A user's guide to lattice QCD

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"Modern Techniques in Hadron Spectroscopy", RUB, July 15-27th, 2024

Review of Continuum QCD:

- Fermion action (for a single flavor):

$$S_{\mathrm{F}}[\bar{\psi}, \psi, A] = \int d^4x\, \bar{\psi}(x) \left(\not{D} + m\right) \psi(x)$$

$$\not{D} = \gamma_\mu D_\mu = \gamma_\mu \left(\partial_\mu + i A_\mu(x)\right)$$

- Gauge action:

$$S_{\mathrm{G}}[A] = \frac{1}{2g_0^2} \int d^4x\, \mathrm{tr}\left\{F_{\mu\nu}(x) F_{\mu\nu}(x)\right\}$$

$$F_{\mu\nu}(x) = -i[D_\mu(x), D_\nu(x)]$$

- Euclidean path integral: $(t = i\tau)$

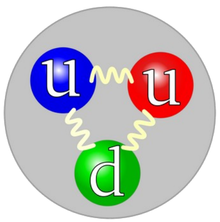
$$\langle O_1(x_1) \ldots O_n(x_n)\rangle = \frac{1}{Z} \int D[\bar{\psi}, \psi] D[A]\, \mathrm{e}^{-S_{\mathrm{F}}[\bar{\psi}, \psi, A]}\, \mathrm{e}^{-S_{\mathrm{G}}[A]} \times$$

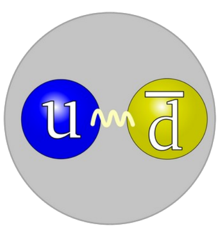
$$O_1(x_1)[\bar{\psi}, \psi, A] \ldots O_n(x_n)[\bar{\psi}, \psi, A]$$

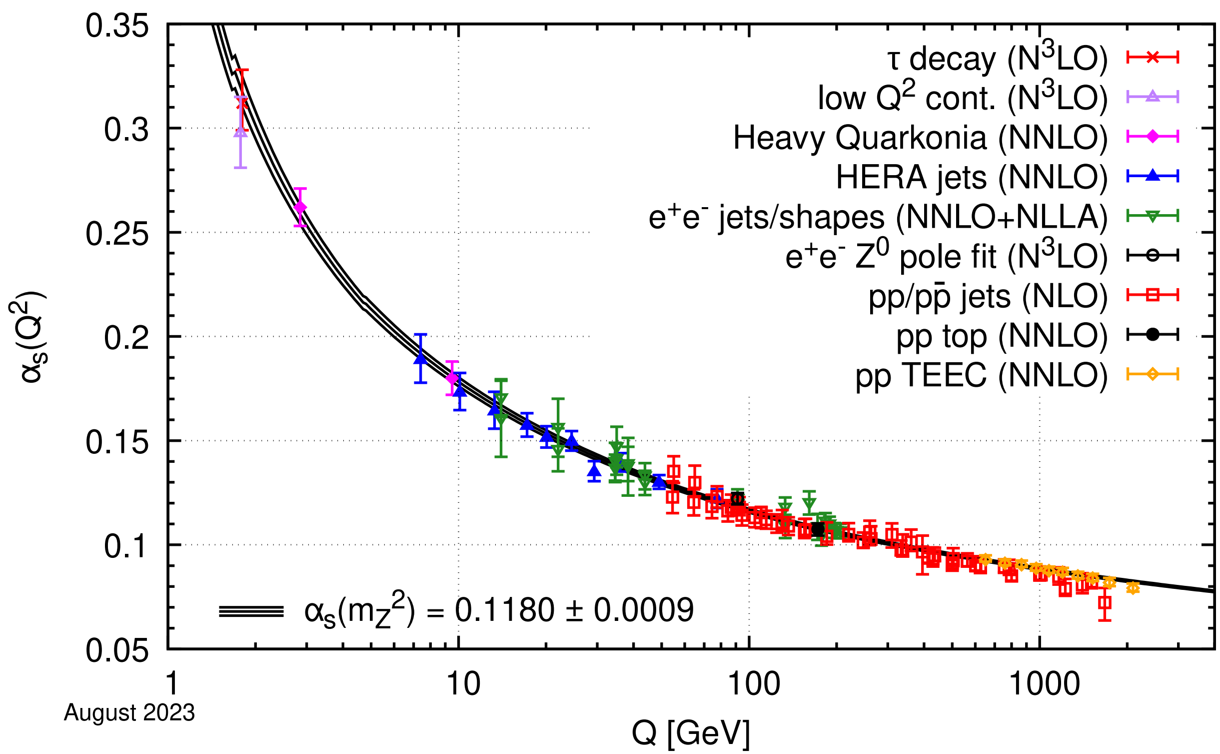
The running coupling: asymptotic freedom

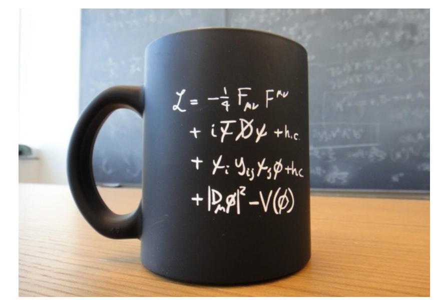
- Interaction strength is scale (and scheme) dependent
- Rate of change given by the beta-function: $(a_\mathrm{s} \equiv \alpha_\mathrm{s}/\pi)$

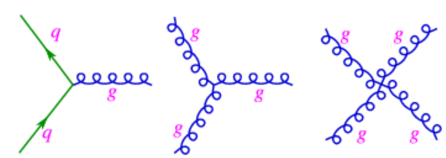
$$\beta(a_s) = Q^2 \frac{da_\mathrm{s}(Q^2)}{dQ^2} = -\frac{a_\mathrm{s}^2}{4}\left(11 - \frac{2}{3}N_\mathrm{f}\right) + \mathrm{O}(a_\mathrm{s}^3)$$





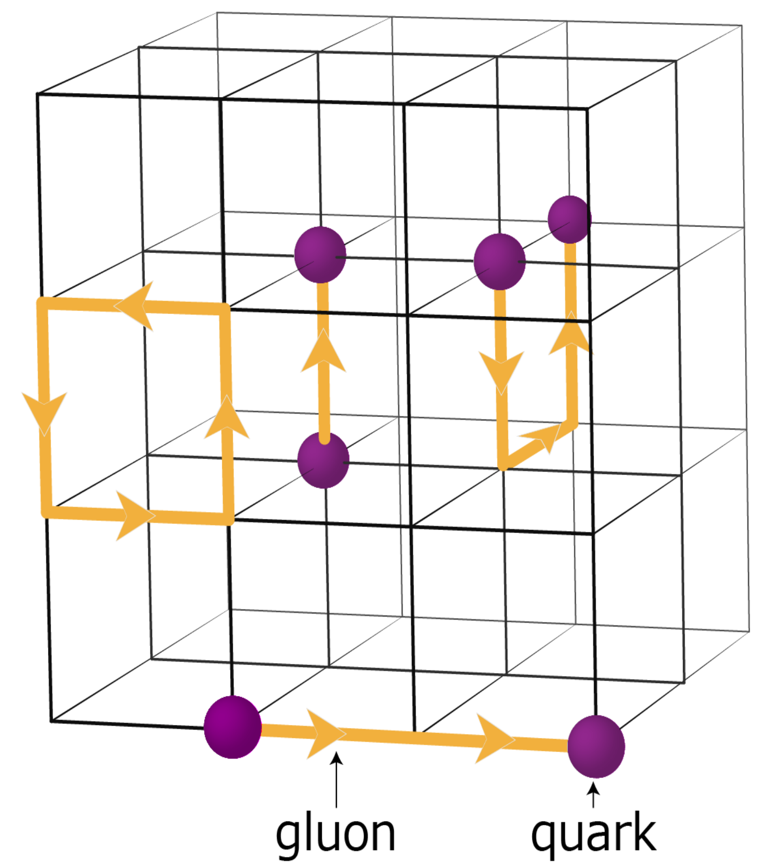






Lattice QCD: a bridge between low and high energies

- Discretization
- Simulation Algorithms
- 'Measurements'



Setup:

- Regular square lattice:

$$\Lambda = \{x = (x_1, x_2, x_3, x_4) \,|\, x_i = n_i a\},$$

$$n_1, n_2, n_3 = 0, \ldots, L/a - 1, \quad n_4 = 0, \ldots, T/a - 1$$

- Boundary conditions must be specified. Usually 'periodic'.

