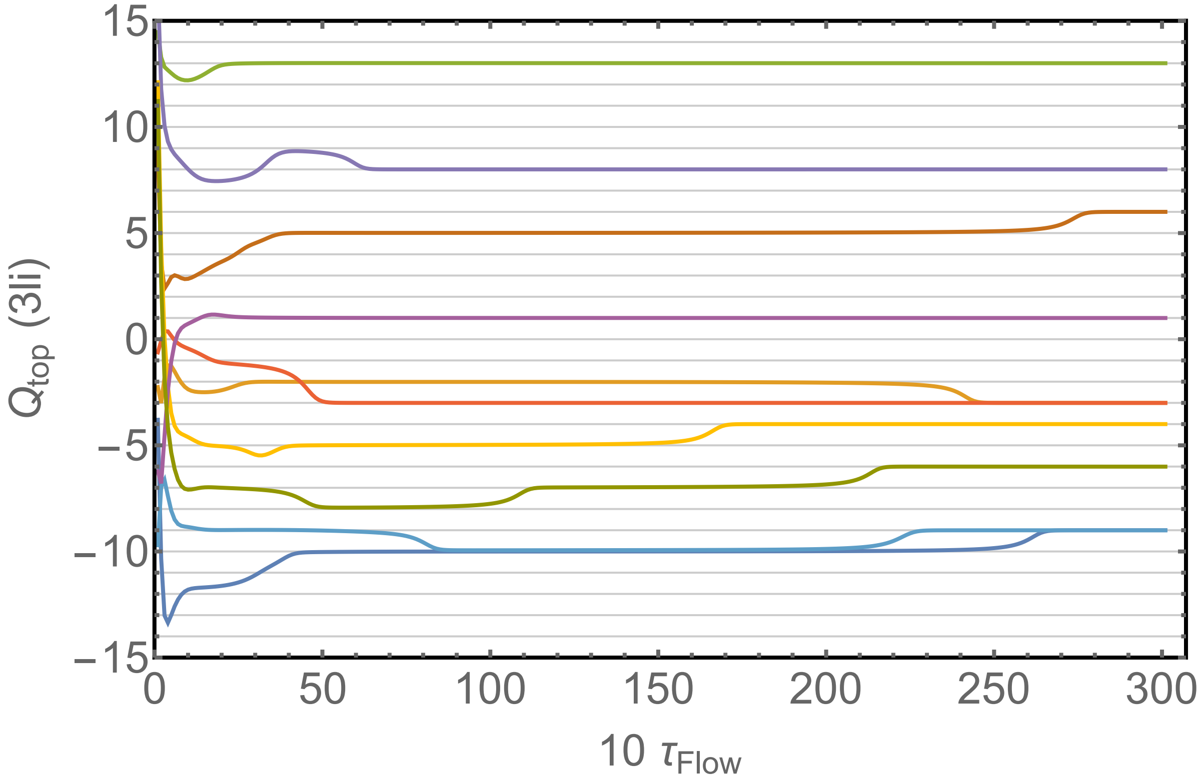


Topological charge

- Gluonic definition of topological charge (not unique)
- configurations require cooling to get integer values
- jumps in charge with cooling iterations due to small instantons "falling through the lattice"



32^3x72, SU(3) YM, β=6.17 (a~0.70 fm)



Anatomy of a lattice QCD computation

1. Generate a statistically uncorrelated ensemble of gauge configurations distributed according to the action for multiple lattice parameters (e.g., lattice spacing, quark masses, etc)
2. Measure operators on background field configurations
3. Estimate expectation values of operators as ensemble averages over background gauge field configurations
4. Use theory to connect expectation values of lattice operators to relevant physical quantities
5. Analysis of data, necessary extrapolations/fits, quantification of all statistical and systematic uncertainties

Understanding uncertainties

- Most numerical work quote two types of uncertainties:
  - **Statistical uncertainties** — are controlled primarily by ensemble size and choice of operators; can be reduced by increased computing resources and improved algorithms
  - **Systematic uncertainties** — can sometimes be controlled/estimated/removed using functional forms predicted by theory (e.g., within an EFT framework)

Uncertainties — controlled by numerics

- Autocorrelations
  - due to algorithmic inefficiency
  - critical slowing down as continuum/chiral limits approached
- Equilibration
- Statistical/fitting
- Tuning of lattice parameters

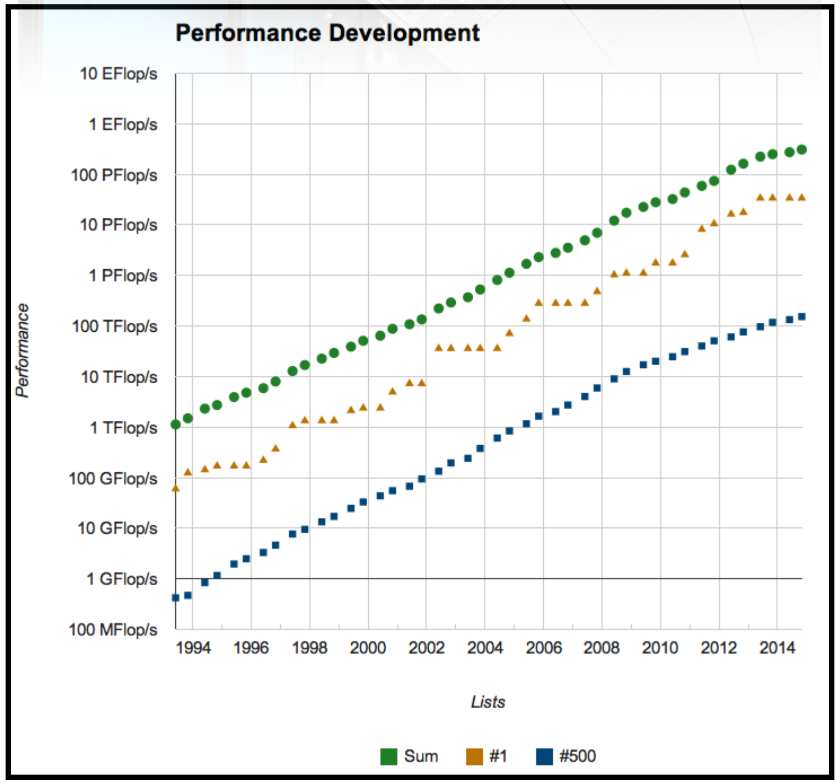
Uncertainties — controlled by theoretical input

- Continuum extrapolation
- Infinite volume extrapolation
- Accounting for thermal effects
- Chiral extrapolation

Consequences of limited resources

- Limited computational resources result in sacrifices…
  - quenched — uncontrolled approximation of the past
  - simulations at unphysical pion masses
  - limited number of lattice spacings — need 3+ for continuum extrapolation
- Limited statistics present significant signal/noise challenges:
  - disconnected contributions to correlators
  - multi-baryon correlators
  - glue-ball correlators

Hardware and algorithms



```
i = blockDim.x/2;
while (i != 0) {
if (cid < i) {
cache[cid].x += cache[cid
cache[cid].y += cache[cid
}
__syncthreads();
i /= 2;
}
if (cid == 0) {
psum[block
```

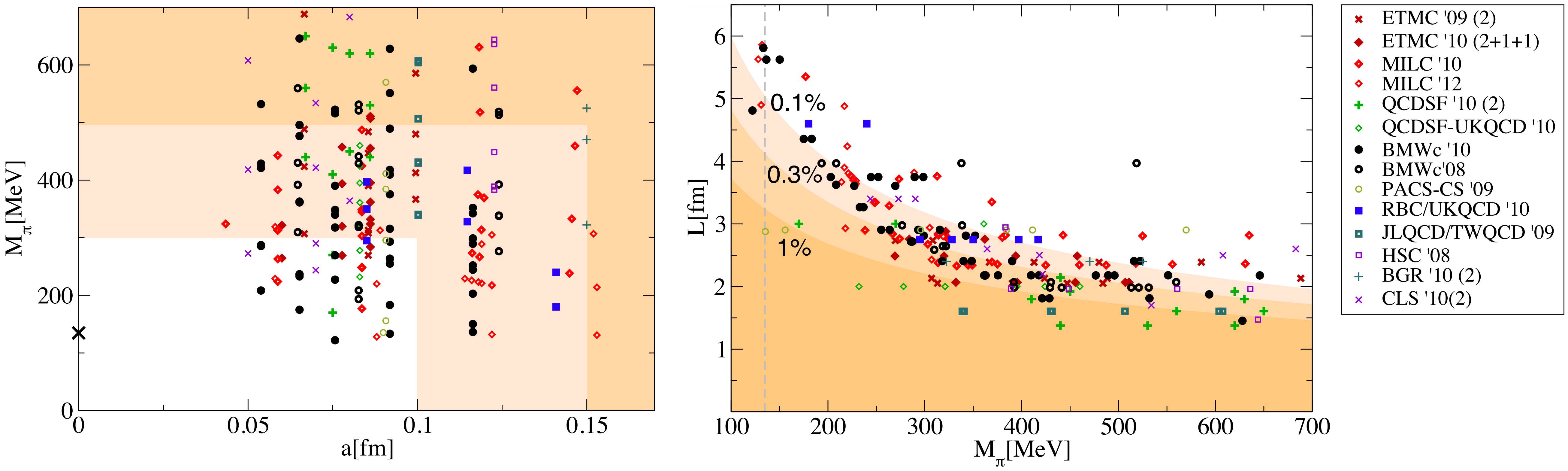
Rapid advances in both **hardware** and **algorithms** have enabled:

— realistic simulations:
   e.g., large volumes, light pions

— increasingly challenging studies

Survey of ensembles

Hoelbling [arXiv:1410.3403]



- N_f = 1+1, 2+1, 1+1+1 and even 1+1+1+1 flavor ensembles
- Typical lattice spacings: a > 0.05 fm
- Typical pion masses greater than 200-300 MeV; state-of-the-art down to the physical pion mass
- Some simulations include dynamical QED

Numerical computation — summary

- Algorithms: Hybrid Monte Carlo
- Considerations for carrying out a lattice QCD calculation to completion
- Understanding and controlling (when possible) systematic/ statistical uncertainties

Outline

- ✓ Basic formalism — QCD on a space-time lattice
- ✓ Numerical computation — hardware, algorithms and analysis
- From lattice to physics — results and challenges

From lattice to physics

Survey of LQCD applications

- Weak decays and matrix elements (Amarjit Soni, K to ππ)
- Hadron structure (Jian-Wei Qiu, parton distribution functions)
- **Hadron spectroscopy and interactions** — a sampling of lattice QCD results, enabled by theoretical, algorithmic and hardware developments
- Nonzero temperature and density: e.g., equation of state, deconfinement transition, dense QCD (complex Langevin)
- …

Correlation functions in Euclidean spacetime

$$C_{ij}(t) = \langle 0|\hat{\mathcal{O}}'_i e^{-\hat{H}t} \hat{\mathcal{O}}^\dagger_j |0\rangle$$

ensemble average over individual correlators

$$= \langle \mathcal{C}_{ij}(t) \rangle_U$$

$$= \sum_n Z'_{in} Z^*_{jn} e^{-E_n t}$$

sum over states

$$\hat{H}|n\rangle = E_n|n\rangle \qquad Z'_{in} = \langle 0|\hat{\mathcal{O}}'_i|n\rangle \qquad Z'_{jn} = \langle 0|\hat{\mathcal{O}}_j|n\rangle$$

Effective mass

linear combination of operators

$$v'^{\dagger} C(t) v = \langle 0 | \left(v'^{\dagger} \hat{\mathcal{O}}' \right) e^{-\hat{H} t} \left(\hat{\mathcal{O}}^{\dagger} v \right) | 0 \rangle \qquad \hat{\mathcal{O}}_v = v^{\dagger} \hat{\mathcal{O}}$$

typically one lattice spacing

$$m_{eff}(t) = -\frac{1}{\Delta t} \log \frac{v'^{\dagger} C(t + \Delta t) v}{v'^{\dagger} C(t) v}$$

exp. suppression at late times

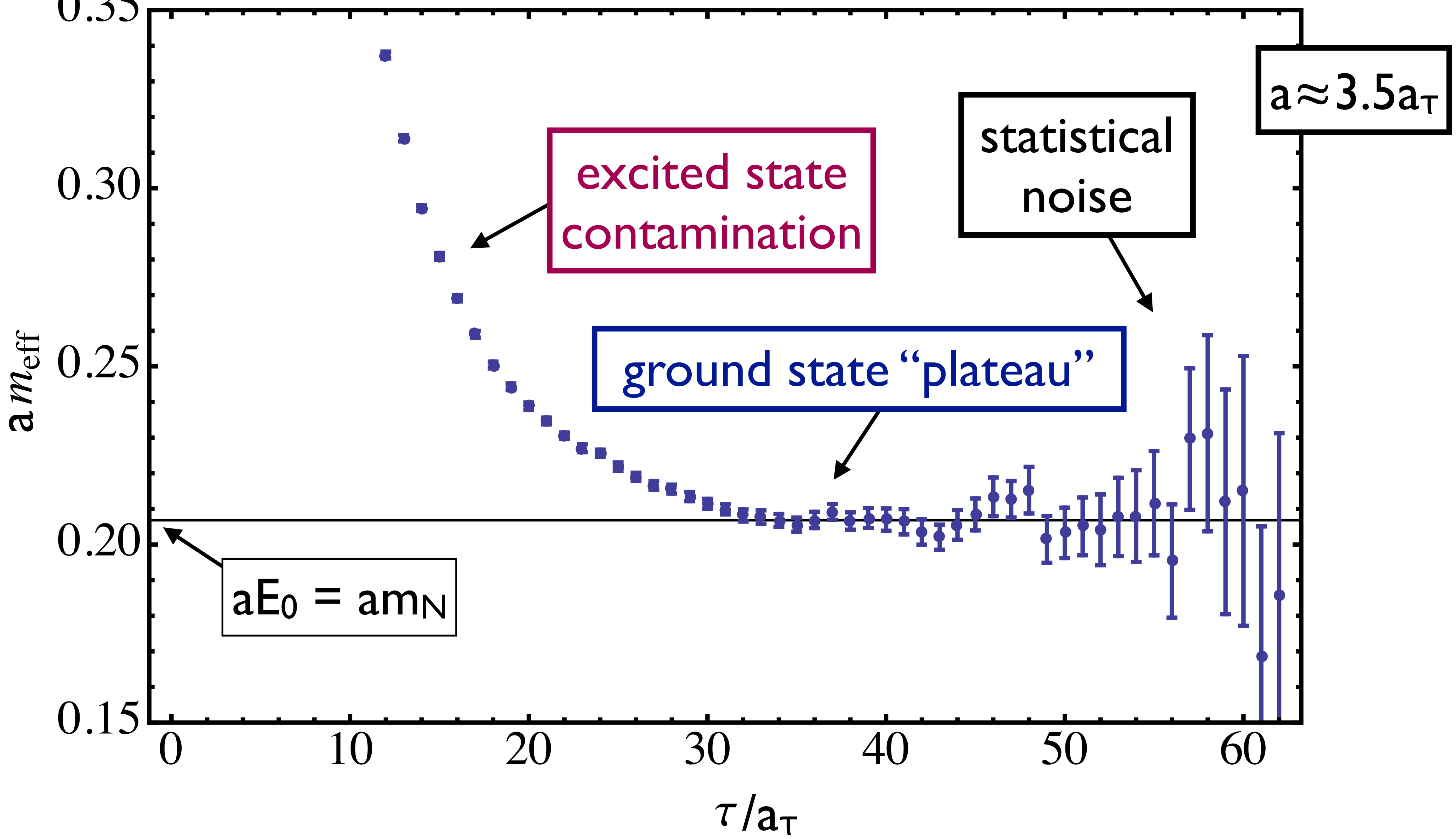
$$\approx \underline{E_0} + \underline{\frac{(v'^{\dagger} Z'_1)(v^{\dagger} Z_1)}{(v'^{\dagger} Z'_0)(v^{\dagger} Z_0)} \left[\frac{1 - e^{-(E_1 - E_0)\Delta t}}{\Delta t} \right] e^{-(E_1 - E_0) t} + \cdots}$$

ground state energy

“excited state contamination”

