Lattice hadron spectroscopy

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LOW ENERGY QCD

- QCD fundamental objects: quarks and gluons
- QCD observed objects: protons, neutrons (π, K, . . .)

! Huge discrepancy: not even the same particles observed as in the Lagrangean

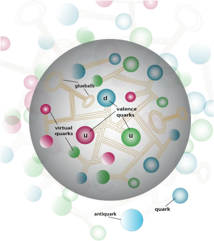
➛ Perturbation theory has no chance

- Need to solve low energy QCD to:
  - Compute hadronic and nuclear properties
    "people who love QCD"
    - Masses, decay widths, scattering lengths, thermodynamic properties, . . .
  - Compute hadronic background
    "people who hate QCD"
    - Non-leptonic weak MEs, quark masses, g-2, . . .

QCD AND HADRONS

What is a hadron?

- Not so easy to define!
- Bound state of quarks and gluons that is not a more complex nucleus?
  - baryons (qqq)
  - mesons ($\bar{q}q$)
  - (glueballs)
  - ? tertaquarks ($\bar{q}q\bar{q}q$)
  - ? pentaquarks ($qqq\bar{q}q$)
  - ? hadronic molecules
  - ? ...



- PDG lists some 1500 hadrons up to $M \sim 3\text{GeV}$
- Only one single hadron is stable in the SM (proton)

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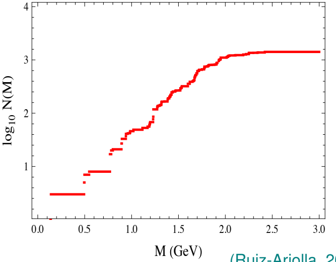

(Ruiz-Ariolla, 2014)

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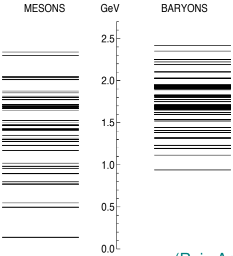

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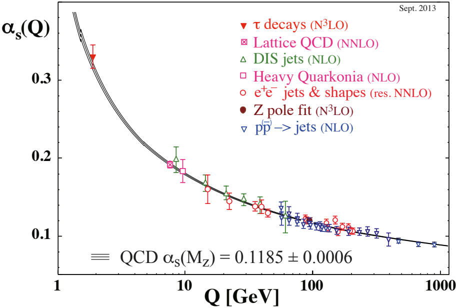
WHY HADRON SPECTROSCOPY?

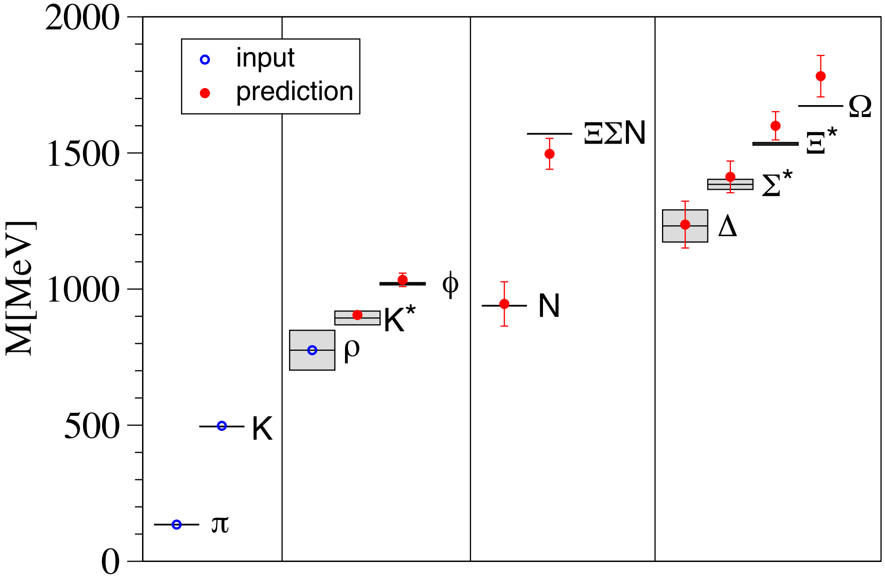
There are many reasons to do hadron spectroscopy:

- Test whether QCD is the correct theory of the strong interaction in the low energy regime
  - QCD itself needs to be validated at low energies
  - Good crosscheck for lattice QCD methods