General Considerations:

- Simulation parameters/outputs are dimensionless:

$$g_0^2,\ am_q \to aM_{\mathrm{H}}$$

- Scale-setting required for dimensionful predictions:

$$a \equiv am_\Omega / m_\Omega^{\mathrm{phys}}$$

- State-of-the-art for lattice dimensions:

$$L/a \sim 64 - 128$$

- UV and IR physics controlled (in principle):
  - Finite-volume effects (single-hadron) at percent level for

$$m_\pi L \gtrsim 4 \quad L \gtrsim 5.6\,\mathrm{fm} \qquad \to a = 0.04 - 0.09\,\mathrm{fm}$$

  - Leading cutoff effects typically quadratic:

$$\mathrm{O}(a\Lambda_{\mathrm{QCD}})^2 \sim 0.01 - 0.05 \quad \mathrm{O}(am_{\mathrm{c}})^2 \sim 0.07 - 0.33$$

Lattice discretization of SU(3) gauge theory:

- Gluons: lattice links (parallel transporter)

contiunuum:

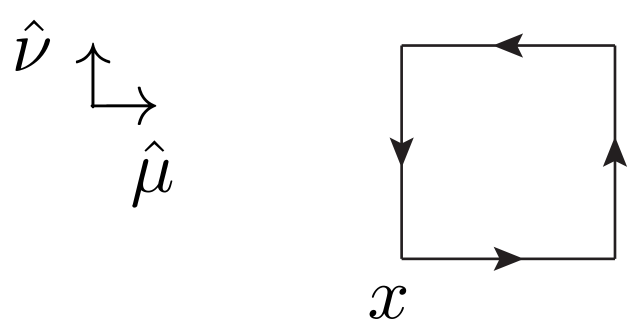
$$G(x,y) = P\exp\left(-\int_{C_{xy}} A\cdot ds\right)$$

lattice:

$$\begin{aligned} U_\mu(x) &= \exp(iaA_\mu(x)) \\ &= 1 + iaA_\mu(x) + \mathcal{O}(a^2) \end{aligned}$$

- ‘Loops’ are gauge invariant, e.g. the ‘plaquette’:

$$P_{\mu\nu}(x) = U_\mu(x)\,U_\nu(x+a\hat{\mu})\,U_\mu(x+a\hat{\nu})^\dagger\,U_\nu(x)^\dagger$$



- Wilson gauge action: K. G. Wilson, Phys. Rev. D 10, 2445 (1974)

$$S_G[U] = \frac{2}{g_0^2} \sum_x \sum_{\mu<\nu} \mathrm{Re}\,\mathrm{tr}\left[1 - P_{\mu\nu}(x)\right]$$

$$= \frac{a^4}{2g_0^2} \sum_x \sum_{\mu,\nu} \mathrm{tr}\left[F_{\mu\nu}(x)\right]^2 + \mathcal{O}(a^2)$$

- Gauge invariance exactly preserved by the lattice regulator!

- No gauge fixing required

Lattice Discretization of Fermions:

Naive fermion action:

$$S_F[\psi, \bar{\psi}, U] = a^4 \sum_x \bar{\psi}(x) \times$$

$$\left(\sum_\mu \gamma_\mu \frac{U_\mu(x)\psi(x + a\hat{\mu}) - U_{-\mu}(x)\psi(x - a\hat{\mu})}{2a} + m\psi(x) \right)$$

$$= a^4 \sum_{xy} \bar{\psi}(x) D(x|y) \psi(y)$$

Fourier Transform: (Ex.)

$$\tilde{D}(p) = m + \frac{i}{a}\sum_{\mu}\gamma_\mu \sin(ap_\mu)$$

Massless propagator:

$$\tilde{D}^{-1}(p) = -ia\frac{\sum_\mu \gamma_\mu \sin(ap_\mu)}{\sum_\mu \sin^2(ap_\mu)}$$

Remarks:

- In continuum, pole at $p = (0,0,0,0)$
- At finite *a*, 15 **additional poles** ('doublers') at

$$p = (\pi/a, 0, 0, 0),\ (0, \pi/a, 0, , 0), \ldots, (\pi/a, \pi/a, \pi/a, \pi/a)$$

- Action must be modified to deal with the doublers!

Theorem (Nielsen+Ninomiya): you can't have all of the following

- $\tilde{D}(p)$ is continuous (periodic) in the Brillouin zone.

  (Equivalently, $D(x|y)$ is local)

- $\tilde{D}(p)$ has the correct continuum limit.

- $\tilde{D}(p)$ is free from doublers.

- Continuum chiral symmetry a finite lattice spacing

$$\{\gamma_5, D\} = 0$$

Naive Fermions:

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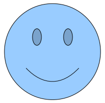

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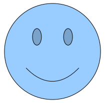

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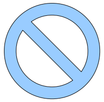
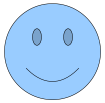


- Continuum chiral symmetry $\{\gamma_5, D\} = 0$



Wilson Fermions:

K. G. Wilson, Phys. Rev. D 10, 2445 (1974)

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- $\tilde{D}(p)$ has the correct continuum limit.

- $\tilde{D}(p)$ is free from doublers.

- Continuum chiral symmetry $\{\gamma_5, D\} = 0$

Wilson Fermions:

- Add an additional term to naive Dirac operator:

$$-a\sum_{\mu}\frac{U_\mu(x)\delta_{x+a\hat{\mu},y}-2\delta_{x,y}+U_{-\mu}(x)\delta_{x-a\hat{\mu},y}}{2a^2}$$

- Explicitly breaks chiral symmetry (in addition to the quark masses)

- Doublers now have mass (see exercises)

$$m+\frac{2\ell}{a}$$

where ℓ is the number of nonzero components

Wilson Fermions:

- Bad news:
  - Wilson term introduces O(a) cutoff effects
  - Wilson term explicitly breaks chiral symmetry

- Good news:
  - No doublers!
  - Dirac operator has concise form. Relatively cheap numerically.

$$D_{\mathrm{W}}(x|y) = \left(m + \frac{4}{a}\right) - \frac{1}{2a} \sum_{\mu=\pm 1}^{\pm 4} (1 - \gamma_\mu) U_\mu(x) \delta_{x-a\hat{\mu},y}$$

$$\gamma_{-\mu} = -\gamma_\mu, \quad U_{-\mu}(x) = U_\mu(x - a\hat{\mu})^\dagger$$

Other Fermion Discretizations:

- Staggered Fermions:
  - Partition Dirac spinors across neighboring sites
  - Very cheap numerically
  - Four doublers (‘tastes’) are still present.
  - Fourth root → non-local action

- Domain-wall fermions
  - Introduce a fifth dimension. Chiral fermions bound to the 4-d ‘domain walls’.
  - A remnant of chiral symmetry as $L_5 \to \infty$
  - Very expensive numerically

Other Fermion Discretizations:

- Twisted-mass fermions:
  - Doublet of Wilson fermions. Mass term has non-trivial isospin structure.
  - Good numerical properties.
  - ‘Automatically’ O(a)-improved
  - Discrete symmetries don’t have usual form

The Symanzik Improvement Program:

- Describe discretization effects by a continuum EFT

- Breakdown scale: $\Lambda = \frac{1}{a}$

- Cutoff effects encoded by additional terms in the action:

$$S_{\rm eff} = \int d^4x \left(\mathcal{L}^{(0)}(x) + a\mathcal{L}^{(1)}(x) + a^2\mathcal{L}^{(2)}(x) + \ldots\right)$$

- Idea: add terms to lattice action to cancel additional terms

Example: removing O(a) cutoff effects from Wilson action

See R. Sommer, hep-lat/9705026

- There are 4 operators at dimension 5

$$\mathcal{L}_1^{(1)}(x) = \bar\psi(x)\,\sigma_{\mu\nu}F_{\mu\nu}(x)\,\psi(x),$$
$$\mathcal{L}_2^{(1)}(x) = \bar\psi(x)\left(\overrightarrow{D}_\mu(x)\overrightarrow{D}_\mu(x) + \overleftarrow{D}_\mu(x)\overleftarrow{D}_\mu(x)\right)\psi(x),$$
$$\mathcal{L}_3^{(1)}(x) = m\,\mathrm{tr}[F_{\mu\nu}(x)F_{\mu\nu}(x)],$$
$$\mathcal{L}_4^{(1)}(x) = m\,\bar\psi(x)\left(\gamma_\mu\overrightarrow{D}_\mu(x) - \gamma_\mu\overleftarrow{D}_\mu(x)\right)\psi(x),$$
$$\mathcal{L}_5^{(1)}(x) = m^2\,\bar\psi(x)\psi(x)$$