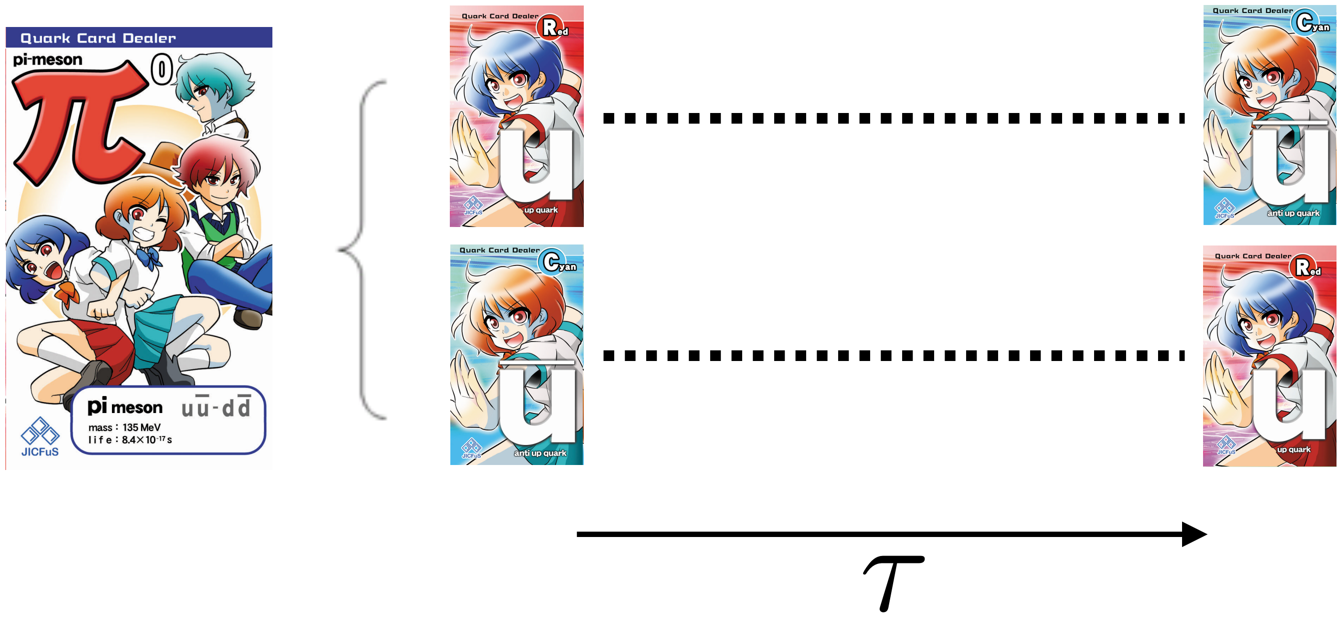
Effective mass — example: the nucleon

(data courtesy of The College of William & Mary)



Energies determined via fit to the "plateau region"

Understanding the origins of noise: pion

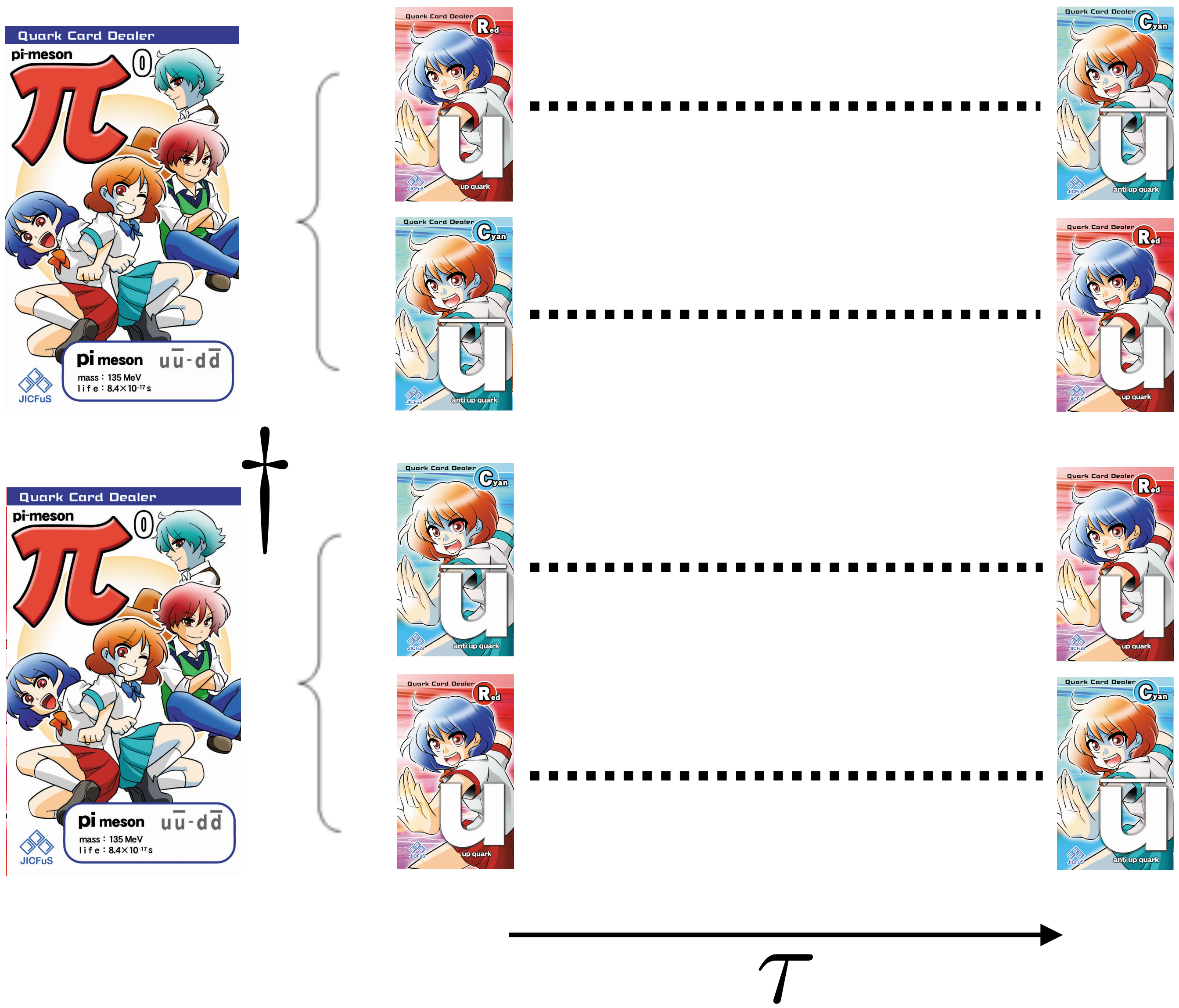


Signal:

$$C(t) = \langle \mathcal{C}(t) \rangle_U \sim e^{-m_\pi t}$$

$$\mathcal{C}(t) \sim D^{-1} D^{-1\dagger}$$

Understanding the origins of noise: pion

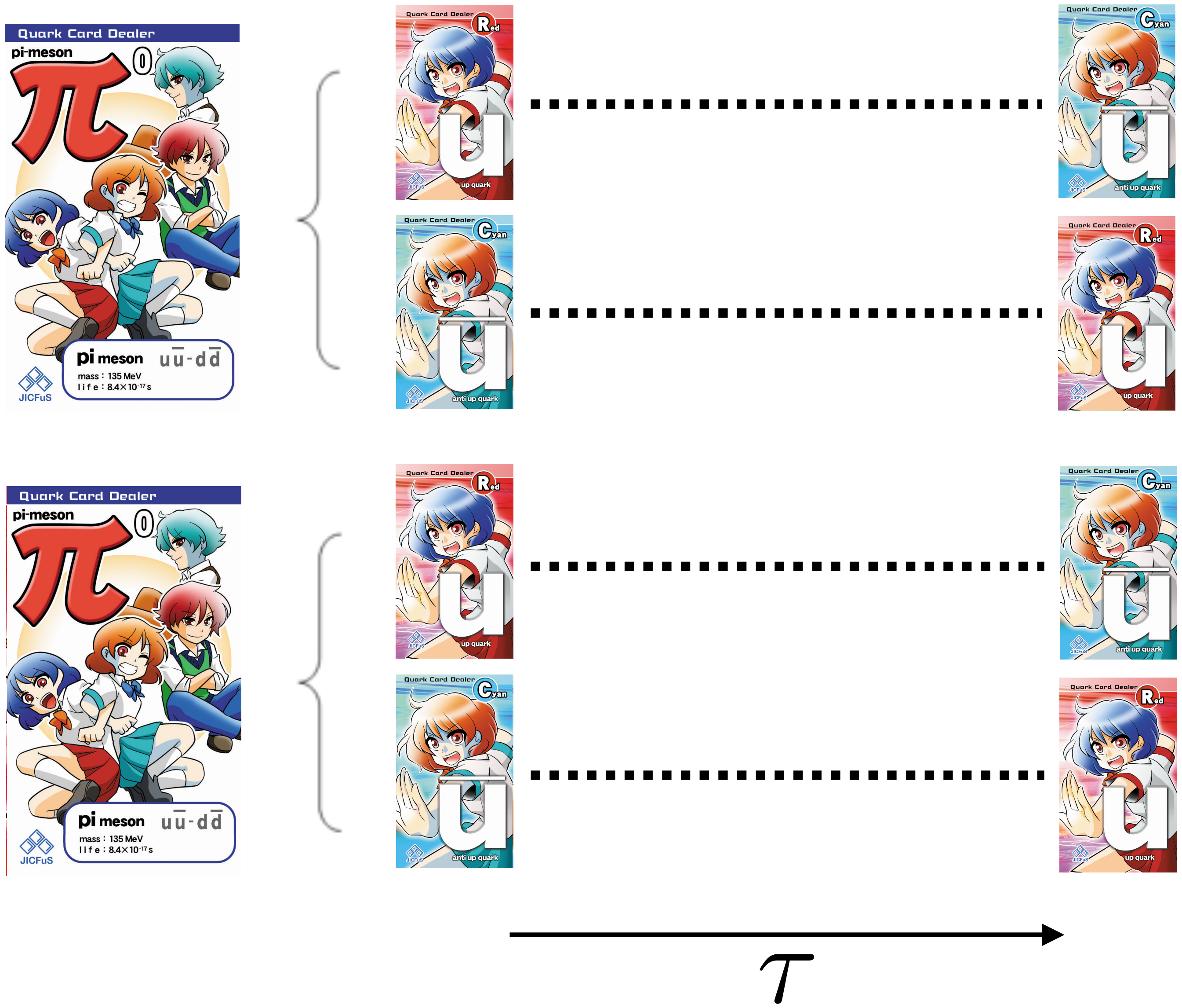


Variance:

$$\sigma^2(t) = \langle|\mathcal{C}(t)|^2\rangle_U - |\langle\mathcal{C}(t)\rangle_U|^2$$

$$|\mathcal{C}(t)|^2 \sim \quad D^{-1}D^{-1\dagger}$$
$$\times \quad D^{-1\dagger}D^{-1}$$

Understanding the origins of noise: pion



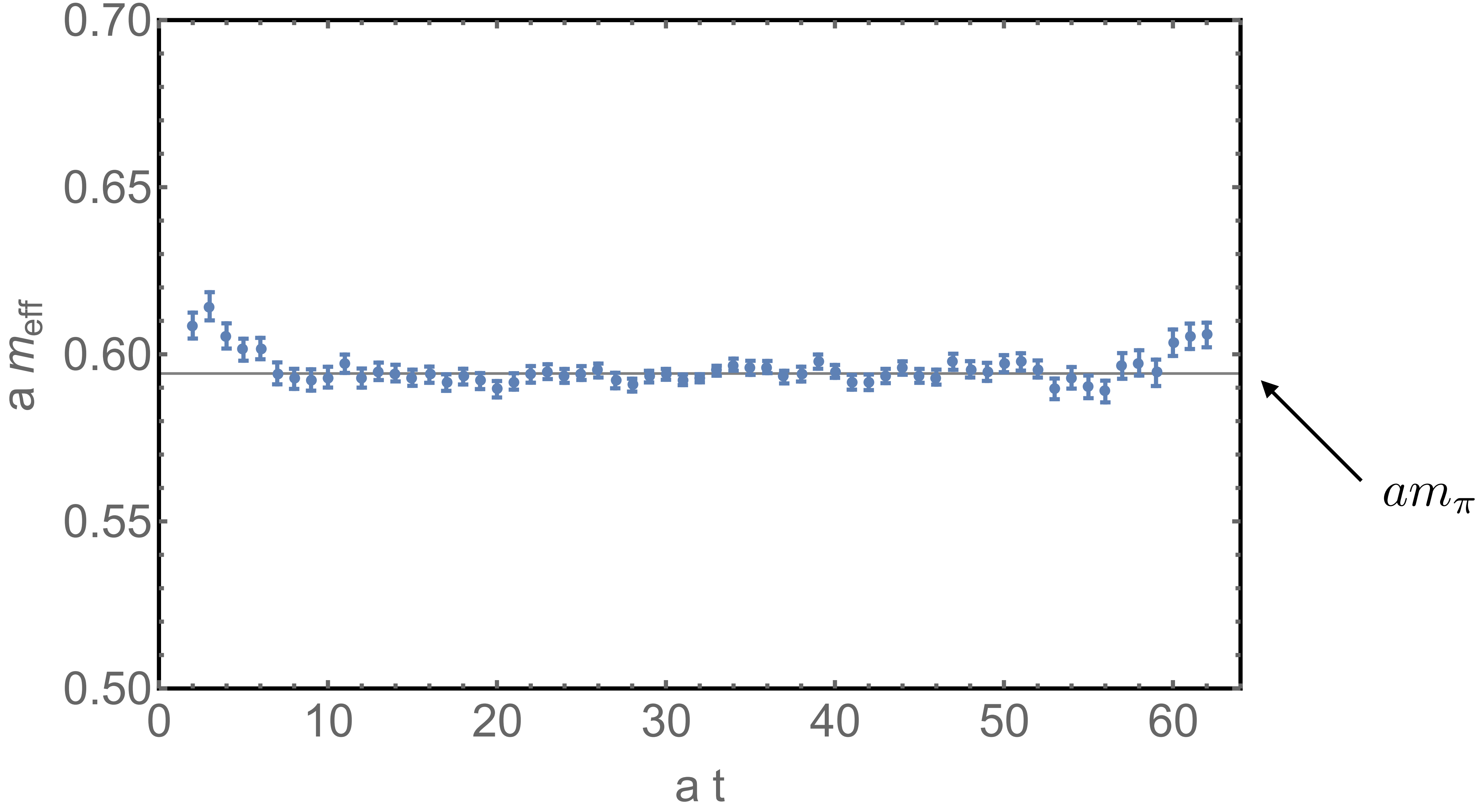
Variance:

$$\sigma^2(t) = \langle |\mathcal{C}(t)|^2 \rangle_U - |\langle \mathcal{C}(t) \rangle_U|^2$$

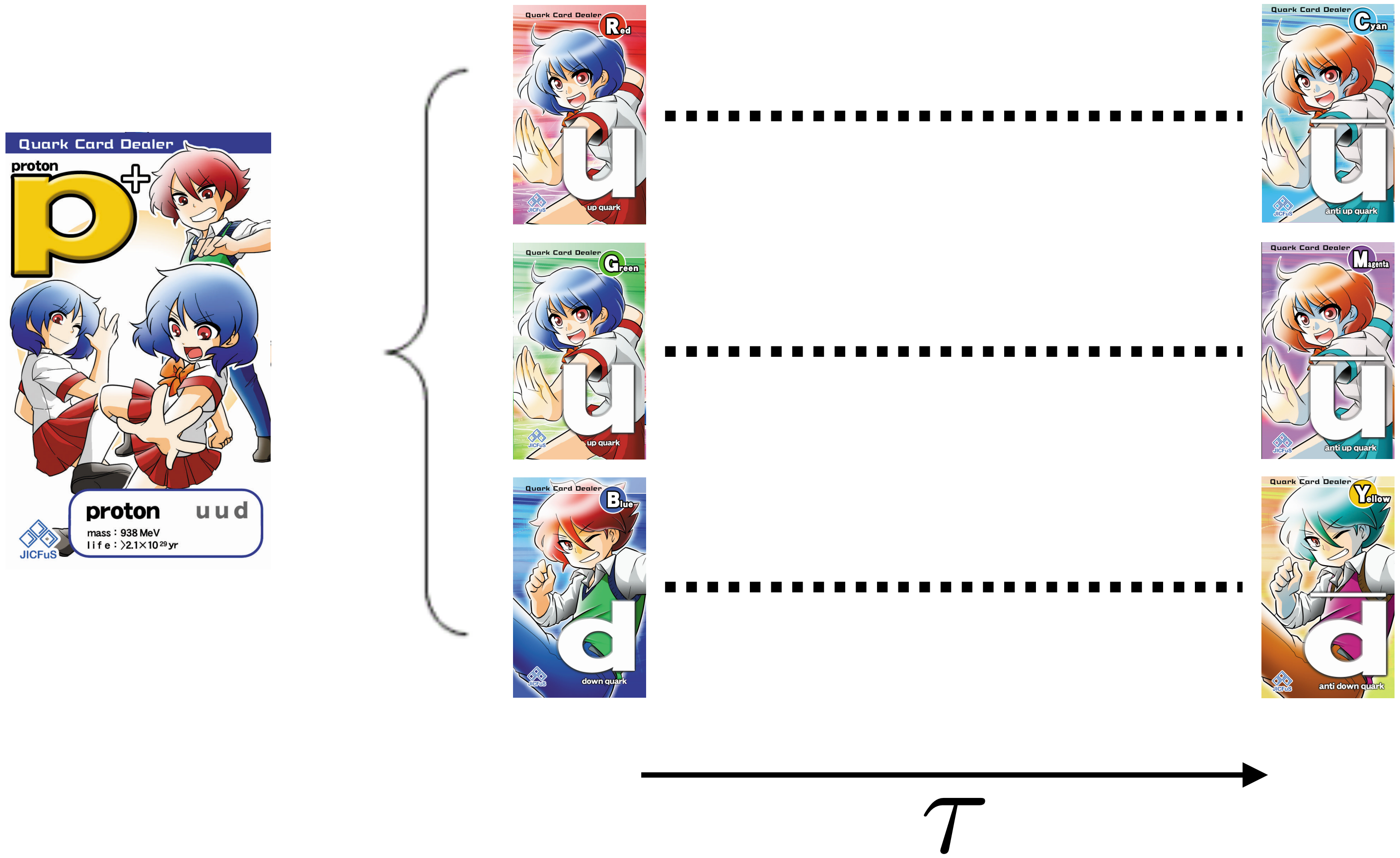
$$\sim e^{-2m_\pi}$$

Understanding the origins of noise: pion

$$s/n \sim C(t)/\sigma(t) \sim \mathcal{O}(1)$$



Understanding the origins of noise: nucleon



Signal:

$$C(t) = \langle \mathcal{C}(t) \rangle_U \sim e^{-m_p t}$$

$$\mathcal{C}(t) \sim D^{-1} D^{-1} D^{-1}$$

Understanding the origins of noise: nucleon

Variance:

$$\sigma^2(t) = \langle|\mathcal{C}(t)|^2\rangle_U - |\langle\mathcal{C}(t)\rangle_U|^2$$

$$\begin{aligned}|\mathcal{C}(t)|^2 \sim \quad & D^{-1}D^{-1}D^{-1} \\ \times \quad & {D^{-1}}^\dagger {D^{-1}}^\dagger {D^{-1}}^\dagger\end{aligned}$$