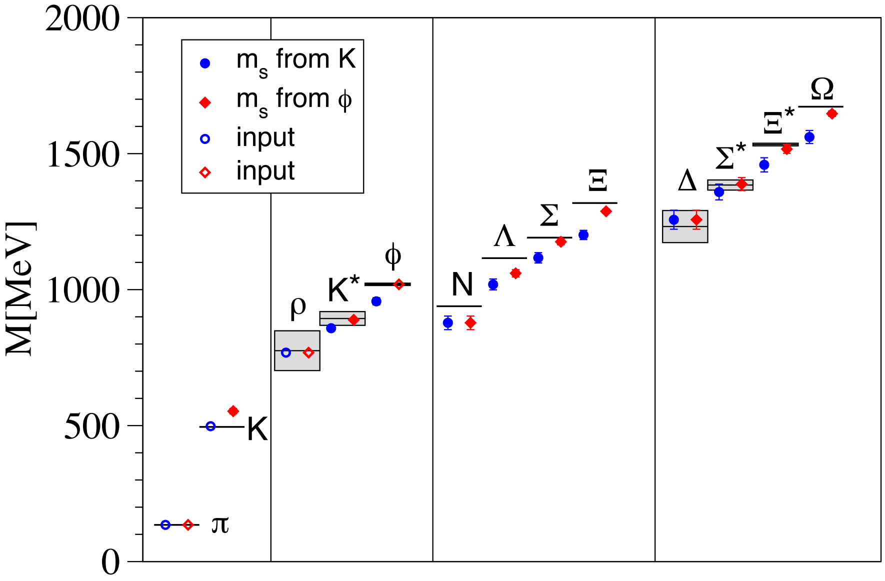


- Predict new states for experiments
- Clarify the nature of (possibly exotic) resonances
- Explore QCD at nonphysical parameters
  - Can reveal interesting properties (e.g. σ terms)
  - Fundamental questions about fine-tuning of our universe

GF11 1993



CP-PACS 2000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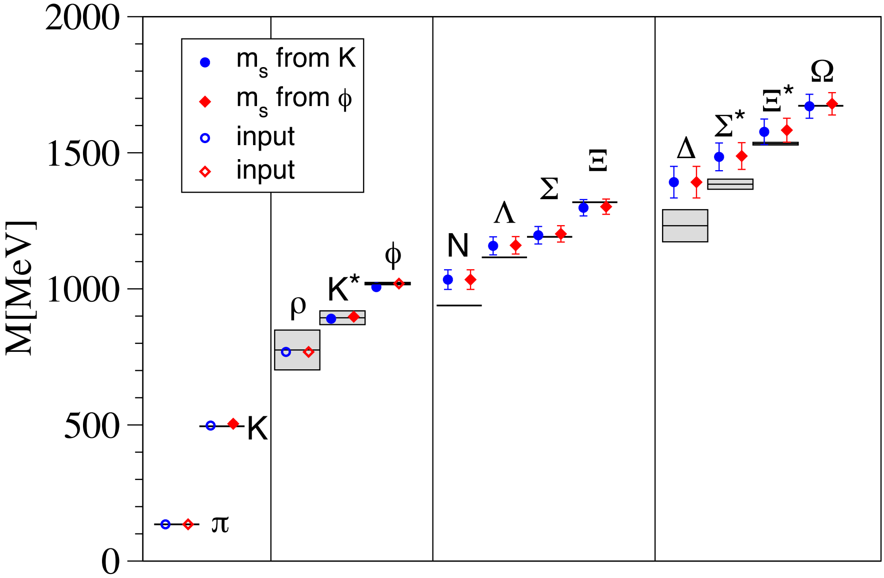
CP-PACS 2002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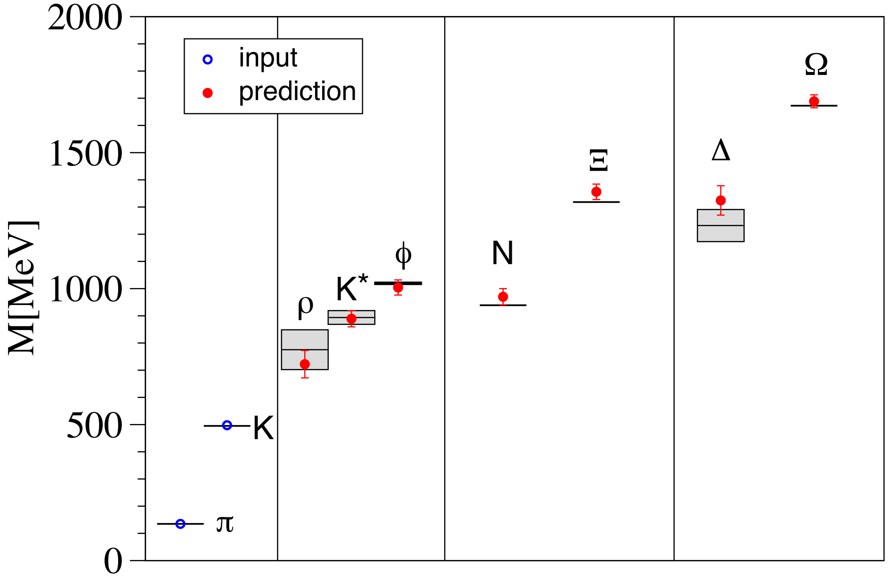
MILC 2010



INGREDIENTS OF A SPECTRUM CALCULATION

Hadron spectrum is the prototypical lattice calculation

- In principle, computing the spectrum is easy:
  - Go to the physical point, measure propagators
  - Read off the target mass

  but the devil lies in the details!
  - Physical point is difficult to reach
  - Identifying the target state contribution to a propagator
  - Eliminate discretization and finite volume effects
  - Obtain sufficient statistical accuracy
- Many intertwined ingredients
- Optimize for cost efficiency (physics output per CPU hour)