- After parameter redefinitions and field eq.'s, only $\mathcal{L}_1^{(1)}(x)$ remains (see exercises)

Wilson fermions → 'clover' fermions

B. Sheikholeslami, R. Wohlert, Nucl.Phys.B 259 (1985) 572

- Define a new Dirac operator:

$$D_{\rm clover}(x|y) = D_{\rm W}(x|y) + a\, c_{\rm SW} \sum_{\mu<\nu} \frac{\sigma_{\mu\nu}}{2} \hat{F}_{\mu\nu}(x)\delta_{x,y}$$

$$\hat{F}_{\mu\nu}(x) = \frac{-i}{8a^2}\left\{Q_{\mu\nu}(x) - Q_{\nu\mu}(x)\right\}$$

where $Q_{\mu\nu}(x)$ is the sum of all plaquettes in the $\hat{\mu}\hat{\nu}$ -plane

- Now all 'spectral' quantities (i.e. masses and energies) are O(a)-improved

$$\frac{am_H}{am_\Omega}(a) = \frac{am_H}{am_\Omega}(0) + \mathrm{O}(a^2)$$

Improvement of composite operators:

- Higher-dimensional counter-terms required to improve correlation functions of composite operators.
- Ex: the axial current

$$A_\mu^a(x) = \frac{1}{2}\bar{\psi}(x)\gamma_\mu\gamma_5\tau^a\psi(x)$$

- Possible counterterms:

$$A_{\mu,1}^a(x) = \frac{1}{2}\bar{\psi}(x)\gamma_5\sigma_{\mu\nu}\left(\overrightarrow{D}_\nu - \overleftarrow{D}_\mu\right)\tau^a\psi(x)$$

$$A_{\mu,2}^a(x) = \frac{1}{2}\partial_\mu\left(\bar{\psi}(x)\gamma_5\tau^a\psi(x)\right)$$

$$A_{\mu,3}^a(x) = \frac{m}{2}\bar{\psi}(x)\gamma_\mu\gamma_5\tau^a\psi(x)$$

Determining improvement coefficients:

- General strategy: impose some continuum property at finite lattice spacing

- Typically: chiral Ward identities

- Best if improvement/renormalization coefficients determined non-perturbatively

- To do a simulation with Wilson Clover fermions, need to tune:

$$g_0^2, \quad am_{\mathrm{light}}, \quad am_{\mathrm{s}}, \quad c_{\mathrm{SW}}$$

- Other renormalization/improvement coefficients should also be non-perturbative.

- Using equations of motion and redefinition of renormalization constant, only one operator required:

$$A^a_{\mathrm{I},\mu}(x) = A^a_\mu(x) + c_\mathrm{A} a \hat{\partial}_\mu P^a(x), \quad P^a(x) = \bar{\psi}(x)\gamma_5 \frac{\tau^a}{2}\psi(x)$$

- Renormalization also required for full O(a)-improvement:

$$A^a_{\mathrm{R},\mu}(x) = Z_A(1 + b_\mathrm{A} am) A^a_{\mathrm{I},\mu}(x)$$

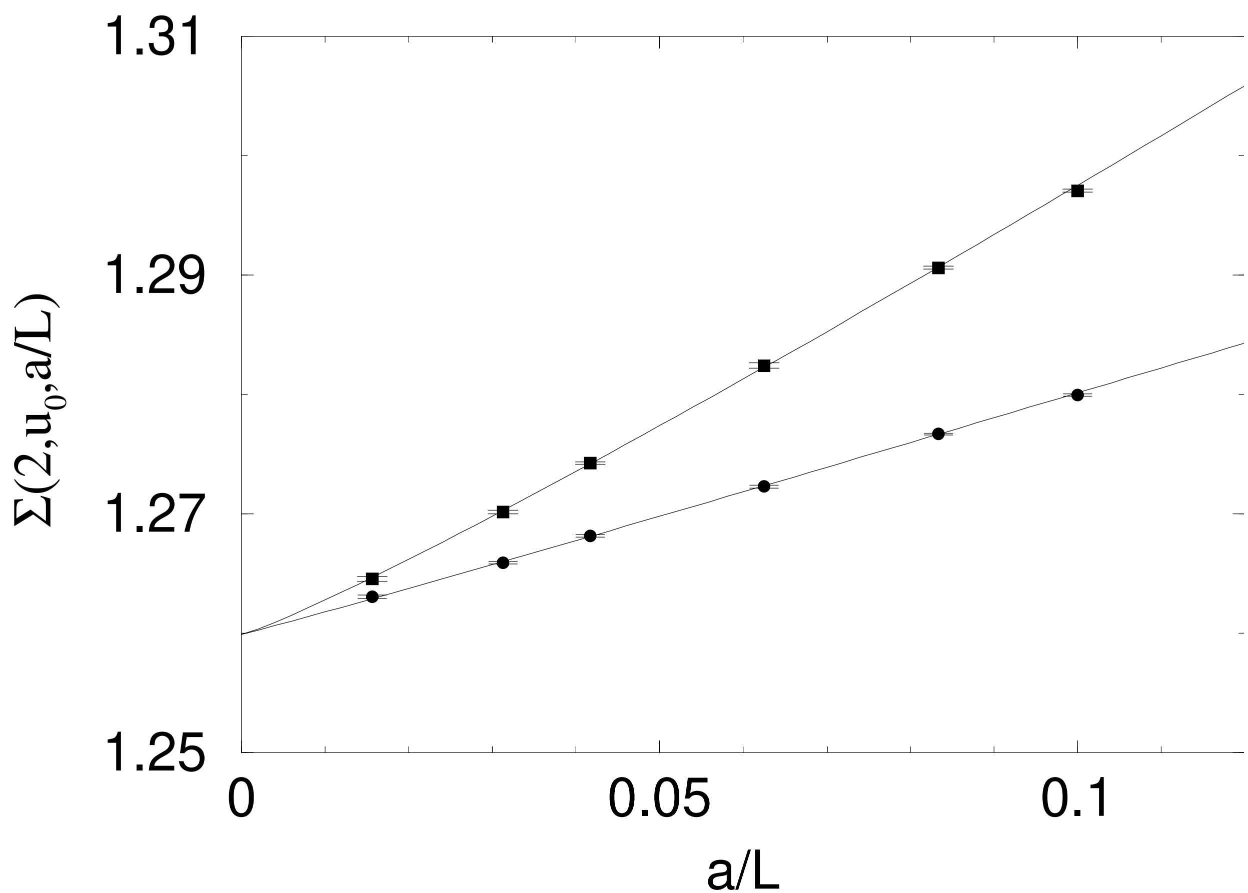
- More complicated for u,d,s quarks. Ex: coupling improvement

$$g^2_{\mathrm{I},0} = g^2_0 \left\{ 1 + \frac{b_g}{3} \sum_f am_f \right\}$$

A word of warning about cutoff effects:

Plot from: J. Balog, F. Niedermayer, P. Weisz, Nucl.Phys.B 824 (2010) 563-615

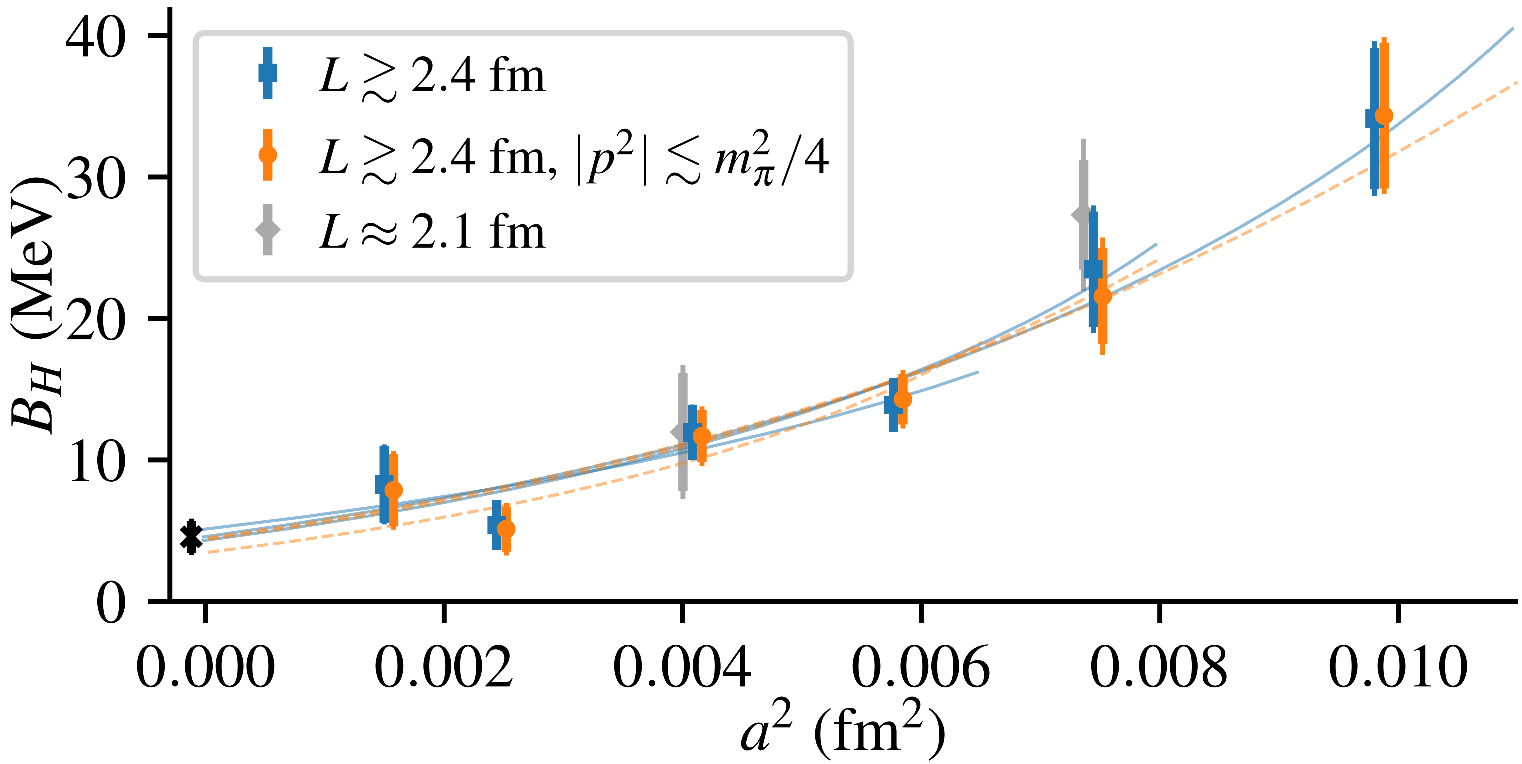
- Symanzik expansion is an asymptotic series
- $\mathrm{O}(a^2)$ could contain large logarithmic corrections.
- Ex: the 2-d non-linear sigma model should have leading $\mathrm{O}(a^2)$



- Data described well by perturbative computation of log corrections

Cutoff effects are important:

- Ex: H-dibaryon binding energy   J. R. Green, et al., Phys.Rev.Lett. 127 (2021) 24, 242003



- Perturbative computation of log-corrections in SymEFT:

N. Husung, P. Marquard, R. Sommer,   Eur.Phys.J.C 80 (2020) 3, 200

Lattice QCD simulation:

- Integrate out the fermions:

$$\langle \mathcal{O}_1(t_1) \cdots \mathcal{O}_n(t_n) \rangle = \frac{1}{Z} \int DU \, \mathrm{e}^{-S_{\mathrm{G}}[U]} \prod_{f=u,d,s} \det D_{\mathrm{clover},f}[U] \times$$
$$\mathcal{O}_1(t_1) \cdots \mathcal{O}_n(t_n)[U]$$

- Determinant is a non-local function of U
- PDF must be positive-definite in order to Monte Carlo sample
- If $m_{\mathrm{u}} = m_{\mathrm{d}}$, can exploit γ_5-hermiticity to show

$$\prod_{f=u,d} \det D_{\mathrm{clover},f}[U] = |\det D_{\mathrm{clover},l}[U]|^2$$

Lattice QCD simulation:

- 'Bosonize' the light quark determinant via 'pseudofermions'

$$|\det D_l[U]|^2 = \pi^N \int D\phi \, \mathrm{e}^{-\phi^\dagger (DD^\dagger)^{-1}\phi}$$

- Introduce a rational approximation for the strange quark:

M. A. Clark, A. D. Kennedy, Nucl.Phys.B Proc.Suppl. 129 (2004) 850

$$|\det D_s[U]| \approx \int D\phi \, \mathrm{e}^{-\phi^\dagger [r(D_s^\dagger D_s)]^{-1}\phi}$$

where $r(x) \approx \sqrt{x}$ and $\frac{1}{r(x)} = \sum_{k=1}^{n} \frac{\alpha_k}{x+\beta_k}$

- Any negative signs treated with 'reweighting'

Markov chain Monte Carlo:

- Construct a Markov Chain with limiting distribution:

$$P[U] = \frac{1}{Z} \mathrm{e}^{-S_{\mathrm{G}}[U]} \prod_{f=u,d,s} \det D_f[U]$$

- Metropolis algorithm:
  - Propose a change (symmetrically) : $U \to U'$
  - Accept change with probability:

$$p_{\mathrm{acc}} = \min\left\{1, \frac{P[U']}{P[U]}\right\}$$

- For pure gauge, local proposal is sufficient
- With fermions a global proposal is required

Markov chain Monte Carlo:

- ‘Thermalization’ is required: run for a while to lose ‘memory’ of starting configuration

- Save gauge configuration every n_{step} updates

- Errors estimated using the Central Limit Theorem, but with modified variance:

$$\sigma_O^2 \to 2\tau_O^{\mathrm{int}}\sigma_O^2$$

$$\tau_O^{\mathrm{int}} = \frac{1}{2} + \lim_{\tau\to\infty}\sum_{t=1}^{\tau}\rho_O(t)$$

where $\rho_O(t)$ is the autocorrelation

Hybrid Monte Carlo (HMC): a global update with a reasonable acceptance

S. Duane, A. D. Kennedy, B. J. Pendleton, D. Roweth, Phys.Lett.B 195 (1987) 216

- Introduce 'momentum' fields $P_\mu(x) \in \mathrm{su}(3)$

$$1 = \frac{1}{Z} \int DP_\mu \, \mathrm{e}^{-\sum_{x,\mu} ||P_\mu(x)||^2/2}$$

- Evolve $\{P_\mu, U_\mu\}$ according to Hamilton's equations:

$$\dot{U}_{\mu,t}(x) = P_{\mu,t}(x) \, U_{\mu,t}(x)$$

$$\dot{P}_{\mu,t}(x) = -\partial_{x,\mu} S[U]$$

- Metropolis accept/reject with 'Hamiltonian'

$$H[P,U] = \frac{1}{2} \sum_{x,\mu} ||P_\mu(x)||^2 + S[U]$$

Hybrid Monte Carlo (HMC): a global update with a reasonable acceptance

- Integration performed over trajectory of length τ
- Interval broken into $n_{\rm step}$ integration steps
- Interplay between autocorrelation, and $\tau,\ n_{\rm step},\ \Delta H,\ P_{\rm acc}$
- Generally: largest cost fraction comes from solving Dirac equation:

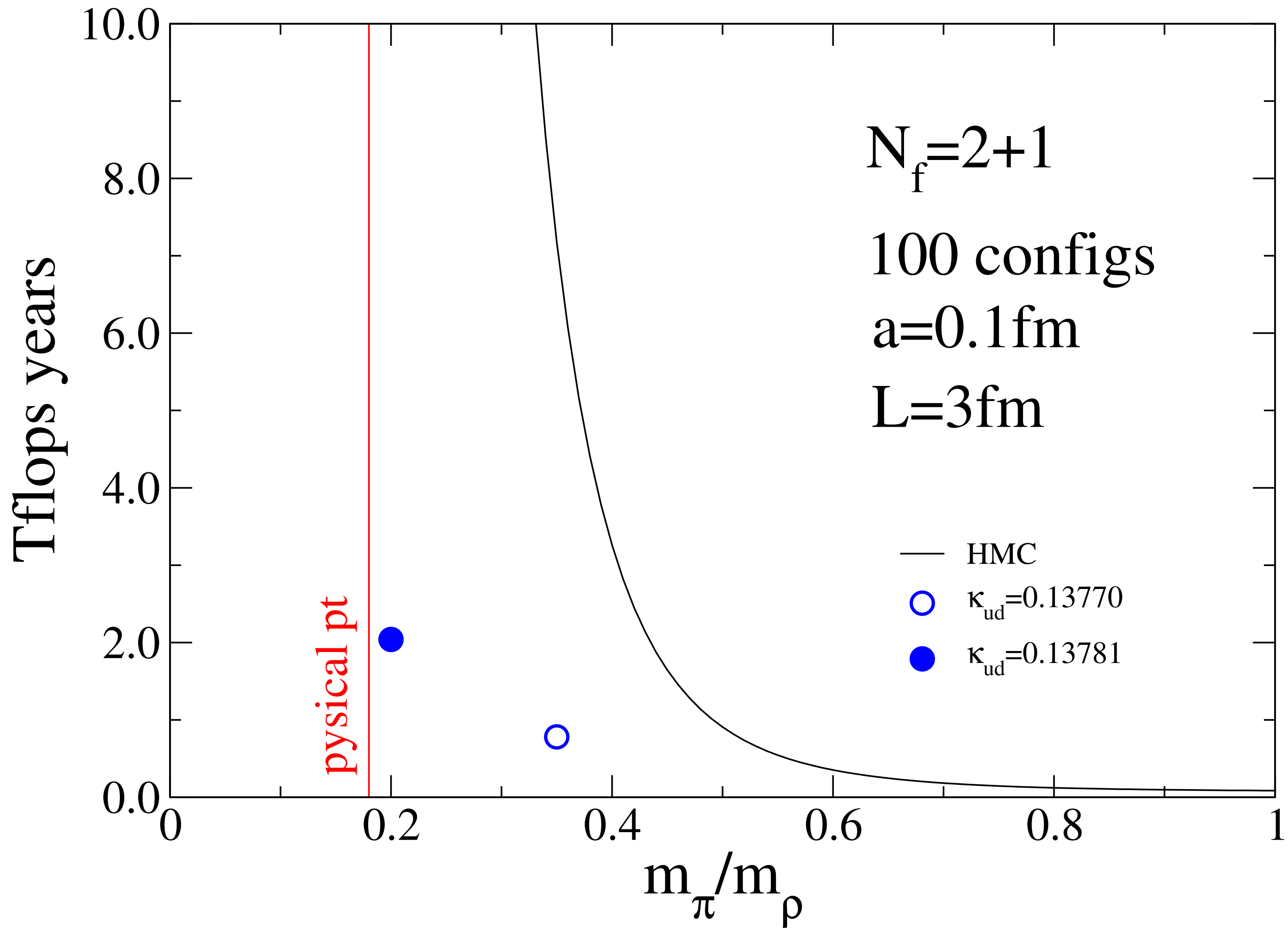
$$\sum_y D(x|y)\phi(y) = \eta(x)$$

- You can run a lattice QCD simulation! See Exercises (pure gauge)

History: breaking down the 'Berlin Wall'

- HMC preconditioners make forces smaller, exploit hierarchies

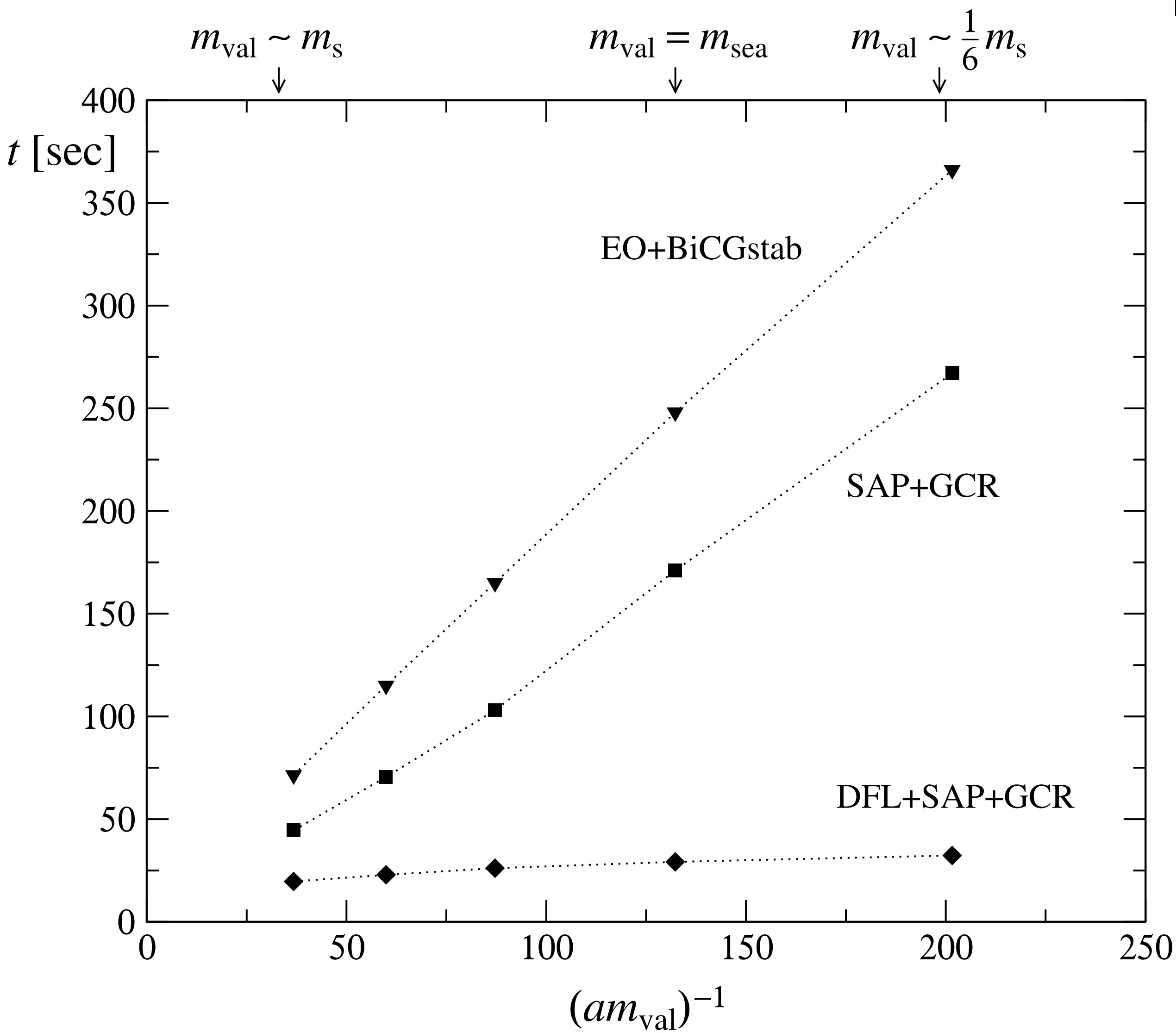
Panel discussion at Lattice '01
Plot from: CP-PACS coll., Phys.Rev.D79:034503,2009



History: breaking down the 'Berlin Wall'

- Improved algorithms for solving the Dirac equation:

Plot from: M. Lüscher, JHEP0707:081,2007



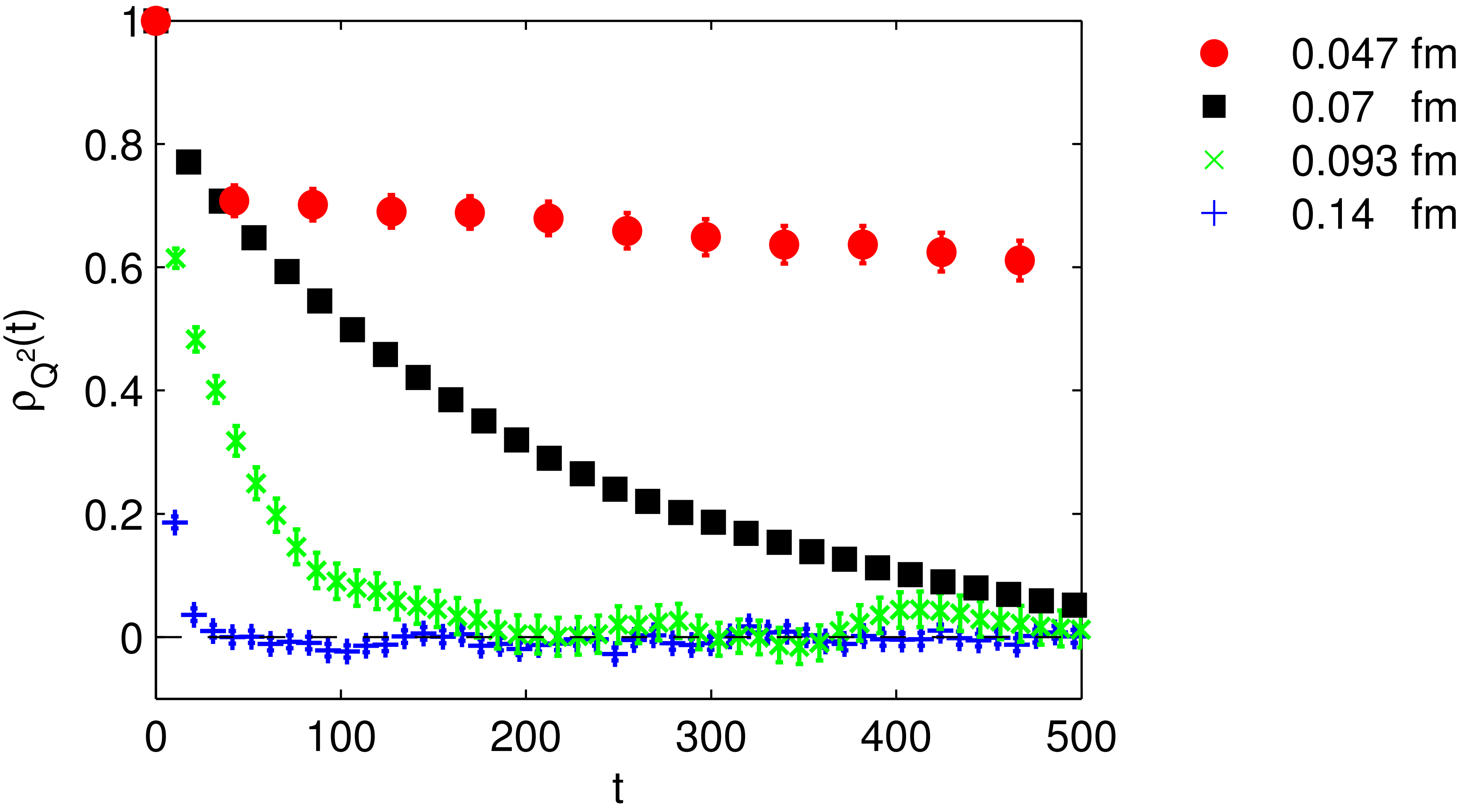
Simulation: summary

- 2+1 flavor simulations are possible down to the physical point for several discretizations

- Isospin-breaking effects are beginning to be added:
  - $m_{\mathrm{u}} \neq m_{\mathrm{d}}$
  - QED

- How should HMC autocorrelations scale? $\tau_{\mathrm{int}} \sim a^{-z}$
  - Random walk: $z = 2$
  - Free field: $z = 1$

Global Topology Freezing:



Plot from: S. Schaefer, R. Sommer, F. Virotta, Nucl. Phys. B845 93 (2011)
arXiv:1009.5228

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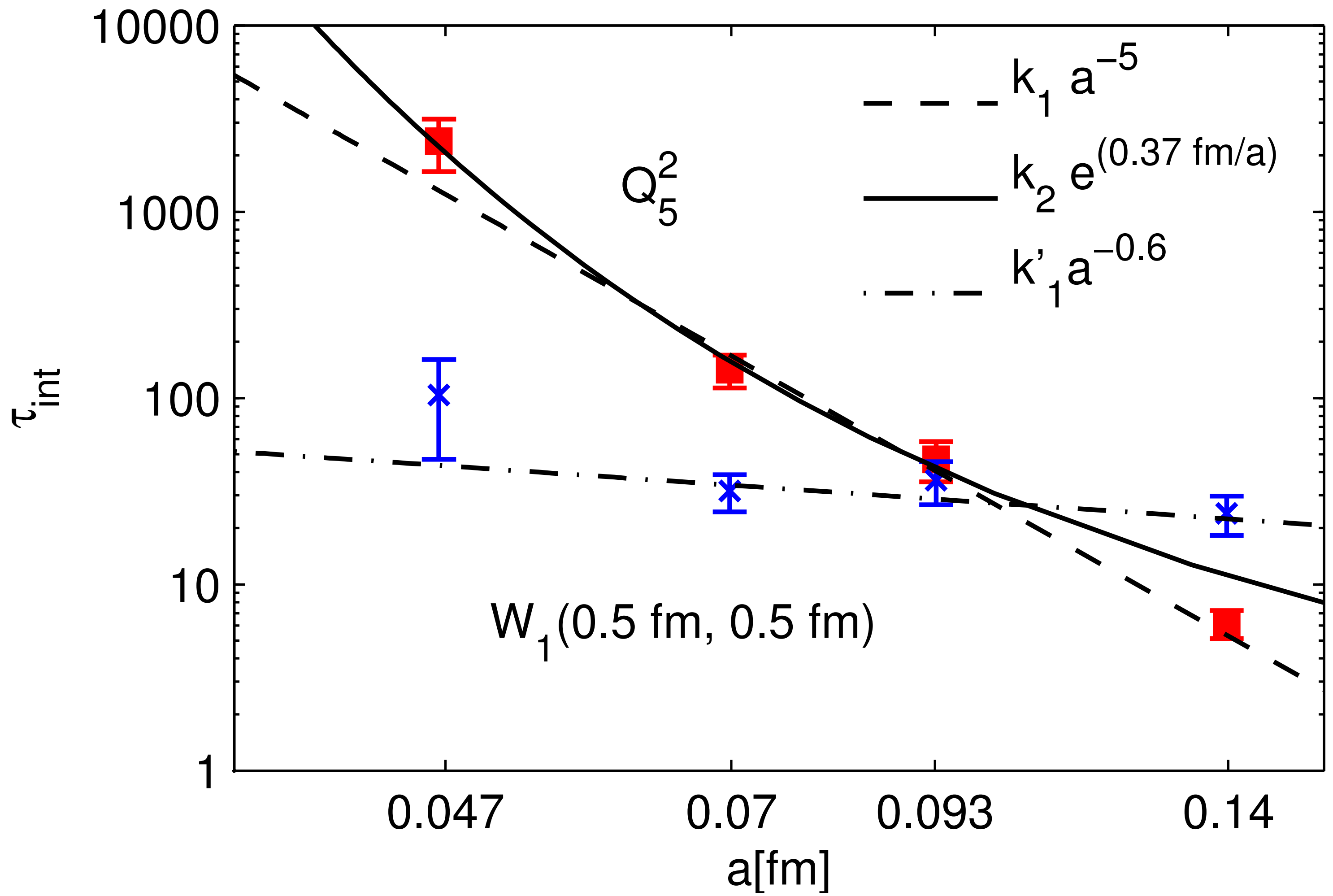


Plot from: S. Schaefer, R. Sommer, F. Virotta, Nucl. Phys. B845 93 (2011)
arXiv:1009.5228

Global Topology Freezing: explanation

M. Lüscher + S. Schaefer, JHEP 04 (2011) 104

- The space of gauge field configurations is not simply connected.