Understanding the origins of noise: nucleon

Variance:

$$\sigma^2(t) = \langle|\mathcal{C}(t)|^2\rangle_U - |\langle\mathcal{C}(t)\rangle_U|^2$$

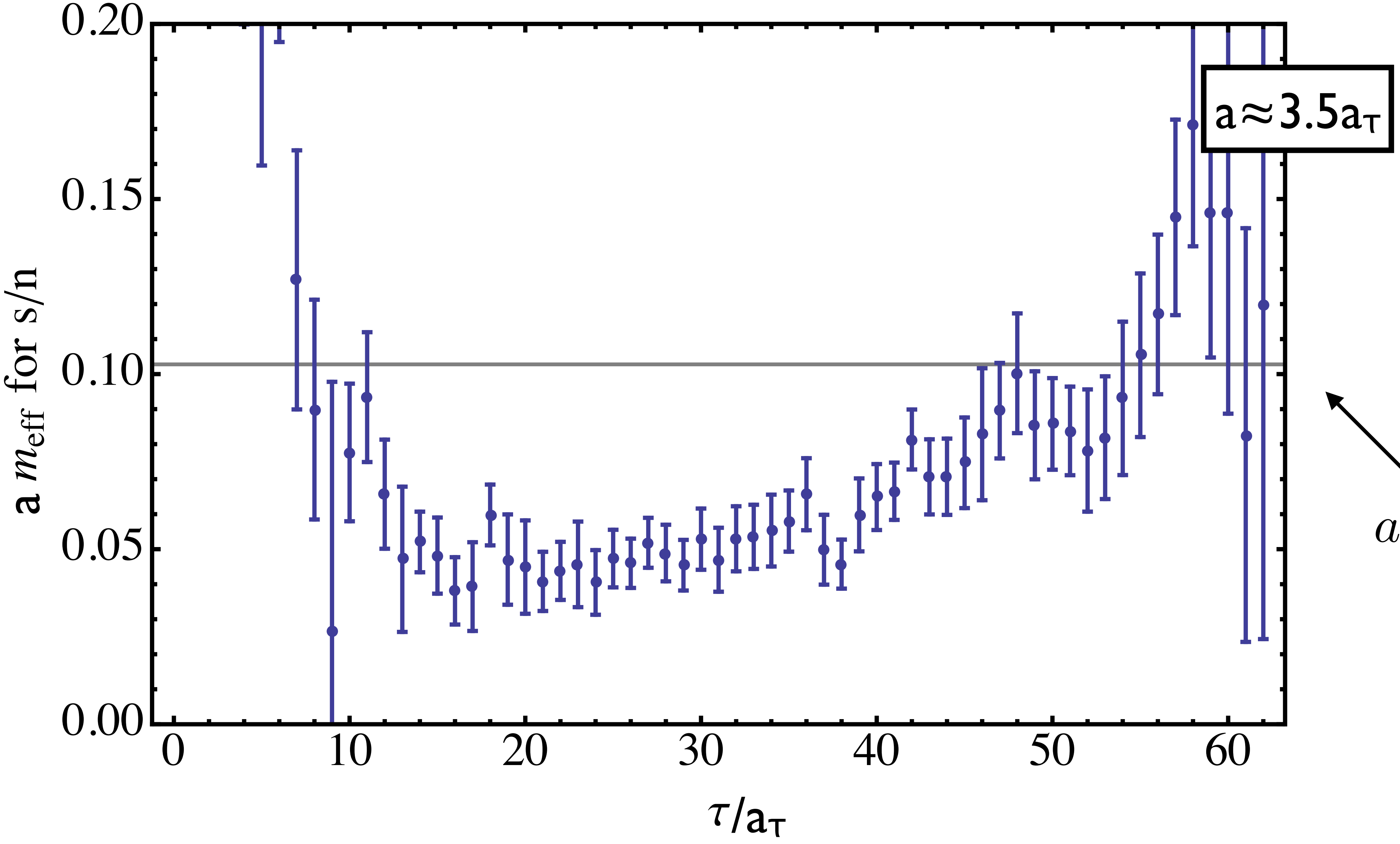
$$\sim e^{-3m_\pi t}$$

Variance is determined by pion physics

Understanding the origins of noise: proton

$$s/n \sim C(t)/\sigma(t) \sim e^{-(m_p - \frac{3}{2}m_\pi)t}$$

(data courtesy of The College of William & Mary)



$am_p - 3/2am_\pi$

Understanding the origins of noise: proton

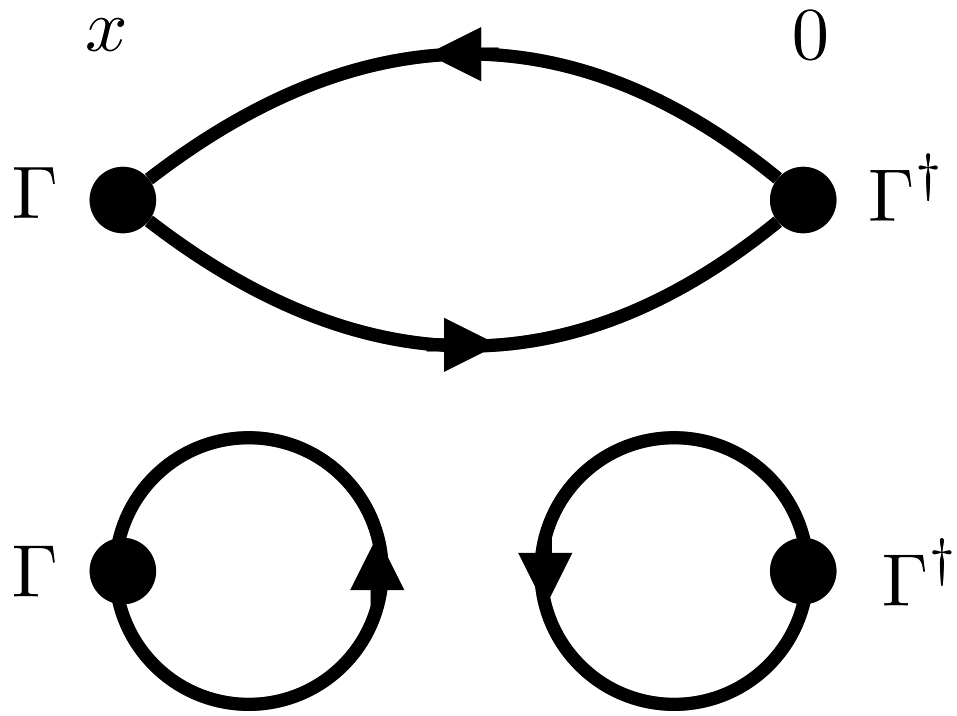
Lepage's argument: $s/n \sim e^{-(E_0 - \frac{3}{2}\tilde{E}_0)t}$

signal ground state

(multi-) pion or vacuum energy

- Generally, variance is governed by the lightest state with vacuum quantum numbers (and nontrivial valence QN)
  - e.g., pions or the vacuum itself
- Multi-baryon systems: exponential degradation with baryon number, e.g., a "signal/noise" problem
- Signal/noise problem is intimately related to the "sign-problem"

Disconnected diagrams



Generate random sources: $\xi_1, \xi_2, \cdots, \xi_M$

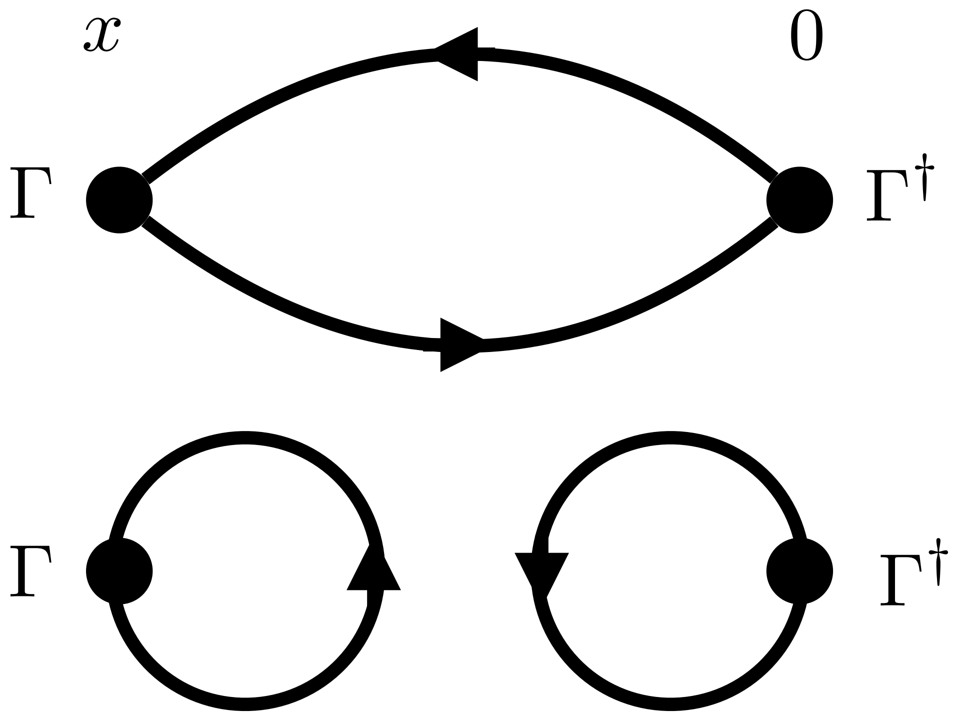
Such that: $\sum_{n=1}^{M} \xi_n \xi_n^\dagger = 1 + \mathcal{O}\left(M^{-1/2}\right)$

Solve: $D\eta_n = \xi_n \longrightarrow \eta_n = D^{-1}\xi_n$

Express correlator in terms of: $D^{-1} \approx \sum_{n=1}^{M} \eta_n \xi_n^\dagger$

$$\begin{aligned} \langle C_{\mathcal{M}}(x) \rangle &= -\left\langle \mathrm{Tr}\left[D_f^{-1}(0,x)\Gamma D_g^{-1}(x,0)\Gamma^\dagger\right]\right\rangle_U \\ &+ \left\langle \mathrm{Tr}\left[D_f^{-1}(x,x)\Gamma\right] \mathrm{Tr}\left[D_g^{-1}(0,0)\Gamma^\dagger\right]\right\rangle_U \delta_{fg} \end{aligned}$$

Disconnected diagrams



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Solve: $D\eta_n = \xi_n \longrightarrow \eta_n = D^{-1}\xi_n$

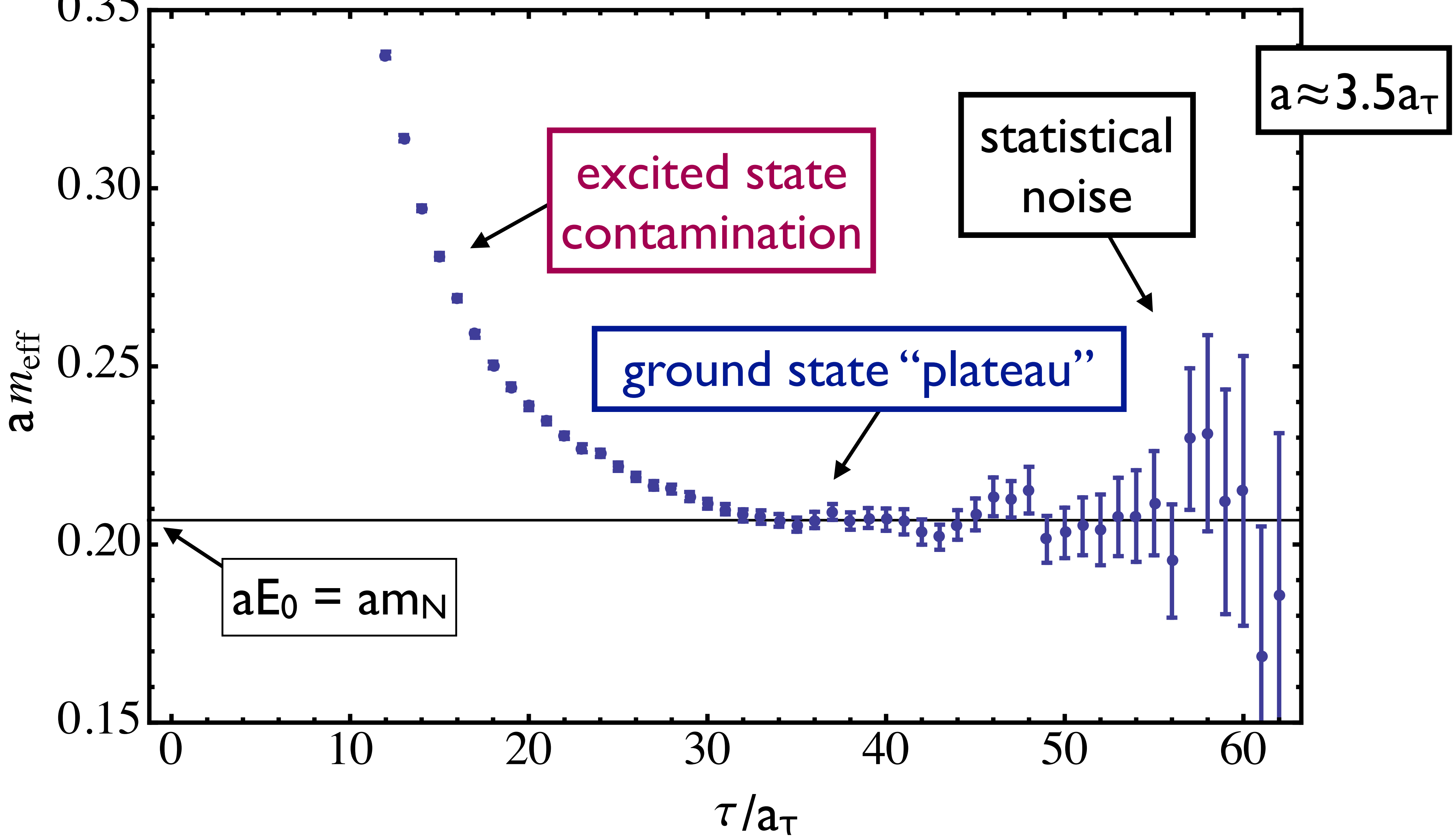
Express correlator in terms of: $$D^{-1} \approx \sum_{n=1}^{M} \eta_n \xi_n^\dagger$$