A CAUTIONARY REMARK

"It is difficult to find a model in the literature that would give a grossly incorrect hadron spectrum"(Hasenfratz, Montvay, 1987)

- $M_\rho = 800 \pm 100$ MeV, $M_{N/\Delta} = 1000 \pm 100$ MeV (Hamber, Parisi, 1981) even though scale was off by a factor 2

Hadron spectroscopy is all about understanding and reducing errors

OUTLINE

Lattice QCD (spectrum relevant)

Extraction of masses

Physical predictions

Isospin and QED

EUCLIDEAN PATH INTEGRAL

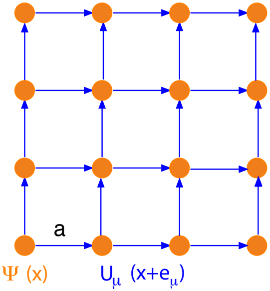
Euclidean correlator:

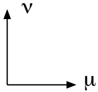
$$\langle 0|T(\mathcal{O}_1(x_1)\cdots\mathcal{O}_n(x_n))|0\rangle_E = \frac{\int [\mathrm{d}\psi]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}A_\mu]\,\mathcal{O}_1(x_1)\cdots\mathcal{O}_n(x_n)\,e^{-S_E[\psi,\overline{\psi},A_\mu]}}{\int [\mathrm{d}\psi]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}A_\mu]\,e^{-S_E[\psi,\overline{\psi},A_\mu]}}$$

Expectation value of $\mathcal{O}_1(x_1)\cdots\mathcal{O}_n(x_n)$
with respect to positive definite measure $[\mathrm{d}\psi]\,[\mathrm{d}\overline{\psi}]\,[\mathrm{d}A_\mu]\,e^{-S_E[\psi,\overline{\psi},A_\mu]}$

LATTICE DISCRETIZATION

- UV cutoff: space-time lattice
- Hypercubic, spacing a
- Momentum cutoff $p_\mu < 2\pi/a$
- Continuum theory: $a \to 0$





☞ anti-commuting $\psi(x)$ quark fields live on the sites

☞ gluon fields $U_\mu(x) = U(x, x + e_\mu)$ live on links

$$U(x, y) = \exp\left(ig \int_x^y dz_\mu \, A_\mu(z)\right) \in SU(3)$$

'reverse' link: $U^\dagger_\mu(x + e_\mu) = U(x + e_\mu, x)$

LATTICE GAUGE INVARIANCE

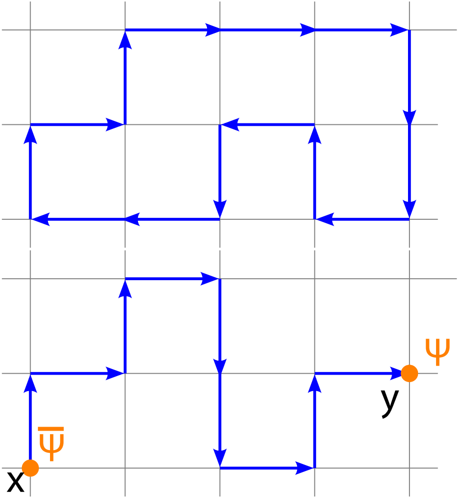
Lattice gauge transformations:

$$U'_\mu(x) = G(x)U_\mu(x)G^\dagger(x+e_\mu)$$
$$\Psi'(x) = G(x)\Psi(x)$$
$$\bar{\Psi}'(x) = \bar{\Psi}(x)G^\dagger(x)$$

with $G(x) \in SU(3)$

- ✎ Gauge symmetry needs to be preserved exactly
- ✎ Action needs to be gauge invariant
- ➠ Construct gauge invariant quantities

GAUGE INVARIANT OBJECTS



Closed gluon loops:

$$\mathrm{Tr}\left(U_{\mu_0}(x)U_{\mu_1}(x+e_\mu)\dots U^\dagger_{\mu_n}(x)\right)$$

$\bar{q}$ q connected by gluon lines:

$$\bar{\Psi}(x)U_{\mu_0}(x)\dots U^\dagger_{\mu_n}(y)\Psi(y)$$

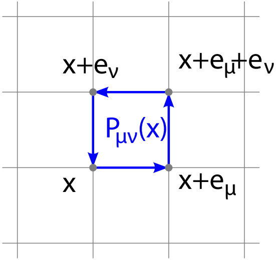
GAUGE ACTION

Continuum gauge action:

$$S_{\mathrm{G}} = \int \mathrm{d}^4 x \frac{1}{4} F_{\mu\nu} F_{\mu\nu}$$

Simplest gauge invariant lattice action (Wilson action):

$$S_{\mathrm{G}}^{\mathrm{W}} = \frac{6}{g^2} \sum_{x,\mu,\nu} \left(1 - \frac{1}{6} P_{\mu\nu}(x)\right) \qquad S_{\mathrm{G}}^{\mathrm{W}} = S_{\mathrm{G}} + \mathcal{O}(a^2)$$



Plaquette: elementary gluon loop

$$P_{\mu\nu}(x) = \mathrm{Tr}\left(U_\mu(x) U_\nu(x+e_\mu) U_\mu^\dagger(x+e_\nu) U_\nu^\dagger(x)\right)$$

IMPROVEMENT

Gauge action is not unique ➛ optimize?