- As the continuum limit is approached, disconnected instanton sectors emerge, with fixed 'winding number'

- Global topological charge:

$$Q = \int d^4x \, q(x) \qquad q(x) = -\frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \, \mathrm{tr}\{F_{\mu\nu}(x) \, F_{\rho\sigma}(x)\}$$

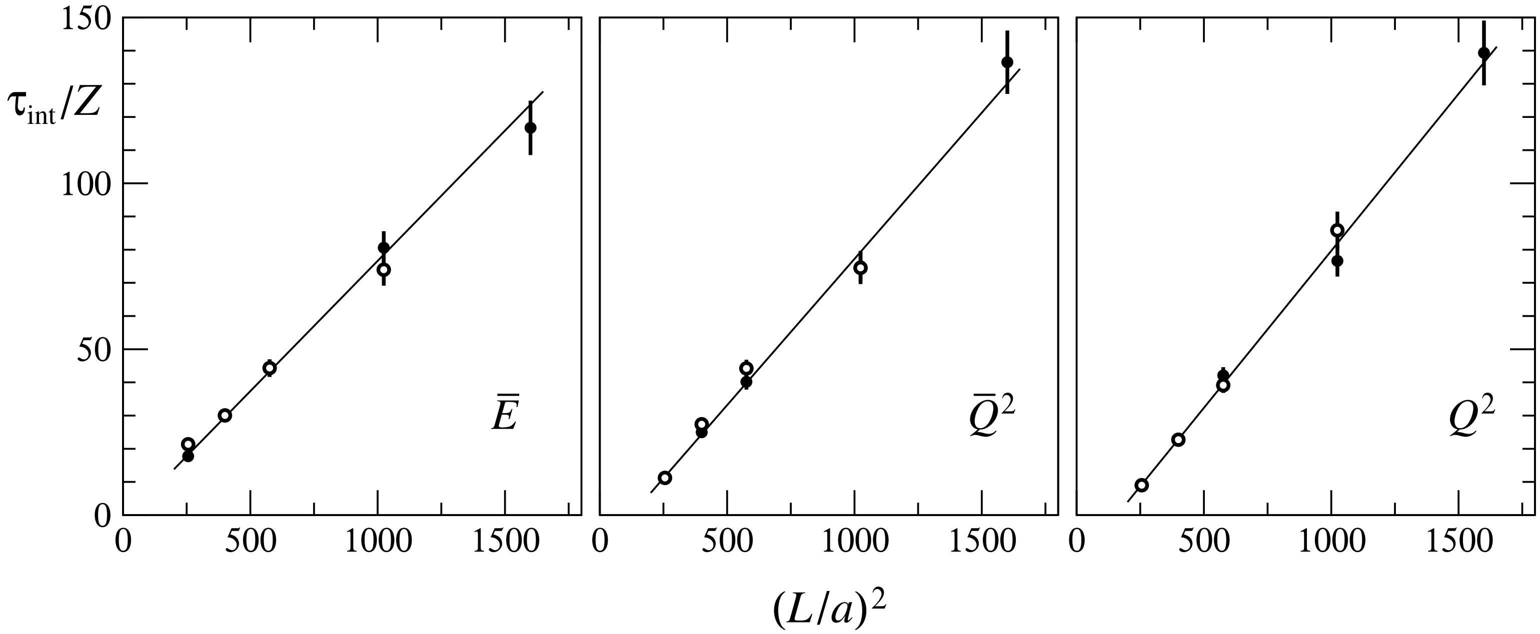
- Made renormalized by applying the Wilson flow

M. Lüscher, JHEP 08 (2010) 071

Global Topology Freezing: topological solution

M. Lüscher + S. Schaefer, JHEP 04 (2011) 104

- Change to open temporal boundary conditions: field space becomes simply connected.



- Langevin scaling achieved

Global Topology Freezing: masterfield solution

M. Lüscher, EPJ Web Conf. 175 (2018) 01002

- Simulate a very large lattice at fixed global topology

- Accumulate statistics from separated space-time regions

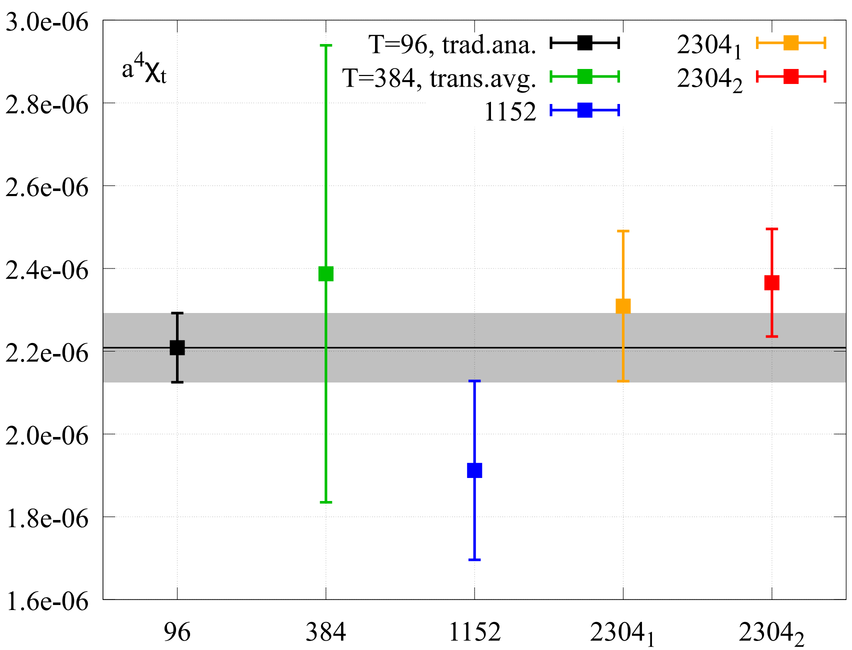
➔ O(1000) gauge configs = 6^4 space time regions of size $m_\pi L \approx 3$

Top. susceptibility comparison:

M. Bruno et al, PoS LATTICE2022 (2023) 368

$$\chi_{\text{top}} = \sum_x \langle q(x)\, q(0) \rangle$$

(only T-direction is large)



Observables from lattice QCD: Euclidean correlation functions

- Large time separation: ground state saturation (Analogy: SHO)

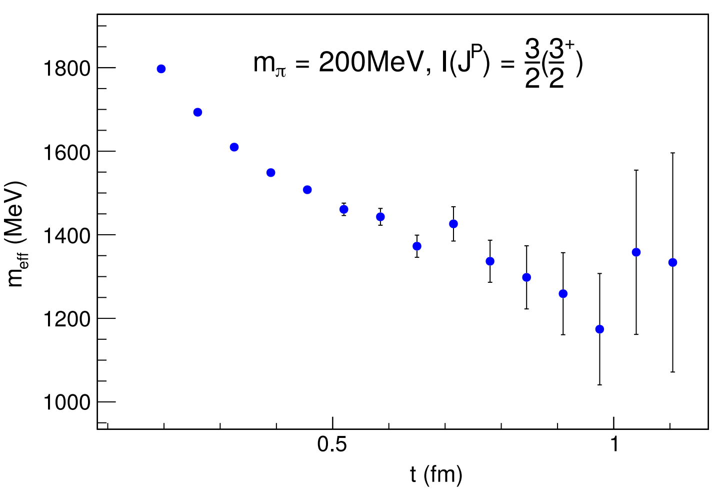
$$C(\tau) = \langle 0|\hat{x}(\tau)\,\hat{x}(0)|0\rangle = \langle 0|\hat{x}\,\mathrm{e}^{-\hat{H}\tau}\,\hat{x}|0\rangle = \sum_n |\langle 0|\hat{x}|n\rangle|^2 \mathrm{e}^{-E_n\tau}$$

- Low-lying states from large-time limit:

$$\lim_{\tau\to\infty} C(\tau) = A\mathrm{e}^{-E_1\tau} \times \left\{1 + \mathrm{O}(\mathrm{e}^{-(E_2-E_1)\tau})\right\}$$

- Signal-to-noise problem → 'Teufelspakt'

$$m_{\mathrm{eff}}(\tau) = \log\left[\frac{C(\tau)}{C(\tau+1)}\right]$$



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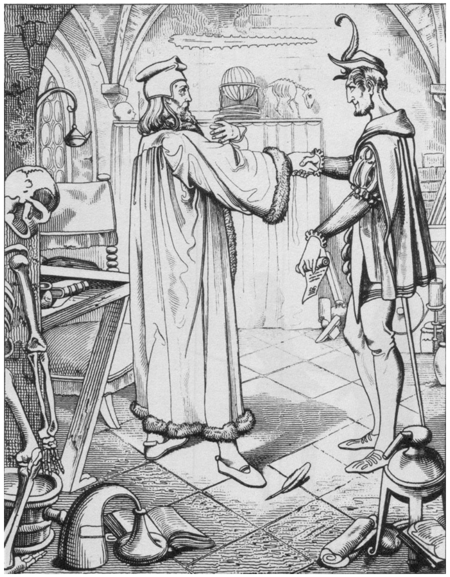


Plot courtesy of C. W. Andersen, apologies to J. W. von Goethe

The Signal-to-noise Problem:

- The variance is also a correlation function. Spectrum can be analyzed.

$$\sigma_\Delta^2(t) \sim \mathrm{e}^{-3m_\pi t}$$

- The signal to noise ratio:

$$\frac{C_\Delta(t)}{\sigma_\Delta(t)} \sim \mathrm{e}^{-(m_\Delta - \frac{3}{2}m_\pi)t}$$

- A general problem in lattice QCD. Exponentially bad.