- Two sources of noise:
  - gauge noise
  - noise associates with stochastic estimate of D^{-1}

tune M so they are comparable

Effective mass — example: the nucleon

(data courtesy of The College of William & Mary)



To extend plateau, one can either:

1) *reduce contamination at early times*
2) *reduce statistical noise at late times*

Variance reduction

- (Semi-) recent algorithmic developments for variance reduction:
  - distillation [arXiv:0905.2160]
  - dilution [arXiv:0505023]
  - low mode averaging [hep-lat/0401011]
  - all mode averaging [arXiv:1208.4349]
  - signal/noise optimization of sources [arXiv:1404.6816]
- Despite advances, signal/noise remains a **significant** challenge for LQCD calculations

Generalized eigenvalue problem

Assuming NxN correlator:

Nucl. Phys. B215, 433 (1983)
Nucl.Phys. B339 (1990) 222-252
Nucl. Phys. B339, 222 (1990)
J. High Energy Phys. 04 (2009) 094

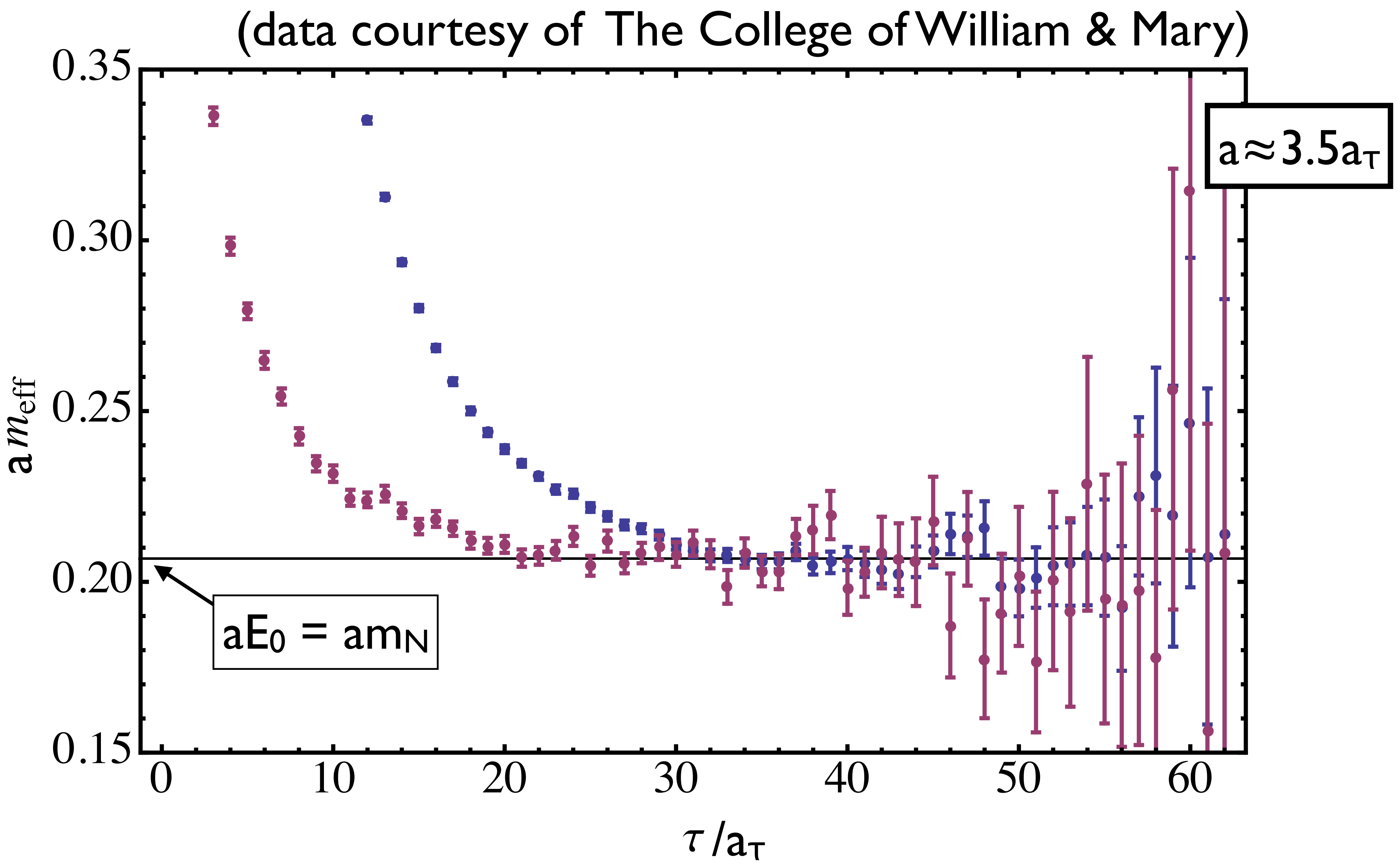
$$C(t) = C^\dagger(t)$$

$$C(t)v_n(t,t_0) = \lambda_n(t,t_0)C(t_0)v_n(t,t_0)$$

$$E_n = -\partial_t \log \lambda_n(t,t_0) + \mathcal{O}\left(e^{-(E_{N+1}-E_n)t}\right) \qquad t_0 < t < 2t_0$$

- **Observation:** correlator is like a truncated transfer matrix
- Solutions to generalized eigenvalue problem yield lowest N energy eigenstates, and operators with maximal overlap
- Enhanced excited state contamination in appropriate regimes
- Works best when operator basis is fairly orthogonal
- Enables extraction of not only ground, but excited states

Effective mass — example: the nucleon



- Other methods exist as well: intuition, Matrix Prony, …
- New/better methods highly desirable

Construction of operator basis

$$\hat{\mathcal{O}}_v = v^\dagger \hat{\mathcal{O}}$$

- Operators should have appropriate quantum numbers
  - definite momentum, parity, other quantum numbers
  - definite transformation properties of a lattice irrep

cubic group with parity:

— 48 group elements
— 10 irreps.
— pos. and neg. parity irreps. correspond to even and odd ℓ respectively

ℓ	decomposition
0	A_1^+
1	T_1^-
2	$E^+ \oplus T_2^+$
3	$A_2^- \oplus T_1^- \oplus T_2^-$
4	$A_1^+ \oplus E^+ \oplus T_1^+ \oplus T_2^+$
5	$E^- \oplus T_1^- \oplus T_1^- \oplus T_2^-$
6	$A_1^+ \oplus A_2^+ \oplus E^+ \oplus T_1^+ \oplus T_2^+ \oplus T_2^+$
9	$A_1^- \oplus A_2^- \oplus E^- \oplus T_1^- \oplus T_1^- \oplus T_1^- \oplus T_2^- \oplus T_2^-$

Construction of operator basis

$$\hat{\mathcal{O}}_v = v^\dagger \hat{\mathcal{O}}$$

Example:

- A_1^+ irrep contains l=0,4,6….
- T_1^- irrep contains l=1,3,5,…

cubic group with parity:

— 48 group elements
— 10 irreps.
— pos. and neg. parity irreps. correspond to even and odd ℓ respectively

ℓ	decomposition
0	A_1^+
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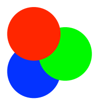
5	$E^- \oplus T_1^- \oplus T_1^- \oplus T_2^-$
6	$A_1^+ \oplus A_2^+ \oplus E^+ \oplus T_1^+ \oplus T_2^+ \oplus T_2^+$
9	$A_1^- \oplus A_2^- \oplus E^- \oplus T_1^- \oplus T_1^- \oplus T_1^- \oplus T_2^- \oplus T_2^-$

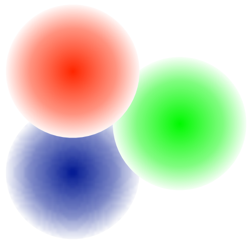
Construction of operator basis

$$\hat{\mathcal{O}}_v = v^\dagger \hat{\mathcal{O}}$$

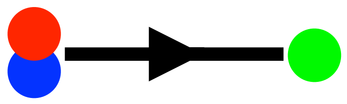
- Operators should have appropriate quantum numbers
  - definite momentum, parity, other quantum numbers
  - definite transformation properties of a lattice irrep
- Target states are extended objects on the lattice
  - point sources not ideal



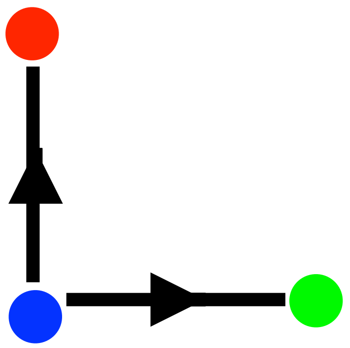
point



smeared



displaced



double displaced

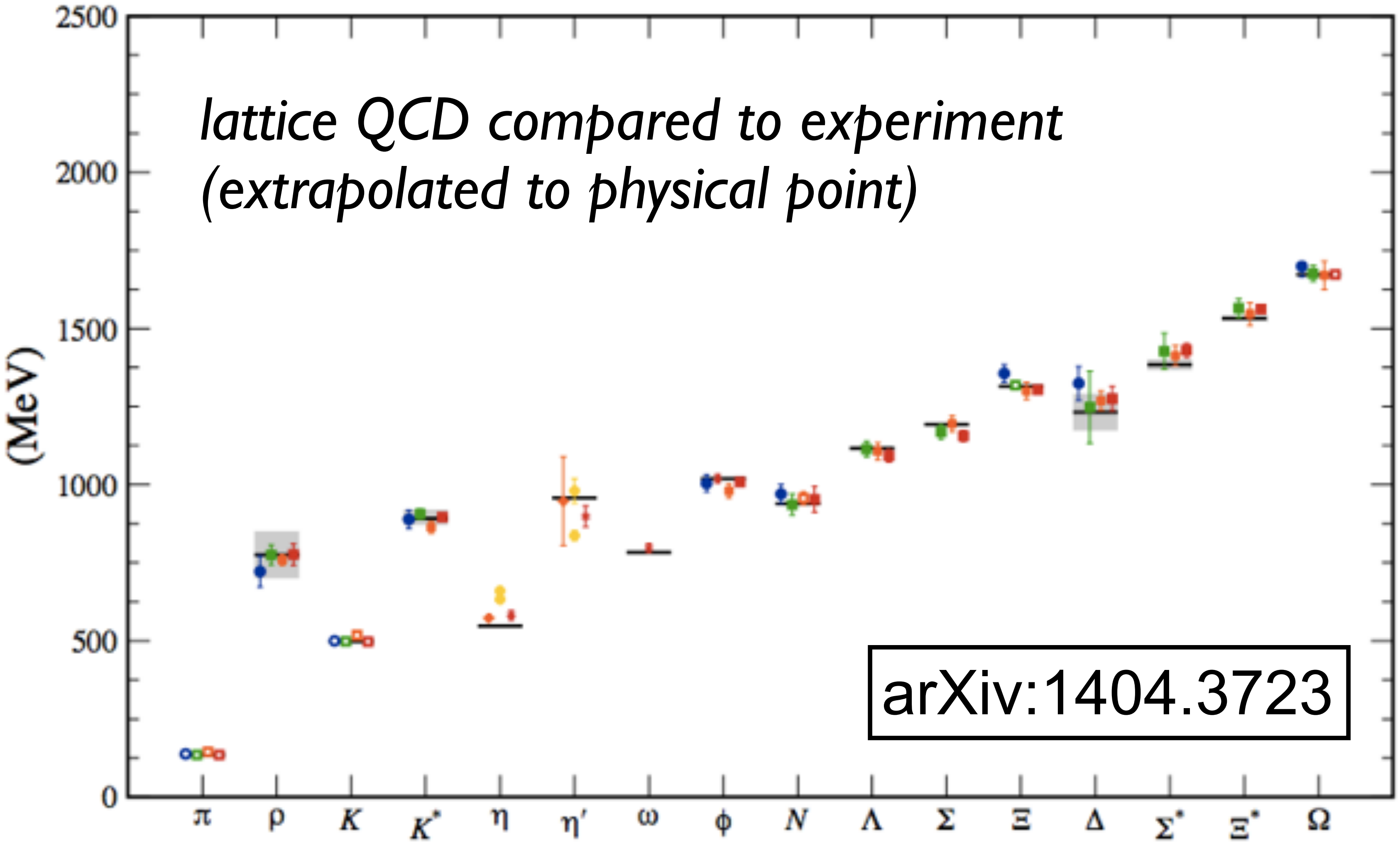
Construction of operator basis

$$\hat{\mathcal{O}}_v = v^\dagger \hat{\mathcal{O}}$$

- Operators should have appropriate quantum numbers
  - definite momentum, parity, other quantum numbers
  - definite transformation properties of a lattice irrep
- Target states are extended objects on the lattice
  - point sources not ideal
- Ideal choice of operators should generally have:
  - low statistical noise
  - large overlap onto target states

not necessarily compatible!

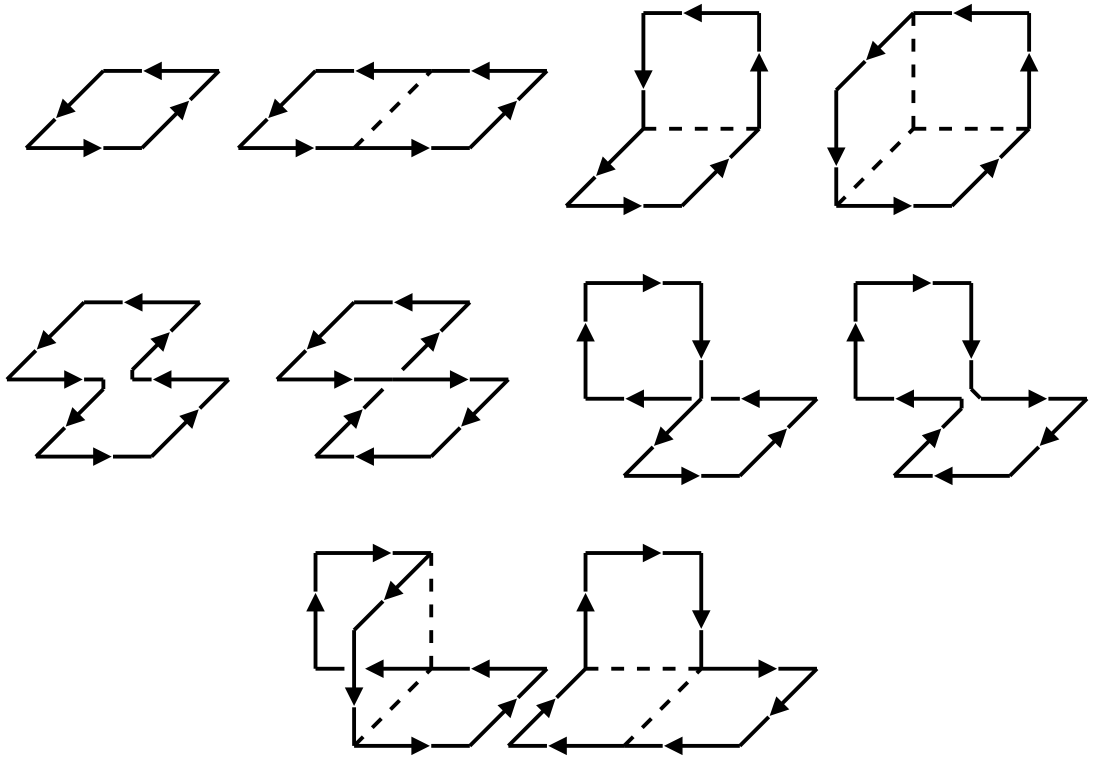
Light hadron spectroscopy

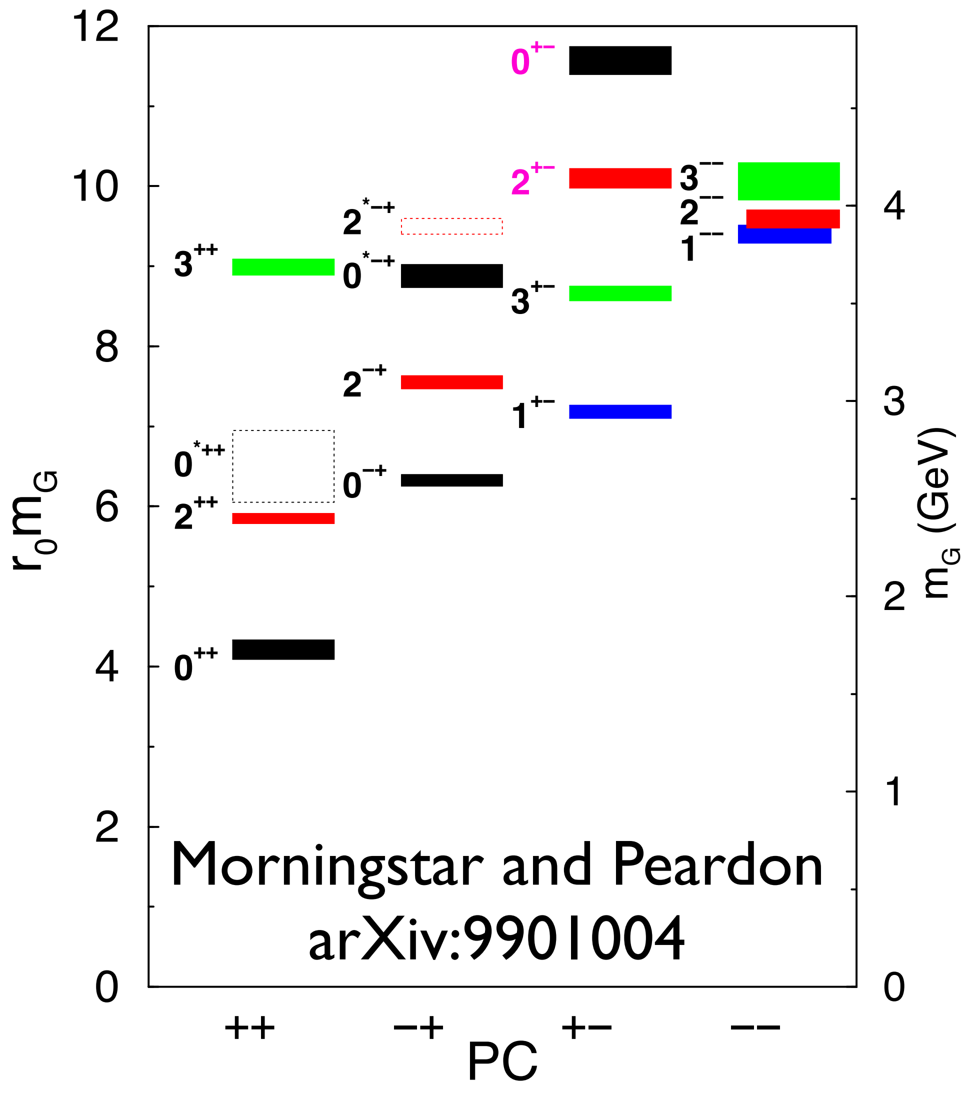


- Summary results: includes MILC, PAC-CS, BMW, QCDSF, RBC&UKQCD and Hadron Spectrum collaborations
- Bars/boxes represent experimentally measured masses/widths
- Agreement: systematics (different for each) are under control