- Lattice actions generically contain discretized derivatives

$$\Delta_a f(x) = \frac{f(x+a) - f(x-a)}{2a} = \sum_{k=0}^{\infty} \frac{a^{2k}}{(2k+1)!} f^{(2k+1)}(x)$$

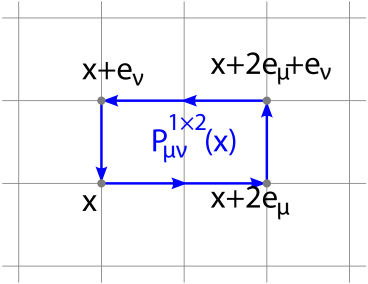
- Closer to derivative by combinations $\Delta_a, \Delta_{2a}, \ldots$
- Take $\Delta_a, \ldots, \Delta_{Na}$ ➛ classically imroved to $O(a^{2N})$
- Quantum theory: radiative corrections

Symanzik improvement (Symanzik 1981)

SYMANZIK IMPROVEMENT

Larger gluon loops possible: e.g. 2×1:

- Same Leading order continuum term
- Different $\mathcal{O}(a^2)$ terms
- Combine with $P_{\mu\nu}$ to cancel $\mathcal{O}(a^2)$ terms



$$S_G^S = \frac{6}{g^2} \sum_{x,\mu,\nu} \left(1 - \frac{1}{6}\left(\frac{5}{3} P_{\mu\nu}(x) - \frac{1}{12} P^{1\times 2}_{\mu\nu}(x)\right)\right) \qquad S_G^S = S_G + \mathcal{O}(a^4)$$

Quantum corrections: $S_G^S = S_G + \mathcal{O}(g^2 a^2)$

Tree level is typically enough and simple

FERMION INTEGRATION

Full lattice QCD action:

$$S = S_G + S_F$$

where the fermionic part in general is a Grassmann bilinear

$$S_F = \bar{\Psi} M \Psi$$

which can be integrated out formally

$$\mathcal{Z} = \int \prod_{x,\mu} [dU_\mu(x)][d\bar{\Psi}(x)][d\Psi(x)] e^{-S_G - S_F}$$
$$= \int \prod_{x,\mu} [dU_\mu(x)] \det(M[U]) e^{-S_G}$$

FERMION PROPAGATORS

Fermion propagators from:

$$\int \prod_{z,\mu} [dU_\mu(z)][d\bar{\Psi}(z)][d\Psi(z)]\Psi_\alpha(x)\bar{\Psi}_\beta(y)e^{-S_G - S_F} =$$

$$\int \prod_{z,\mu} [dU_\mu(z)]M^{-1}_{x,\alpha;y,\beta}[U]\det(M[U])e^{-S_G}$$

Under lattice gauge transformation:

$$M'^{-1}_{x;y}[U] = G(x)M^{-1}_{x;y}[U]G^\dagger(y)$$

$$\Psi'(x) = G(x)\Psi(x)$$

$$\bar{\Psi}'(y) = \bar{\Psi}(y)G^\dagger(y)$$

$$U'_\mu(x) = G(x)U_\mu(x)G^\dagger(x+e_\mu)$$

GAUGE INVARIANT OBJECTS

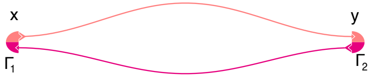
From the basic ingredients:

Fermion propagators $M'^{-1}_{x;y}[U]$

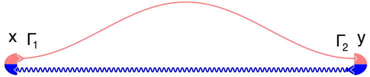
Gauge connections $U(x, y)$

we can build e.g.

Meson propagators ...



... with one static quark

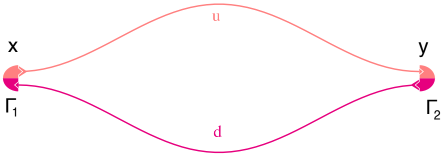


Fermion loops

FERMIONIC OBSERVABLES

$$\mathcal{O}(x,y) = \mathcal{O}_2^\dagger(y)\mathcal{O}_1(x) = \left(\bar{\Psi}^u \Gamma_2^\dagger \Psi^d\right)_y \left(\bar{\Psi}^d \Gamma_1 \Psi^u\right)_x$$ fermionic operator

$$\langle 0|T(\mathcal{O}(x,y))|0\rangle =$$
$$\frac{1}{\mathcal{Z}}\int D\bar{\Psi} D\Psi DU \left(\bar{\Psi}^u \Gamma_2^\dagger \Psi^d\right)_y \left(\bar{\Psi}^d \Gamma_1 \Psi^u\right)_x e^{-S_G - S_F} =$$
$$\frac{1}{\mathcal{Z}}\int DU \mathrm{Tr}_{c,s}\left(\Gamma_1 M_{x,y}^{-1,u}(U)\Gamma_2^\dagger M_{y,x}^{-1,d}(U)\right) \det(M[U]) e^{-S_G}$$