- More examples in the exercises

Computing Correlation functions:

- Wick's theorem (for a fixed gauge field):

$$\langle \eta_{i_1} \eta_{i_2} \ldots \eta_{i_N} \, \bar{\eta}_{j_1} \bar{\eta}_{j_2} \ldots \bar{\eta}_{j_N} \rangle = \sum_{\{k_1,\ldots,k_N\} \in P(i_1,\ldots,i_N)} \; \sum_{\{l_1,\ldots,l_N\} \in P(j_1,\ldots,j_N)} \epsilon_{k_1 \ldots k_N} \epsilon_{l_1 \ldots l_N} \, [D^{-1}]_{k_1 l_1} \ldots [D^{-1}]_{k_N l_N}$$

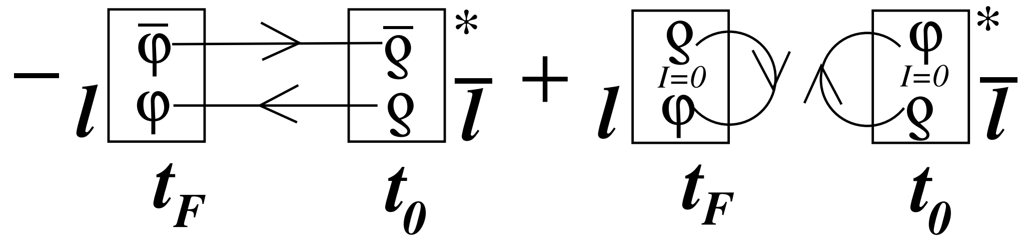
- Recall: computations of inverse are computationally costly

- Better if only 'point-to-all' propagators are required: $D^{-1}(x|0)$
  (12 Dirac equation solves)

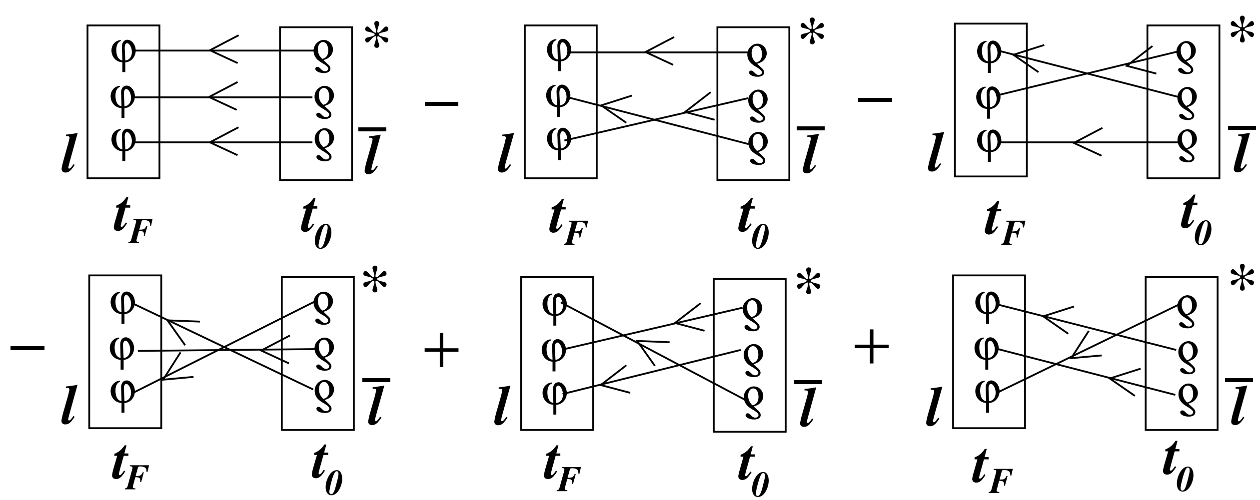
- The full 'all-to-all' propagator is costly: $D^{-1}(x|y)$

Valence quark-line diagrams: examples

- Single meson:



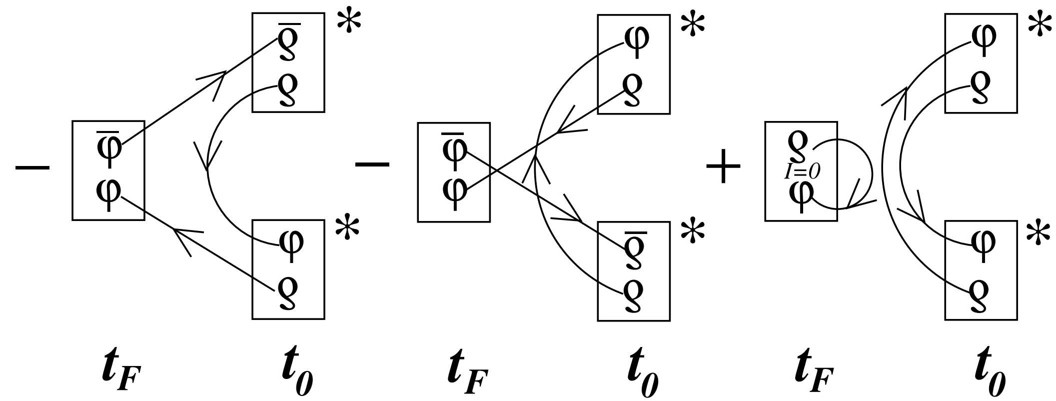
- Single baryon:



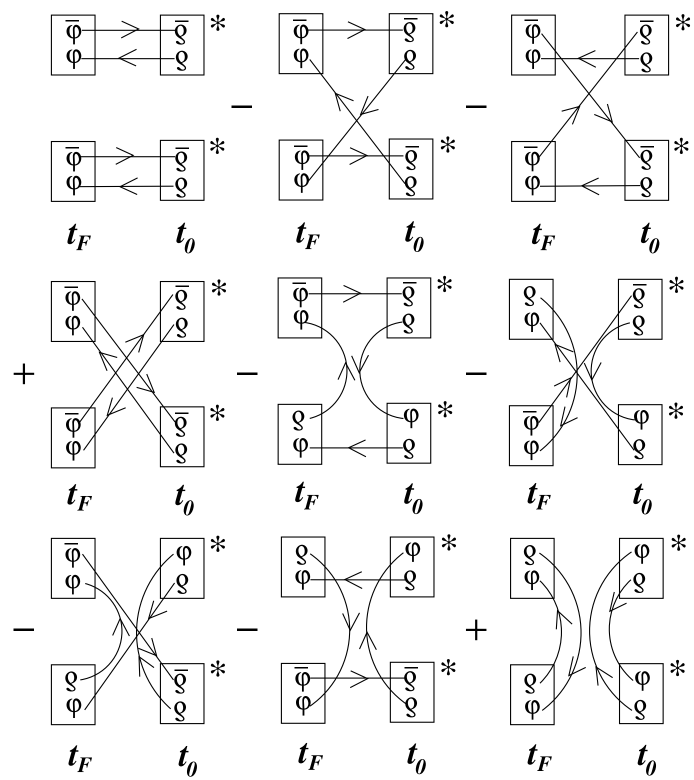
Diagrams from C. Morningstar et al., Phys.Rev.D 83 (2011) 114505

Valence quark-line diagrams: examples

- Meson-to-two-meson:



- Two-meson:



Diagrams from C. Morningstar et al., Phys.Rev.D 83 (2011) 114505

Conclusions:

- Lattice QCD enables non-perturbative computation of low-energy QCD

- Subtleties of lattice regularization:
  - Chiral symmetry/Fermion doubling
  - O(a) improvement

- Algorithms and computing power have improved. Simulations at the physical quark masses (with controlled errors) are possible.

- Some correlation functions are difficult to compute! Signal-to-noise problems are everywhere, especially bad for baryons.

THANKS!