Glueball spectrum (pure YM)

- Operator basis: gauge invariant combinations of Wilson loops
- Glueball spectrum extracted using variational method (GEVP)
- Continuum limit, identification of continuum quantum numbers

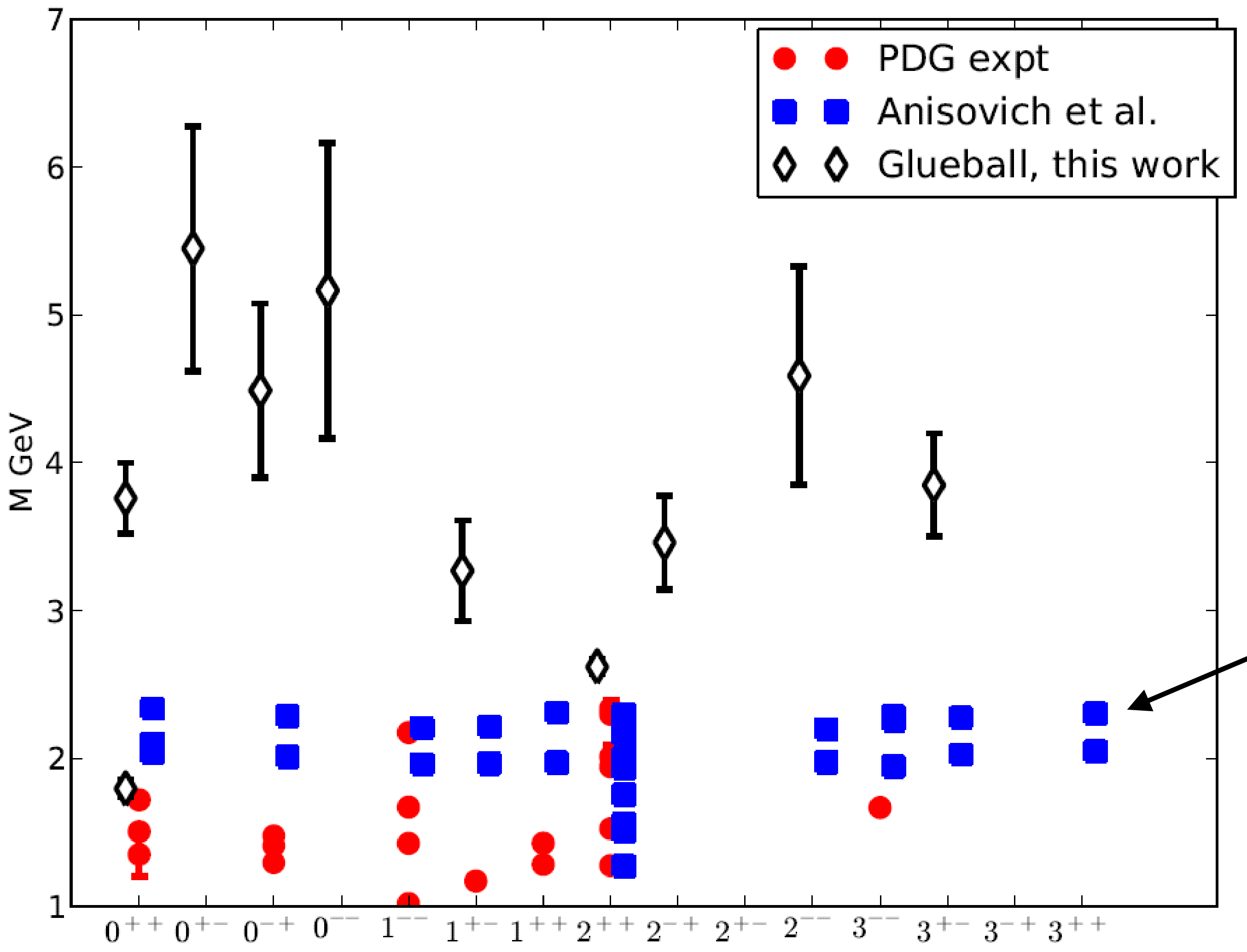




Morningstar and Peardon arXiv:9901004

J^{PC} notation; spin J, parity P and charge conjugation parity C

Glueball spectrum (QCD)

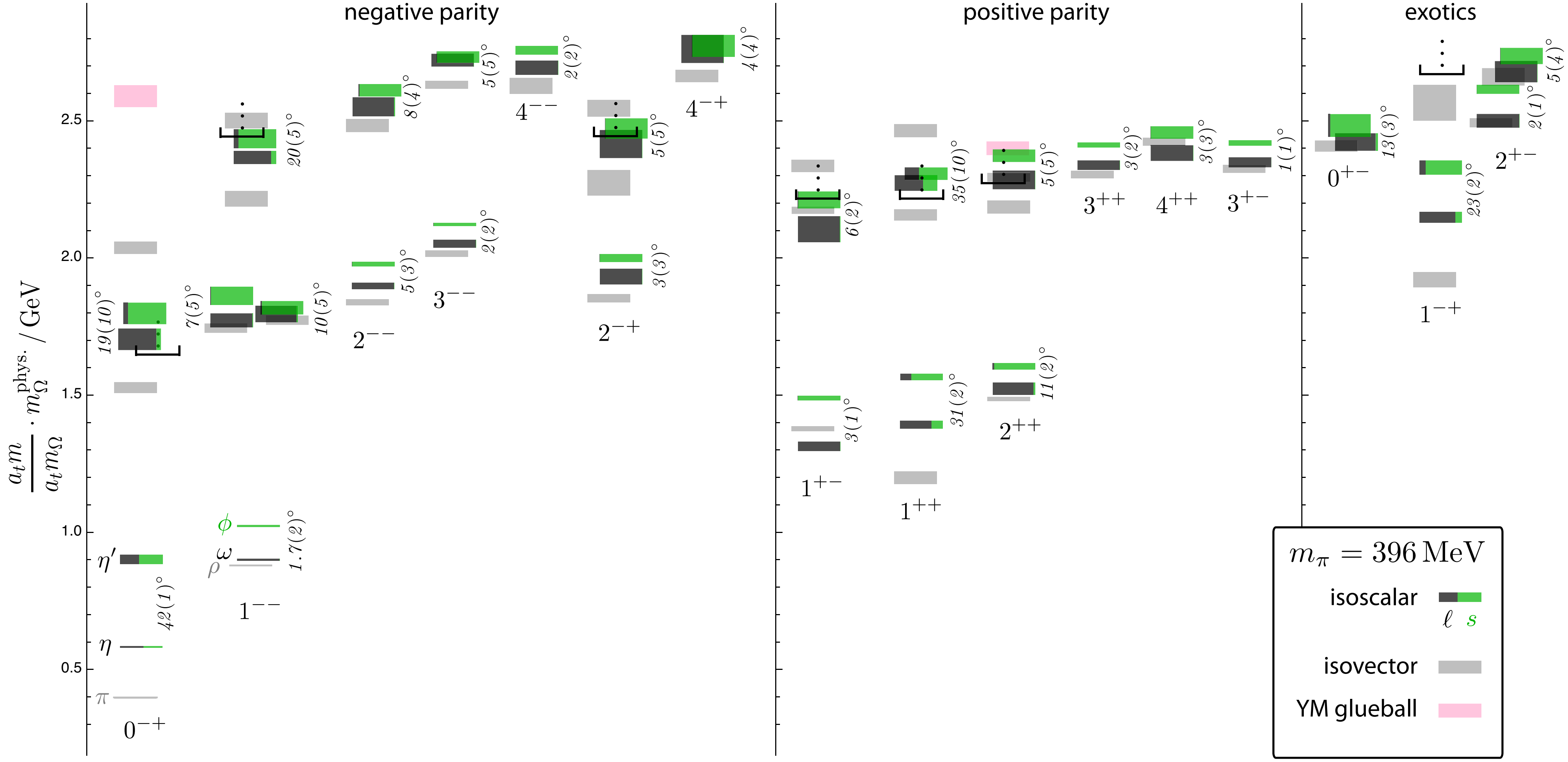


Gregory, et al. [arXiv:1208.1858]

I=0 meson masses (experiment)

- 2+1 flavors, a = 0.092 fm, 360 MeV pions
- Variational analysis using O(30) glueball operators
- Assignment of quantum numbers a challenge (e.g., multiple ℓ in a lattice irrep)
- Consistent with quenched studies, although continuum extrapolation needed

Light meson spectrum



Hadron Spectrum Collaboration: arXiv:1102.4299

- Isoscalar meson spectrum (labeled J^{PC})
- Black/green mixing angle between light/strange quark basis states; determined from overlap factors obtained from GEVP

Maiani-Testa no-go theorem/Luscher formalism

- Monte Carlo calculations are performed in Euclidean space; Wick rotation required for measure positivity of path integral
  - single hadron energies remain straight-forward to extract
  - in general, scattering matrix elements cannot be extracted from infinite volume Euclidean space correlation functions
- Luscher developed formalism for relating two particle infinite volume elastic scattering phase-shifts to energy shifts in a finite volume
- Recent extensions of the formalism to three particles in a finite box
  - Polejaeva, & Akaki [arXive:1203.1241]
  - Briceno & Davoudi [arXive:1212.3398]
  - Hansen & Sharpe [arXiv:1408.5933]

Luscher's formula: two particle s-wave phase shifts

$$p \cot \delta(p) = \frac{1}{\pi L} S\left(\frac{pL}{2\pi}\right)$$

quantization condition for three-momentum $p = |\mathbf{p}|$

$$S(\eta) = \sum_{\mathbf{n}}^{\Lambda} \frac{1}{\mathbf{n}^2 - \eta^2} - 4\pi\Lambda$$

well-defined limit as Λ removed

$$p \cot \delta(p) = -\frac{1}{a} + \frac{r}{2} p^2 + \cdots$$ (higher order shape parameters)

scattering length

effective range

Luscher's formula: two particle s-wave phase shifts

$$p \cot \delta(p) = \frac{1}{\pi L} S\left(\frac{pL}{2\pi}\right)$$

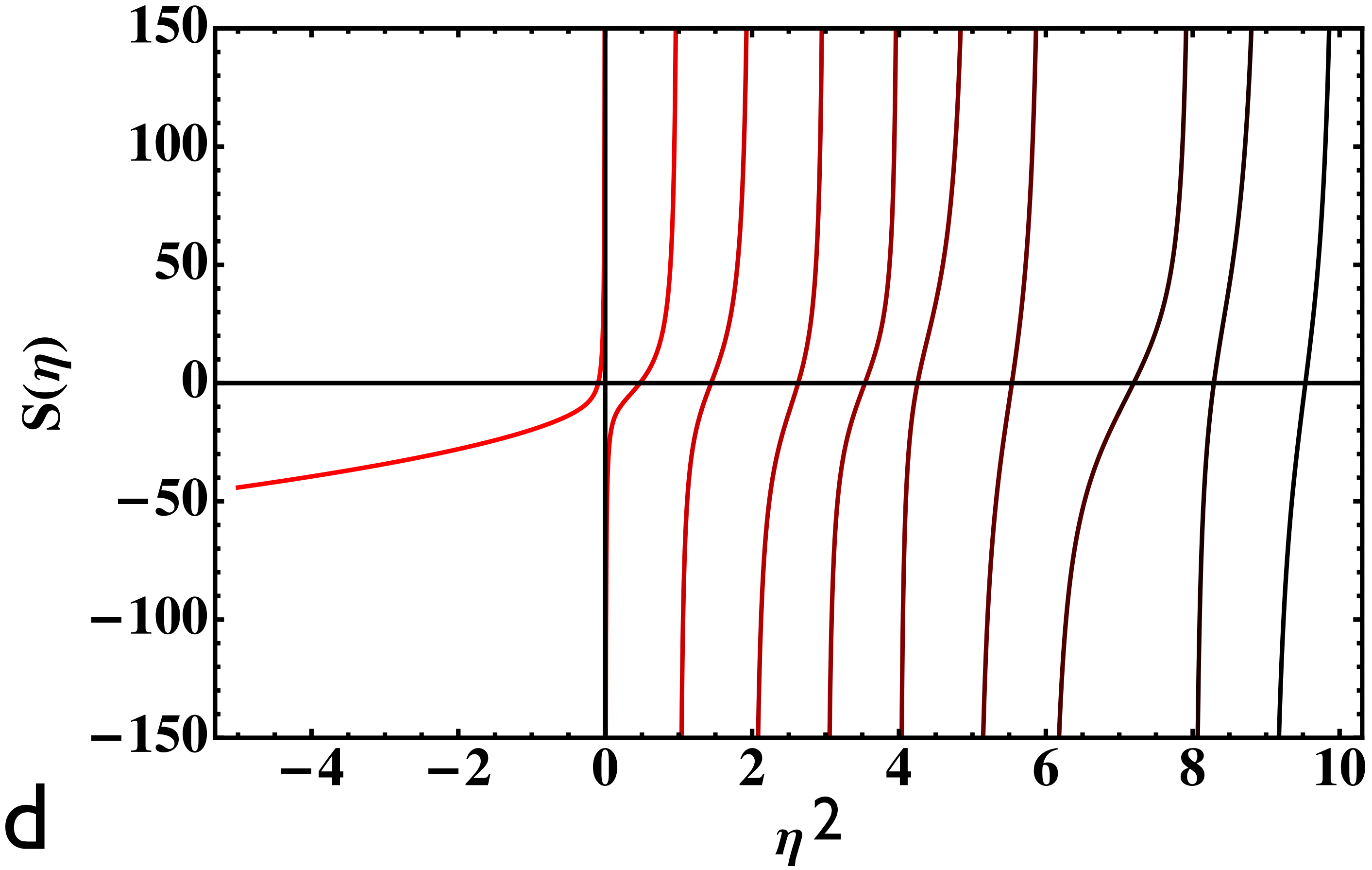
quantization condition for three-momentum $p = |\mathbf{p}|$

$$S(\eta) = \sum_{\mathbf{n}}^{\Lambda} \frac{1}{\mathbf{n}^2 - \eta^2} - 4\pi\Lambda$$

well-defined limit as Λ removed

Above assumes:

- r<<L
- no assumption on a
- s-wave scattering (generalizes to $\ell \neq 0$)
- below inelastic threshold