WICK CONTRACTIONS

Expectation value of $\mathcal{O}(x,y) = \left(\bar{\Psi}^u \Gamma_2^\dagger \Psi^d\right)_y \left(\bar{\Psi}^d \Gamma_1 \Psi^u\right)_x$

with respect to the action $S_\mathrm{G} + S_\mathrm{F}$

is equivalent to

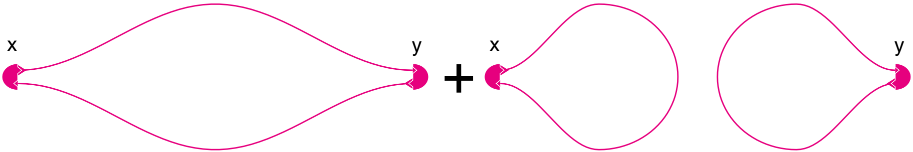
Expectation value of $\mathrm{Tr}_{\mathrm{c,s}}\left(\Gamma_1 M^{-1,u}_{x,y}(U)\Gamma_2^\dagger M^{-1,d}_{y,x}(U)\right)$

with respect to the action $S_\mathrm{G} - \ln\det(M[U])$

DISCONNECTED CONTRIBUTIONS

$$\mathcal{O}(x,y) = \mathcal{O}^\dagger(y)\mathcal{O}(x) = \left(\bar{\Psi}\Psi\right)_y \left(\bar{\Psi}\Psi\right)_x$$ fermionic operator

$$\langle 0|T(\mathcal{O}(x,y))|0\rangle = \frac{1}{\mathcal{Z}} \int DU e^{-S_G} \det(M[U]) \left(\mathrm{Tr}\left(M^{-1}_{x,y}(U) M^{-1}_{y,x}(U)\right) + \mathrm{Tr}\left(M^{-1}_{x,x}(U)\right)\left(M^{-1}_{y,y}(U)\right)\right)$$



EXTRACTING ENERGY LEVELS (IN PRINCIPLE)

We are interested in the mass of a hadronic state $|h\rangle$:

- Chose (possibly identical) operators $\langle h|\mathcal{O}_{1/2}|0\rangle \neq 0$
- Compute the correlator

$$G(t,0) = \langle 0|\mathcal{O}_2^\dagger(t)\mathcal{O}_1(0)|0\rangle = \langle 0|e^{\mathcal{H}t}\mathcal{O}_2^\dagger e^{-\mathcal{H}t}\mathcal{O}_1|0\rangle$$

- Inserting a complete set of energy eigenstates $\mathbb{1} = \sum_n |n\rangle\langle n|$ with $\mathcal{H}|n\rangle = E_n|n\rangle$, $E_0 = 0$

$$G(t,0) = \sum_n \frac{\langle 0|\mathcal{O}_2^\dagger|n\rangle\langle n|\mathcal{O}_1|0\rangle}{2E_n} e^{-E_n t}$$

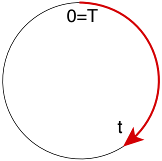
- One of the states is $|h\rangle$ and we can in principle extract it

GROUND STATE MASS

In practice, only ground state is relatively simple:

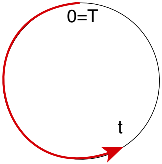
- For infinite time extent ($T \to \infty$), ground state $|h\rangle$ dominates asymptotically:

$$G(t,0) \stackrel{t\to\infty}{\longrightarrow} \frac{\langle 0|\mathcal{O}_2^\dagger|h\rangle\langle h|\mathcal{O}_1|0\rangle}{2E_h} e^{-E_h t}$$



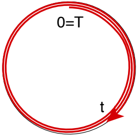
- There is also a backward contribution (torus topology):

$$G(t,0) \stackrel{T-t\to\infty}{\longrightarrow} \pm\frac{\langle 0|\mathcal{O}_1|\tilde{h}\rangle\langle \tilde{h}|\mathcal{O}_2^\dagger|0\rangle}{2E_{\tilde{h}}} e^{-E_{\tilde{h}}(T-t)}$$

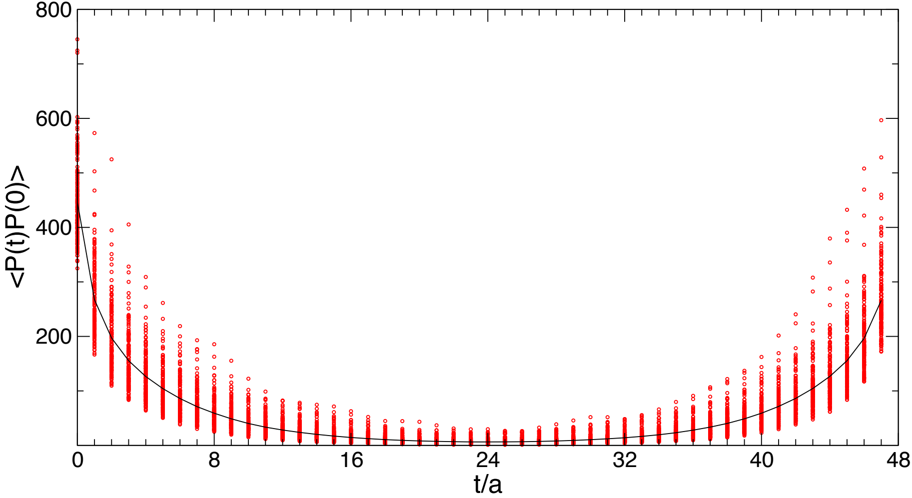


- And multiple windings for finite T that can be summed

$$e^{-E_h t}\sum_{n=0}^{\infty} e^{-E_h nT} = \frac{e^{-E_h t}}{1-e^{-E_h T}}$$



NICE PROPAGATOR EXAMPLE



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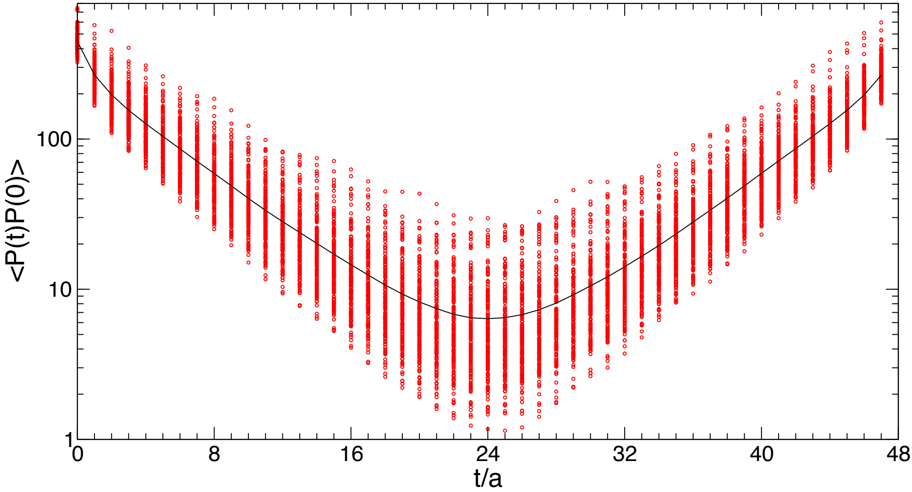
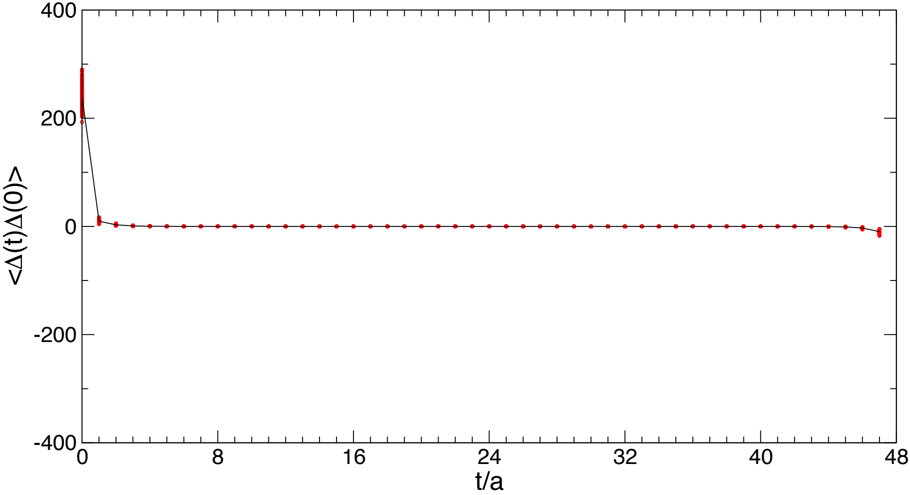


NOT SO NICE PROPAGATOR EXAMPLE



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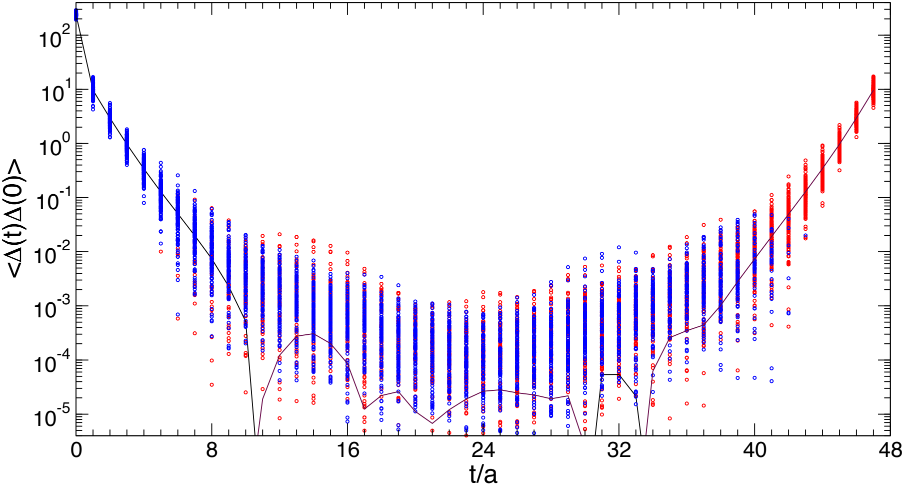