Luscher's formula: two particle s-wave phase shifts

$$p \cot \delta(p) = \frac{1}{\pi L} S\left(\frac{pL}{2\pi}\right)$$

quantization condition for three-momentum $p = |\mathbf{p}|$

- If scattering phase shifts are known as a function of momentum, then the allowed scattering momenta (and therefore) energy spectrum is predicted in a finite box

$$\delta(p) \longrightarrow p_n \longrightarrow E_n = 2\sqrt{m^2 + p_n^2}$$

- If energies spectrum in known in a finite box (determined via numerical calculation) then the scattering phase shifts can be determined at the corresponding scattering momenta

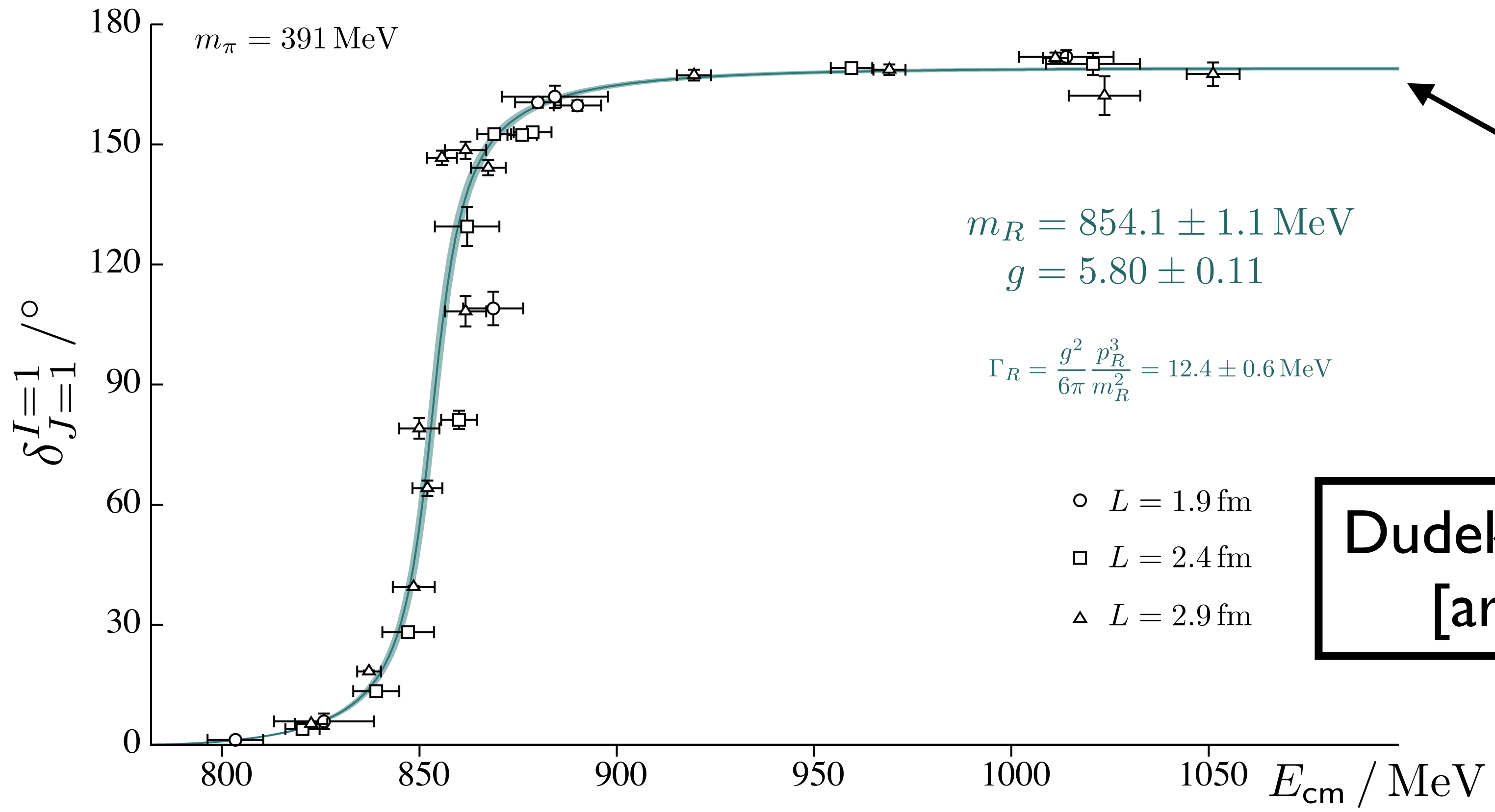
$$\delta(p_n) \longleftarrow p_n \longleftarrow E_n = 2\sqrt{m^2 + p_n^2}$$

Luscher's formula: two particle s-wave phase shifts

$$\delta(p_n) \longleftarrow p_n \longleftarrow E_n = 2\sqrt{m^2 + p_n^2}$$

- Practical issue:
    - Luscher's formula gives δ(p) for discrete values of p, determined by two-particle energy eigenstates of the system
    - a scan in δ(p) requires accessing more energies; changing lattice volume computationally expensive
- Methods developed for accessing wider range of energies from a single simulation, e.g.,
    - use of asymmetric lattices, include nonzero total momentum operators
    - imposing twisted boundary conditions

I=1 P=1 ππ scattering (contains ρ resonance)



Breit-Wigner fit

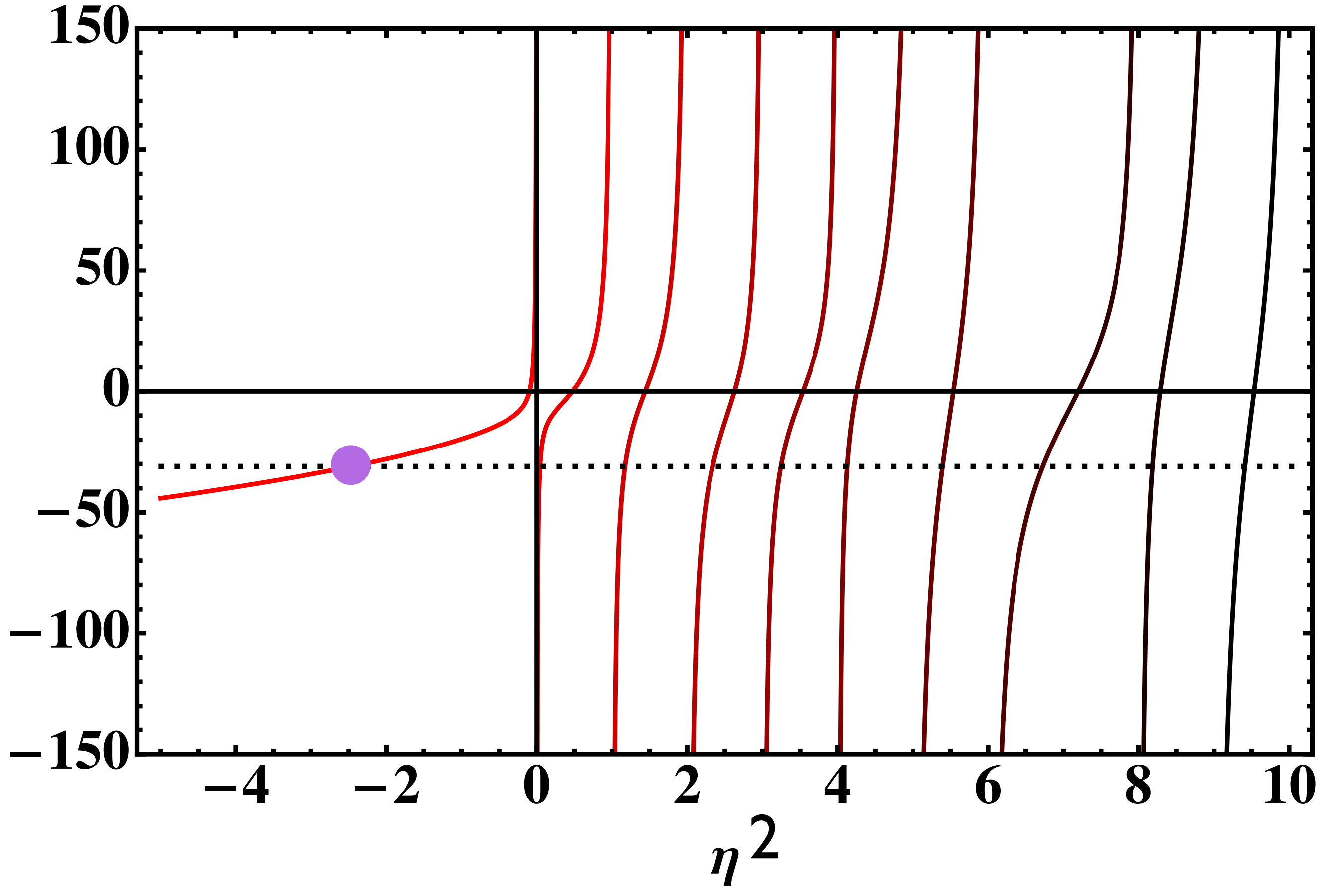
Dudek, Edwards, Thomas [arXiv:1212.0830]

- Resonances appear as rapid change in scattering phase shift in the corresponding scattering channel
- Mapping out δ requires:
  - basis includes single hadron and multi-hadron operators
  - determination of many energy levels (e.g., using GEVP)
  - use of $\ell = 1$ form of Luscher's formula

Luscher's formula — bound states

$$p \cot \delta(p) = \frac{1}{\pi L} S\left(\frac{pL}{2\pi}\right)$$

$$S(\eta) = \sum_{\mathbf{n}}^{\Lambda} \frac{1}{\mathbf{n}^2 - \eta^2} - 4\pi\Lambda$$

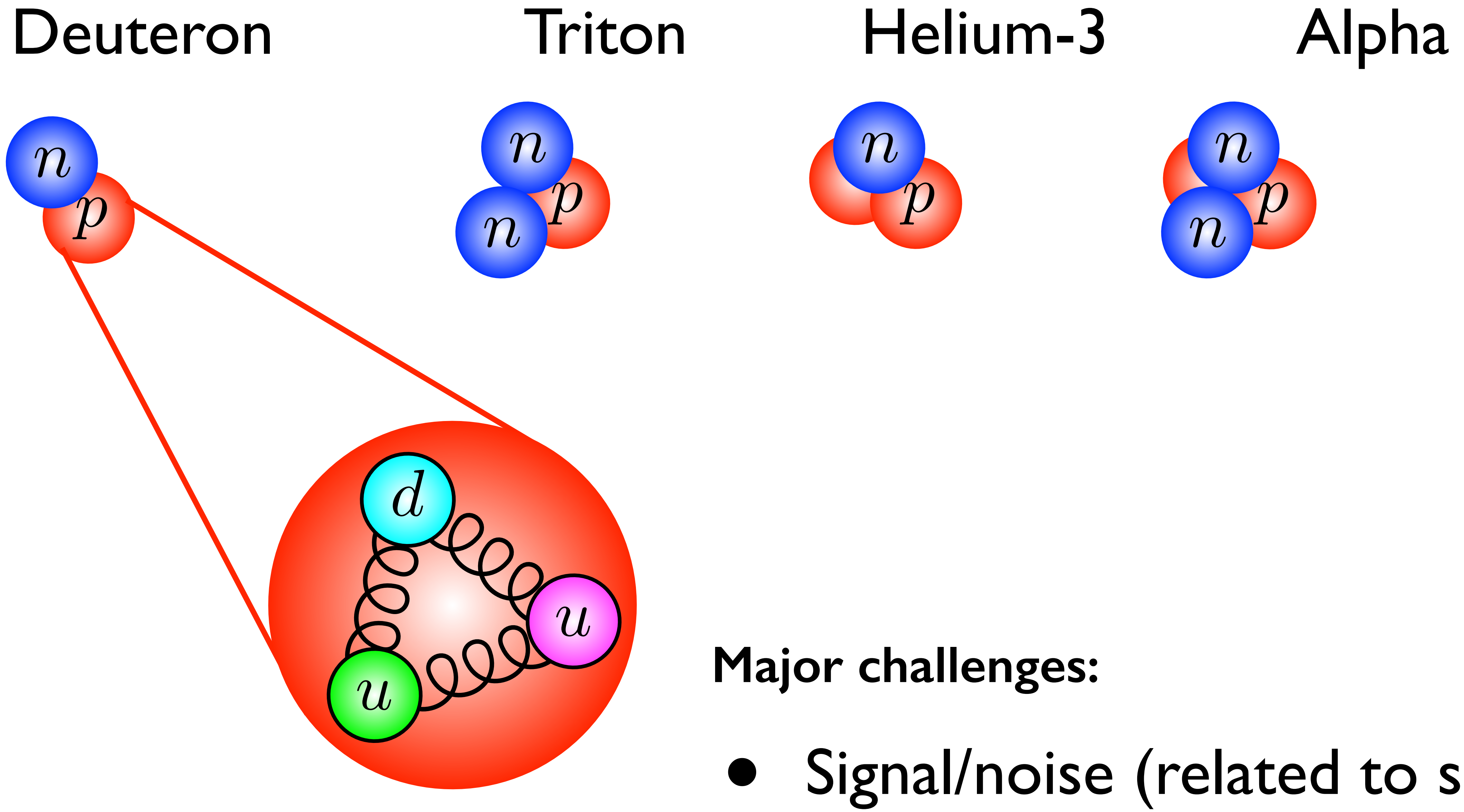


Beane, et al, hep-lat/0312004

$L \gg |a|$ $$E_{-1} = -\frac{\gamma^2}{m}\left[1 + \mathcal{O}(e^{-\gamma L})\right]$$ $$\gamma + p \cot \delta(p)|_{p^2=-\gamma^2} = 0$$

finite vol. corrections controlled by γL, where γ is the binding momentum

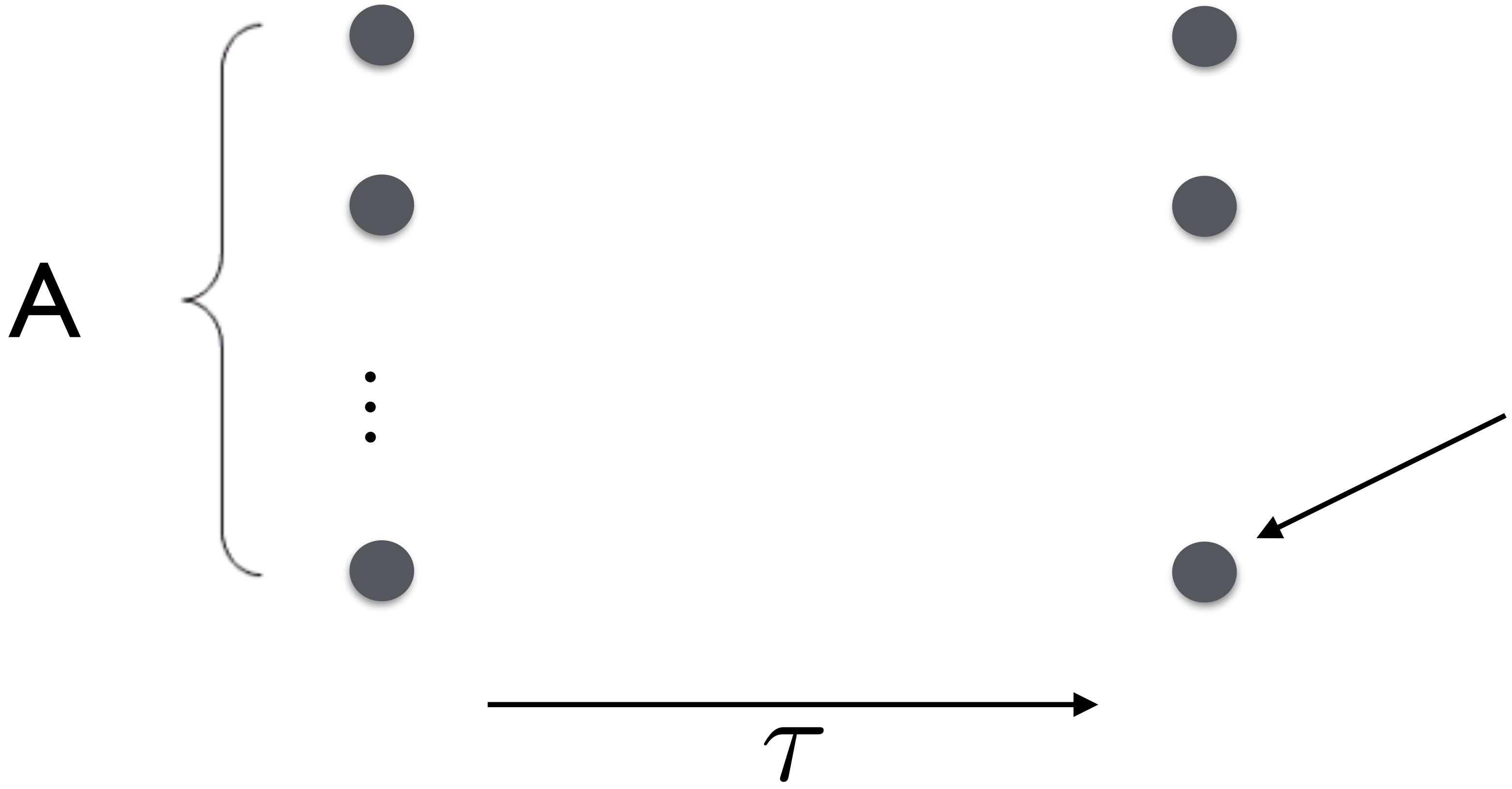
Many hadron systems — nuclei



Major challenges:

- Signal/noise (related to sign problem)
- Contraction problem

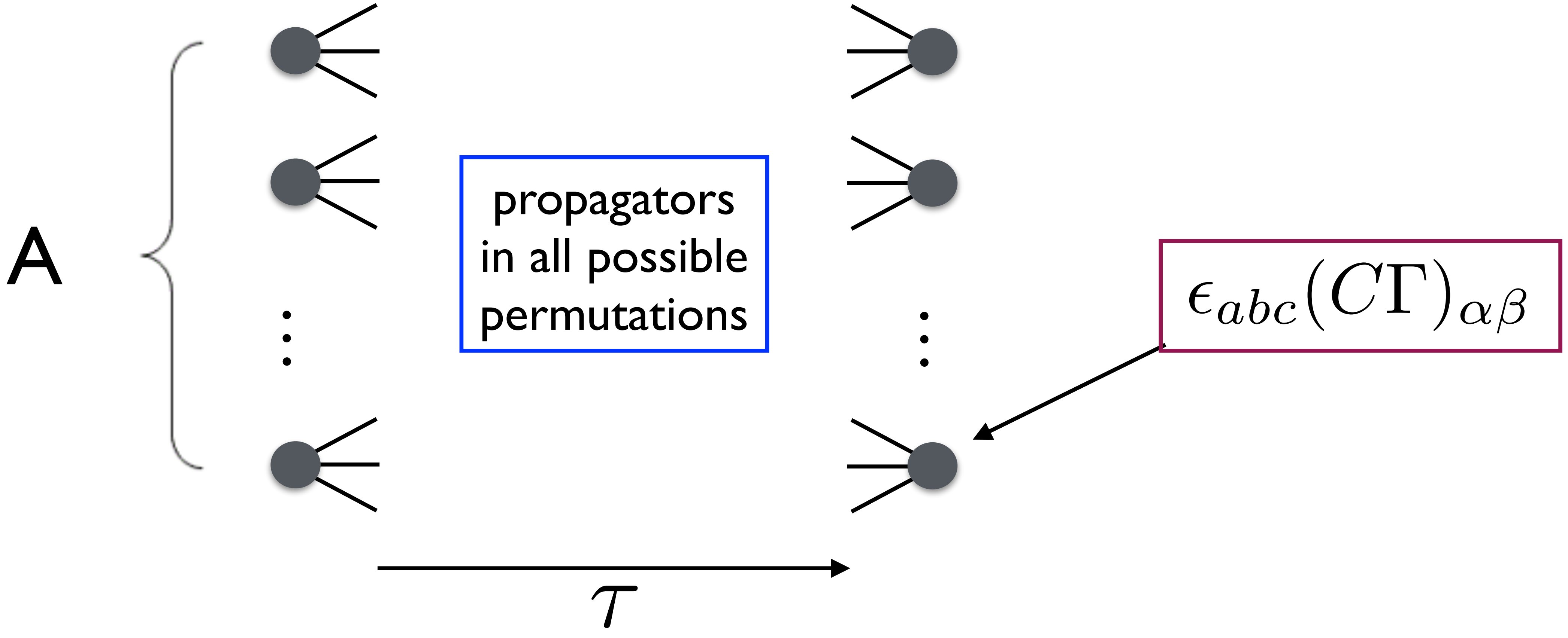
Multi-baryon contractions



nucleon:

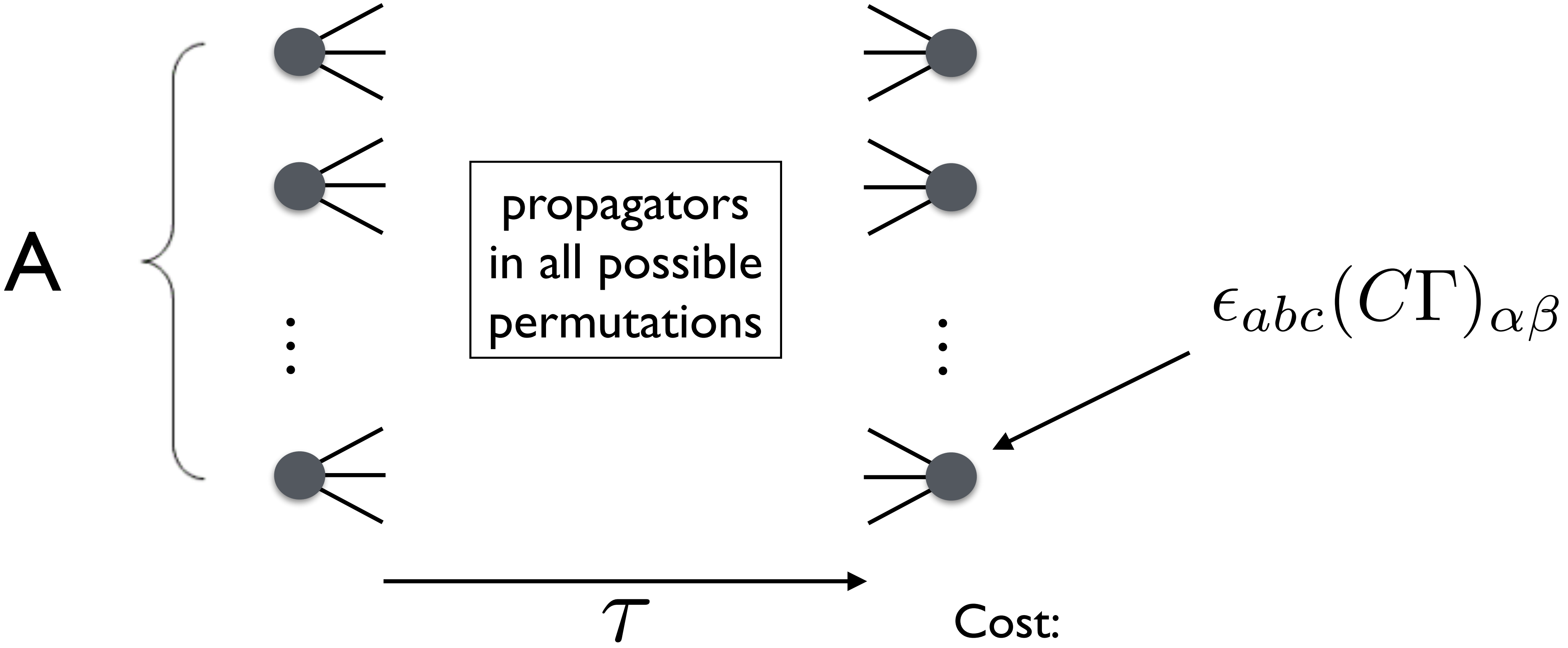
$N \sim (q^T C\Gamma q)q$

Multi-baryon contractions



$$\langle \mathcal{O}(U,\bar{q},q)\rangle = \frac{1}{Z}\int [dU]\, e^{-S_G[U]} \det D[U] \underbrace{\mathcal{O}^{[U]}_{i_1,\cdots,i_N;j_N,\cdots,j_1}}_{\text{products of } \epsilon \text{ and } C\Gamma} \underbrace{\Delta^{[U]}_{i_1,\cdots,i_N;j_N,\cdots,j_1}}_{\text{Wick contractions}}$$

Multi-baryon contractions



propagators in all possible permutations

$\epsilon_{abc}(C\Gamma)_{\alpha\beta}$

Cost:

$^{3}\mathrm{H}: 191102976 \times 2880$

$^{3}\mathrm{He}: 191102976 \times 2880$

$^{4}\mathrm{He}: 110075314176 \times 518400$

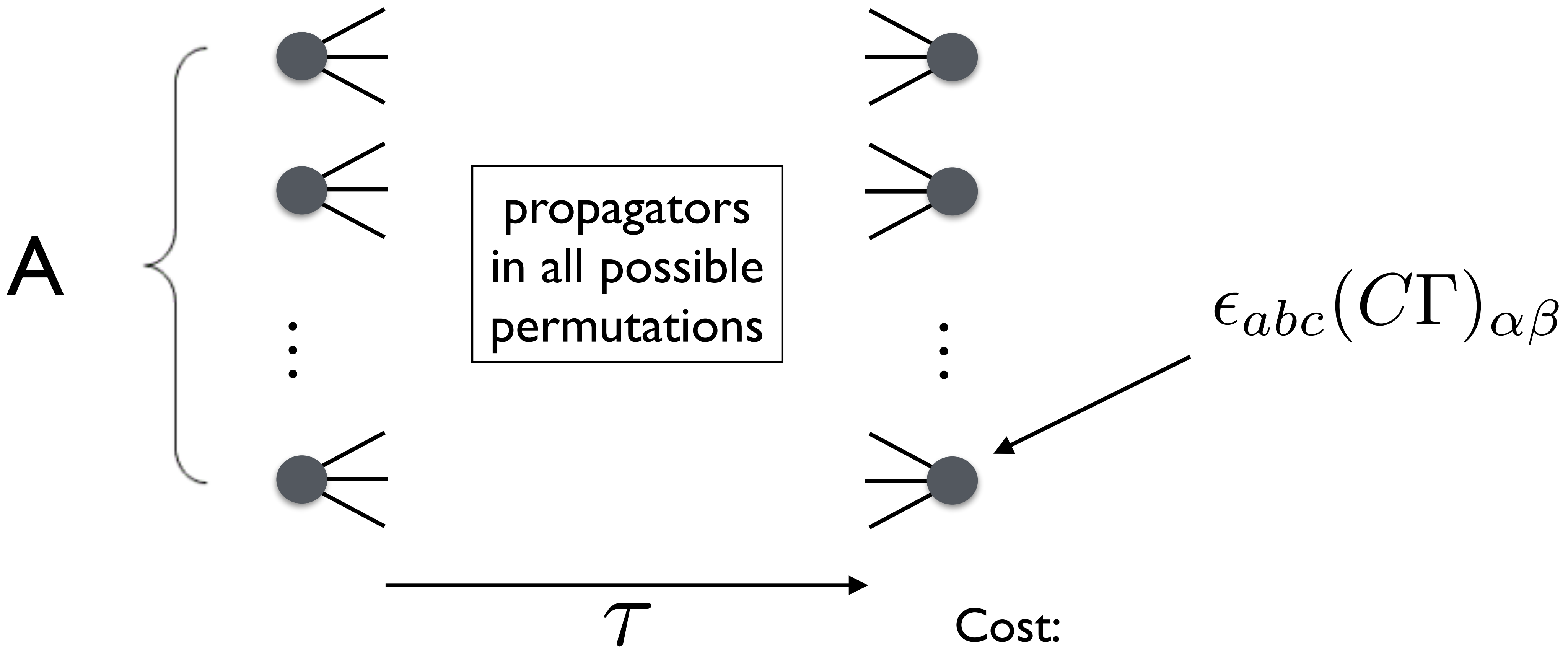
cost/config $\sim 6^{2A} 4^{2A} N_u! N_d!$

color

spinor

quark perms (naive)

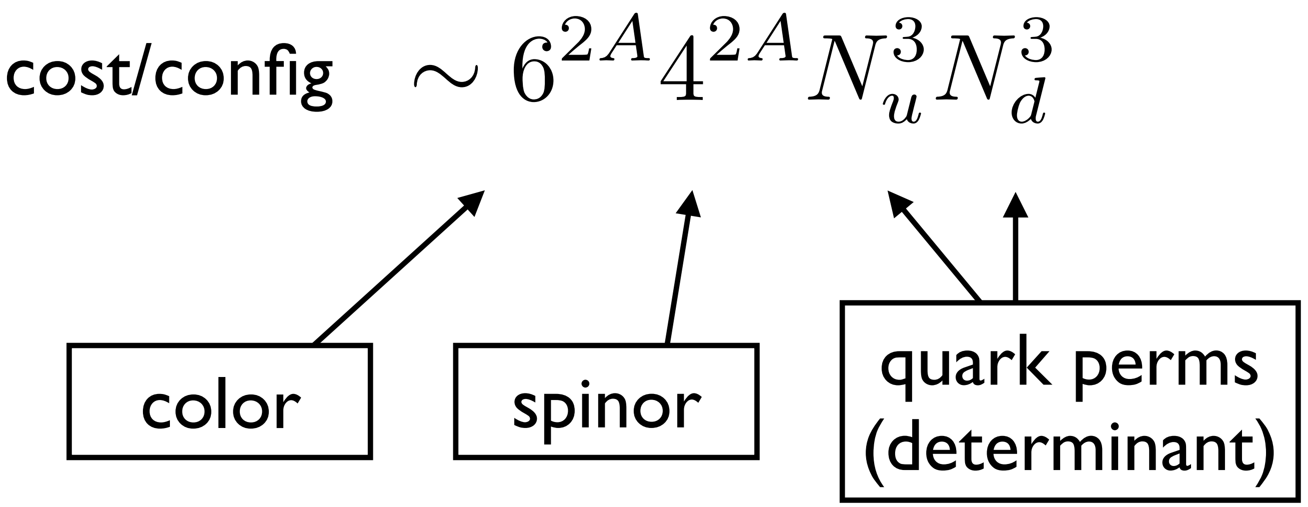
Multi-baryon contractions



propagators in all possible permutations

$\epsilon_{abc}(C\Gamma)_{\alpha\beta}$

τ



cost/config $\sim 6^{2A} 4^{2A} N_u^3 N_d^3$

Cost:

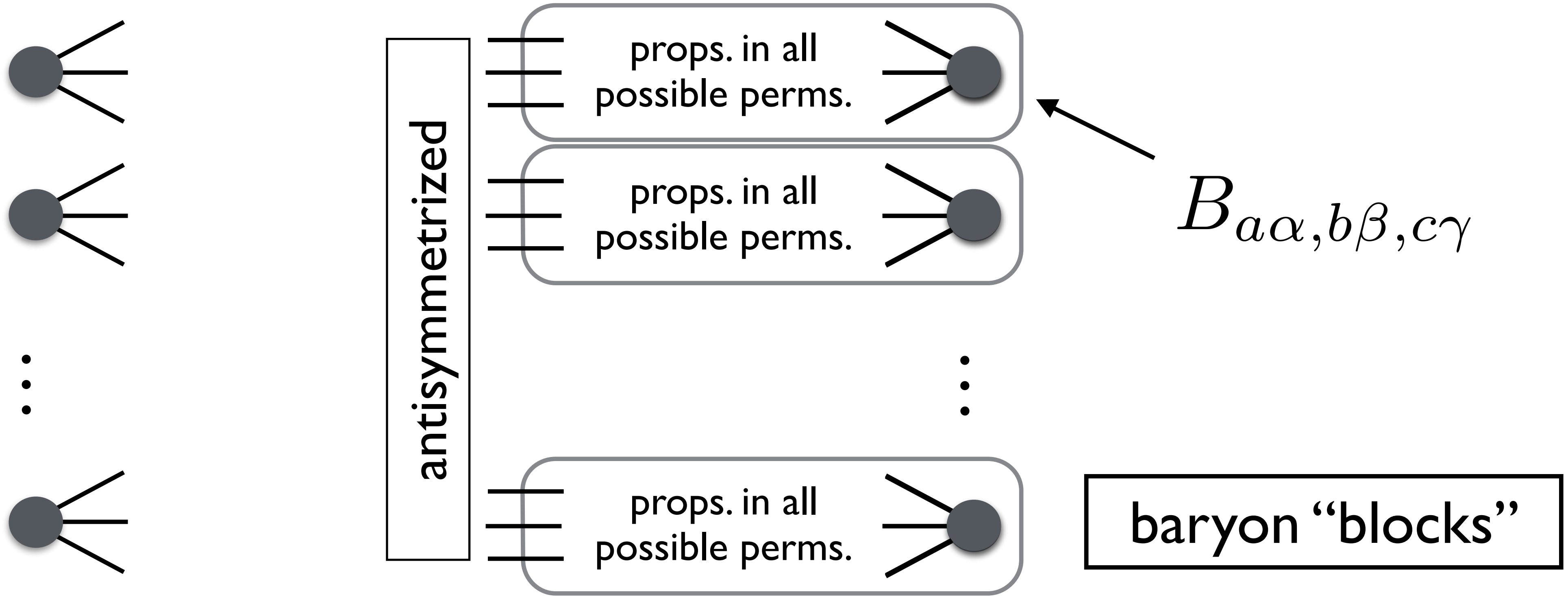
$^3\mathrm{H} : 191102976 \times 8000$

$^3\mathrm{He} : 191102976 \times 8000$

$^4\mathrm{He} : 110075314176 \times 46656$

Multi-baryon contractions

$\mathcal{C}_{ij}(\phi) =$



baryon "blocks"

$$\text{cost/config} \quad \sim \underbrace{6^A}_{\text{color}}\underbrace{4^A}_{\text{spinor}}\frac{N_u!N_d!}{2^A}$$

Cost:

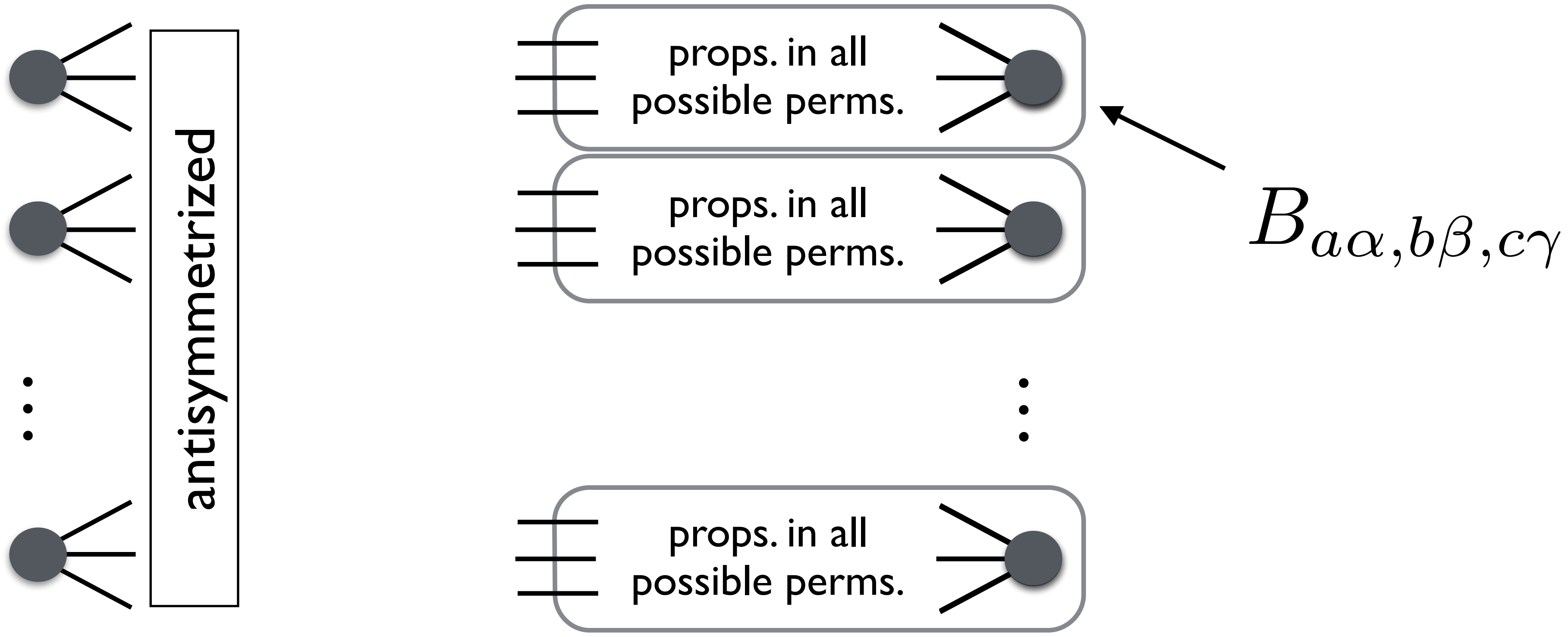
$^3\text{H} : 13824 \times 1000$

$^3\text{He} : 13824 \times 1000$

$^4\text{He} : 331776 \times 2916$

Multi-baryon contractions

$$\mathcal{C}_{ij}(\phi) =$$



S = sparse $\quad\quad$ D = dense

arXiv:1205.0585

$$S_{i_1,\cdots,i_{3A}} D_{\underline{[i_1,\cdots,i_{3A}]}} = S_{\underline{[i_1,\cdots,i_{3A}]}} D_{i_1,\cdots,i_{3A}}$$

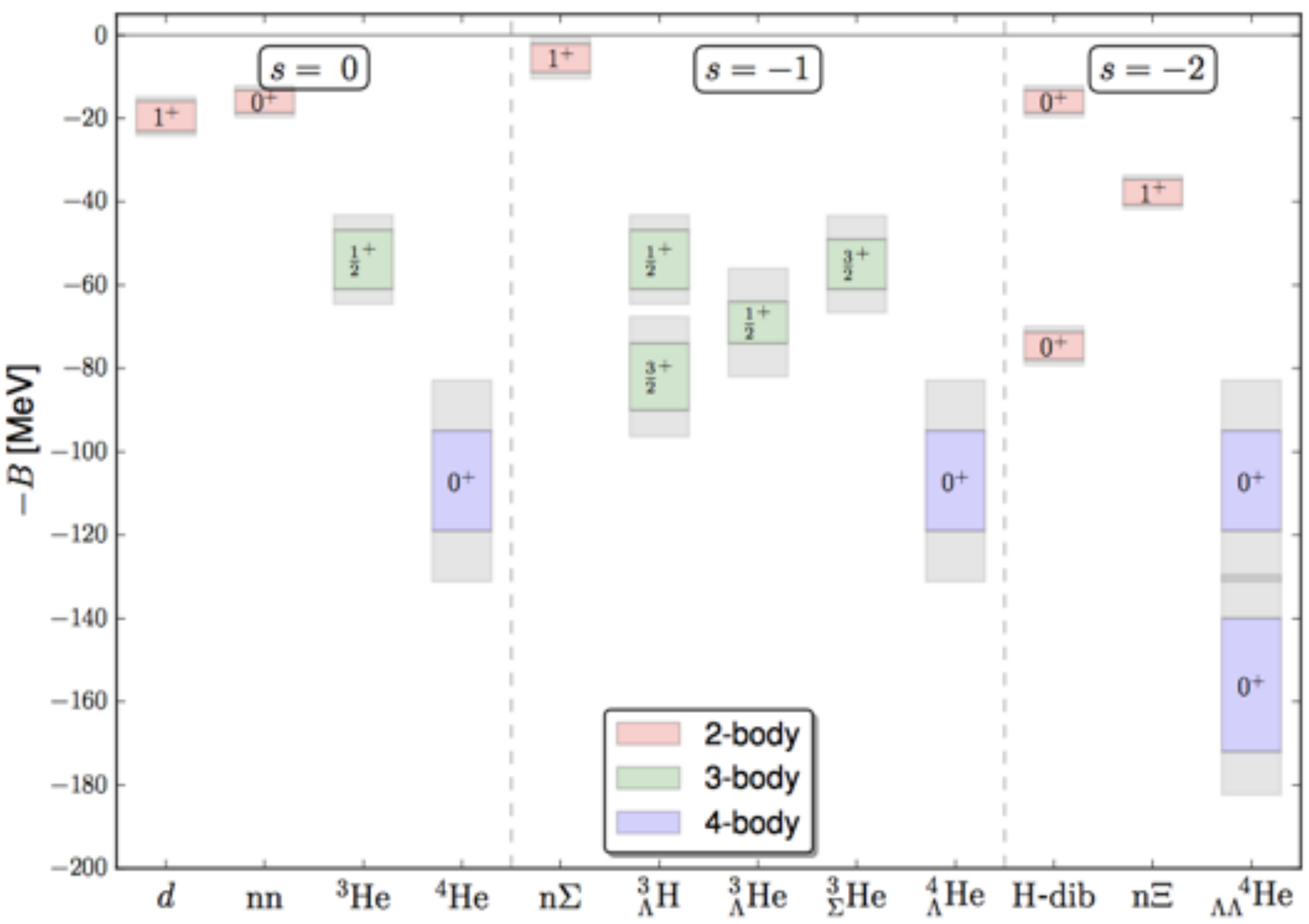
field independent contraction list—compute only once

extremely sparse

Multi-baryon contractions

- General strategies now exist which eliminate all redundancies for multi-baryon correlation functions
  - unified contraction lists [arXiv:arXiv:1205.0585]
  - underlying principle: takes advantage of Pauli exclusion
  - exponential reduction in computational cost
  - efficient methods developed for construction of contraction lists needed: use of recursion relations [arXiv:1207.1452] and [arXiv:1301.4895]
- Multi-baryon contractions methods enable A>4 calculations, however signal/noise remains an issue

Lattice QCD: light nuclei and hypernuclei



$m_\pi \sim 800\text{MeV}$

S. Beane, et al. (NPLQCD),
Phys. Rev. D 87, 034506 [arXiv:1206.5219]

- A<4, strangeness<2
- SU(3) flavor limit, single lattice spacing a~0.145 fm
- Infinite volume extrapolated

Isospin breaking effects on hadron masses

- Lattice QCD simulations often performed in the isospin limit
  - $m_\pi \sim 140$ MeV; $m_N \sim 940$ MeV
  - isospin breaking effects are very small by comparison:
  - e.g., neutron is heavier than the proton: m_N-$m_P \sim 1.29$ MeV
- Isospin breaking effects are only important when numerical precision reaches a level where they can be measured
- Isospin breaking is nonetheless important in nature, e.g.,

Isospin breaking effects on hadron masses

- Two sources for isospin breaking:
  - strong breaking due to $m_d > m_u$ (dictated by Yukawa couplings in the SM of weak interactions)
  - electromagnetic breaking due to $Q_u \neq Q_d$
- According to experiment, contributions to $m_N - m_P$ are comparable in size, but opposite in sign; cancelation of effects
  - $(m_N - m_P)_{strong} \sim 2.0$ MeV
  - $(m_N - m_P)_{e+m} \sim -0.8$ MeV
- Interesting to understand interplay of these contributions as a function of the fundamental parameters of nature

Introducing lattice QED into the mix

Noncompact lattice formulation of U(1) gauge theory:

$$F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) \qquad \partial_\mu = \text{forward difference lattice operator}$$

Gauge transformations:

vanishes on the lattice

$$A_\mu(x) \to A_\mu(x) - \partial_\mu \alpha(x) \qquad F_{\mu\nu}(x) \to F_{\mu\nu}(x) - \cancel{[\partial_\mu, \partial_\nu]}\alpha(x)$$

Gauge invariant lattice gauge action:

$$\mathcal{L}_{QED} = \frac{1}{4e^2} F_{\mu\nu}^2$$

Noncompact action requires gauge fixing
(e.g., Coulomb gauge on the lattice)

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Coupling to matter:

transforms as a site variable

$$q(x) \to e^{iQa\alpha(x)} q(x) \qquad Q = \mathrm{diag}(Q_u, Q_d, \cdots)$$

$$e^{iQaA_\mu(x)} \to e^{iQa[A_\mu(x) - \partial_\mu \alpha(x)]} = e^{iQa\alpha(x)} e^{iQaA_\mu(x)} e^{iQa\alpha(x+ae_\mu)}$$

transforms as a link variable

Gauge invariant lattice fermion action:

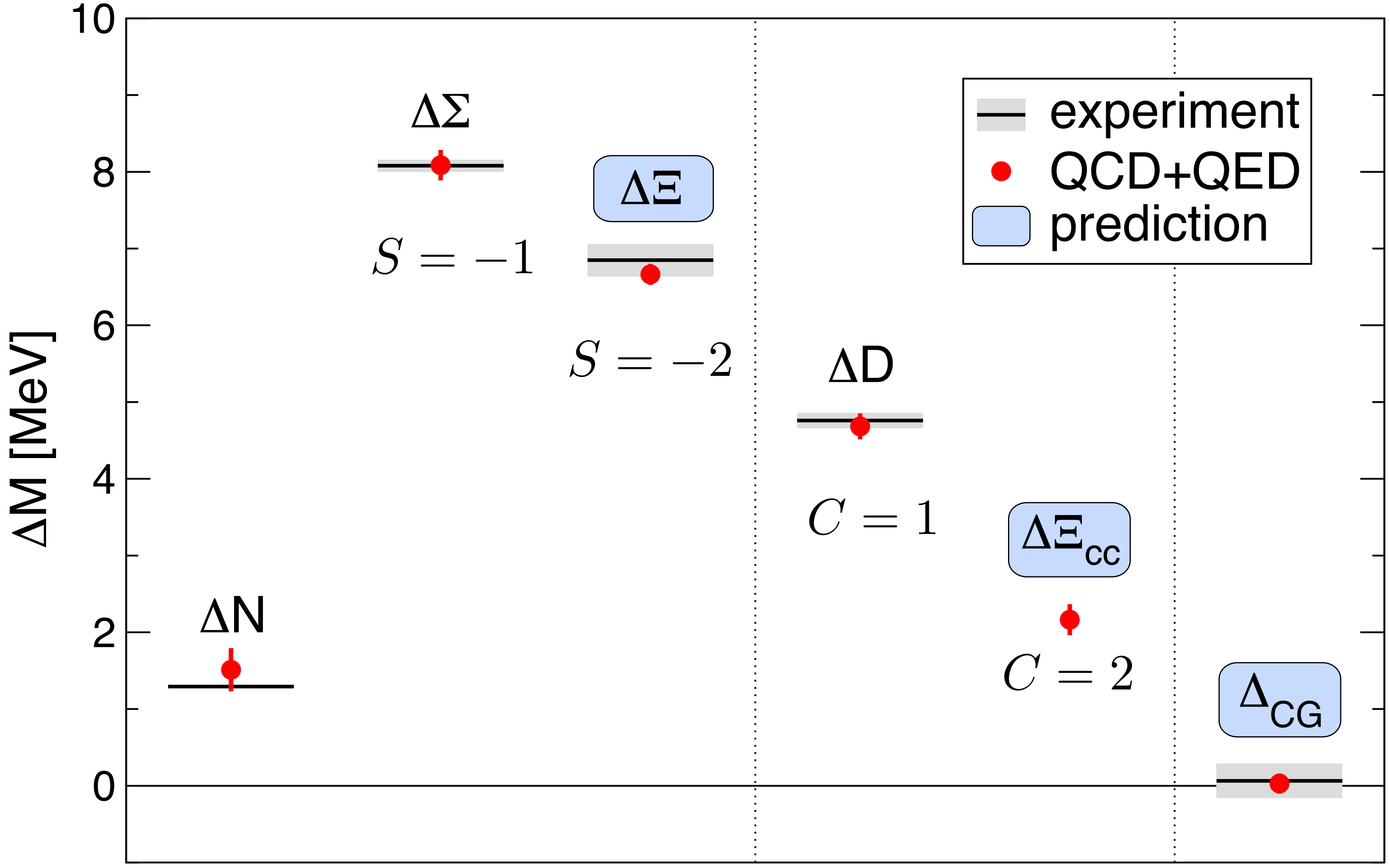
$$U_\mu(x) \to U_\mu(x) e^{iQaA_\mu(x)}$$

$$S_F[U, \bar{q}, q] = a^4 \sum_x \bar{q} D[U] q \qquad D = D_{naive}, D_W, D_{st}, D_{ov}, \cdots$$

Introducing lattice QED into the mix

- Finite volume effects:
  - QED is a long-range interaction; expect power-law finite volume effects — need large volumes
  - Finite volume effects accounted for within an EFT framework [e.g., Davoudi & Savage, arXiv:1402.6741]
- Number of studies using QED quenched approximation:
  - can use currently available QCD configs
  - numerical tricks for reducing noise: +/-e averaging, exploiting correlations in ratios of correlators to suppress excited state contamination
- Recent results for full QCD+QED

Mass differences, including QED effects



BMW [arXiv:1406.4088]

$$\Delta N = n - p$$
$$\Delta\Sigma = \Sigma^- - \Sigma^+$$
$$\Delta\Xi = \Xi^- - \Xi^0$$
$$\Delta D = D^\pm - D^0$$
$$\Delta\Xi_{cc} = \Xi_{cc}^{++} - \Xi_{cc}^{+}$$
$$\Delta_{\mathrm{CG}} = \Delta N - \Delta\Sigma + \Delta\Xi$$

- 1+1+1+1 flavors of Wilson fermions
- Full accounting of systematic errors, physical pion masses, continuum limit
- Predictions — errors exceeding those of experiment

Physics results — summary

- Extraction of energies from correlation functions:
  - designing operators with correct quantum numbers, large overlap onto states of interest
  - challenges with signal/noise
  - many fermion contractions
- Random sampling of specific applications to:
  - hadron spectroscopy and interactions
  - nuclei and hypernuclei
  - measurement of isospin breaking effects in QCD

Thank you!