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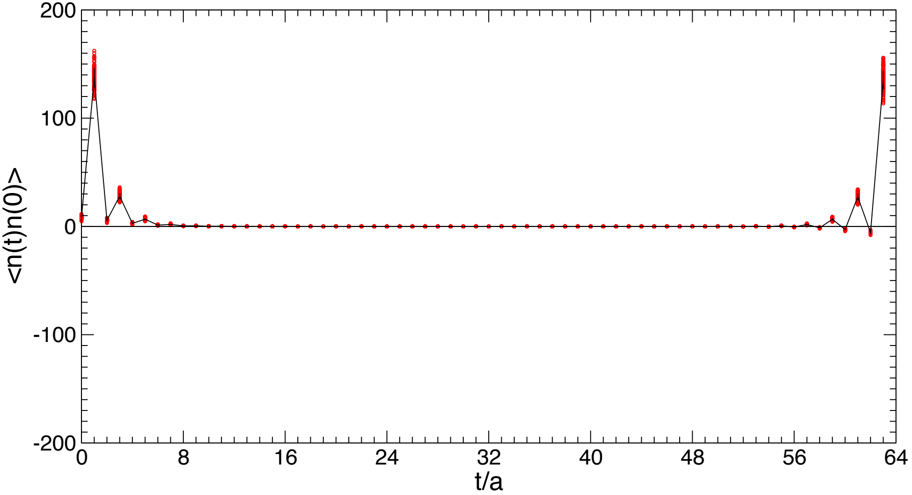

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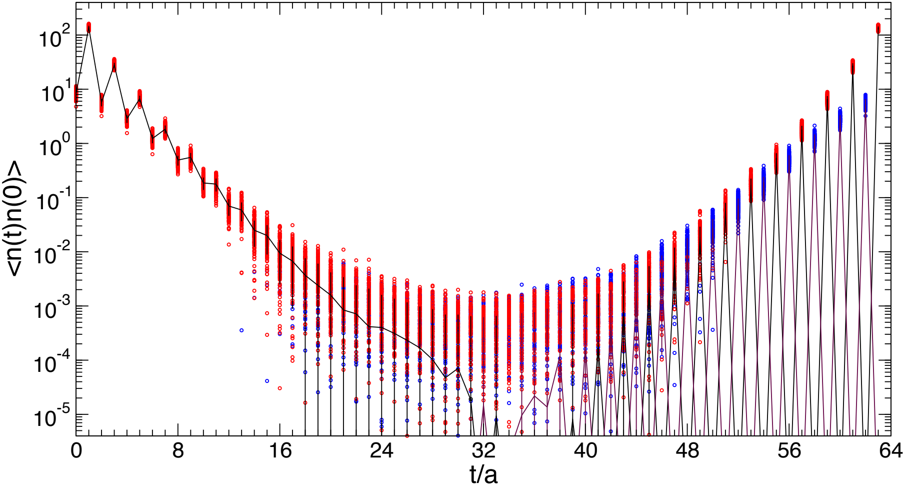
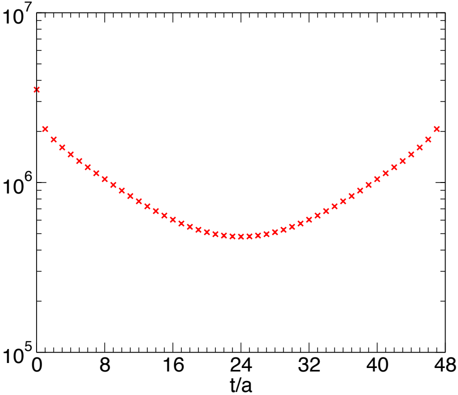
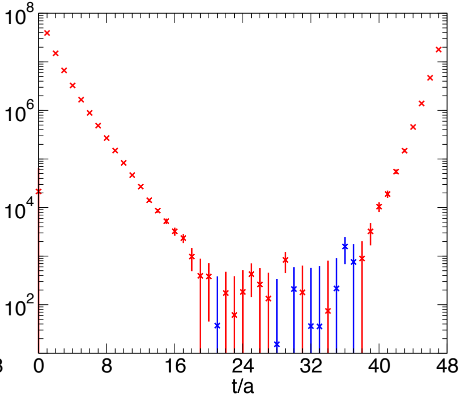


SIGNALS FROM PROPAGATORS

Numerical challenge can vary significantly

- Target state coupling may be small
- Signal decays exponentially, noise not always
- Sign fluctuations in propagators, except for *PP*





EFFECTIVE MASSES

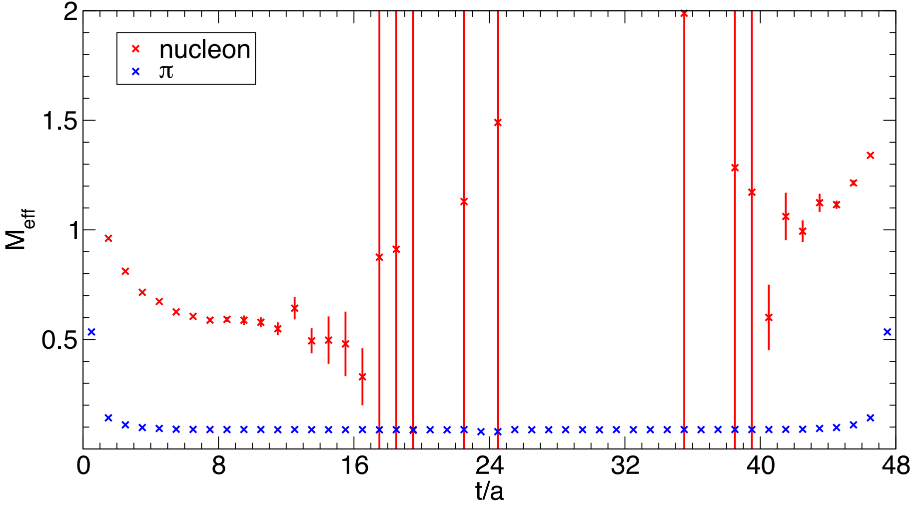
To identify asymptotic region, define an effective mass:

$$M_{\text{eff}}(t) = \frac{1}{l} \ln \frac{C(t - l/2)}{C(t + l/2)}$$

- Lag l: typically 1 or 2
- Modified versions including backward contributions
- Analytical 3-point expression for symmetric case:

$$M_{\text{eff}}(t) = acosh \frac{c_{t+1} + c_{t-1}}{2c_t}$$

MASS PLATEAUX EXAMPLE



EXTRACTING GROUND STATES

Which particle masses can we extract as ground states?

- Stable with respect to the *simulated* theory
  - Weak decays not present
  - Lattice kinematically forbidden decays (large M_π, minimum $\vec{p}$)
  - Broken continuum symmetries can induce unphysical mixing
    - Depends on lattice discretization
- Open window between excited state decay and signal loss

Of course, we need to connect them to physical states later on

- All this depends crucially on the fermion discretization
  - Should be fast
  - Should have little symmetry breaking (low statistical noise)
  - Should allow going to physical point

FERMION OPERATORS

Free continuum theory:

$$S_F = \int d^4x\, \overline{\psi}(\gamma^\mu \partial_\mu + m)\psi$$

Naively discretized:

$$S_F^N = a^4 \sum_x \left(\bar{\Psi}(x)\gamma_\mu \frac{\Psi(x+e_\mu) - \Psi(x-e_\mu)}{2a} + m\,\bar{\Psi}(x)\Psi(x) \right)$$

Inverse propagator:

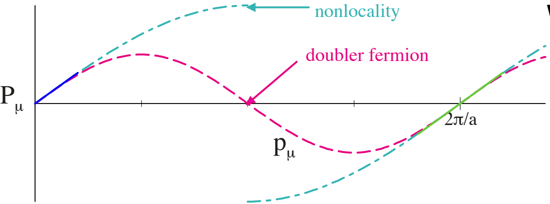
$$G_N^{-1}(p) = \mathrm{i}\gamma_\mu \frac{\sin p_\mu a}{a} + m$$

- ✗ 16 zeros at $p_\mu = \{0, \pm\frac{\pi}{a}\}$ in 1st Brillouin zone
- ✗ In d dimensions 2^d fermions instead of 1 (fermion doubling)

NIELSEN-NINOMIYA THEOREM

Chirally invariant ($\{D, \gamma_5\} = 0$) Dirac operator:

$$D(p) = \sum_\mu \gamma_\mu P_\mu(p)$$



We require:

- Correct continuum limit: $P_\mu(p_\mu) \stackrel{p\to 0}{\rightarrow} p_\mu$
- Periodicity: $P_\nu(p_\mu) = P_\nu(p_\mu + 2\pi/a)$

➠ doubler fermions or nonanalyticity (nonlocality) or give up chirality

WILSON FERMIONS

Breaking chiral symmetry: $S_F^W = S_F^N + \underbrace{a\frac{r}{2}a^4 \sum_x \bar{\Psi}(x)\Box\Psi(x)}_{\text{Wilson term}}$

with

$$\Box\Psi(x) = \frac{\Psi(x+e_\mu) - 2\Psi(x) + \Psi(x-e_\mu)}{a^2}$$

Wilson parameter: $r \in (0,1]$, usually $r = 1$

$$G_W^{-1}(p) = G_N^{-1}(p) + \frac{2r}{a}\sum_\mu \sin^2\frac{ap_\mu}{2} = \begin{cases} i\gamma_\mu p_\mu & \text{all} \quad p_\mu \sim 0 \\ i\gamma_\mu p_\mu + \mathcal{O}(\frac{r}{a}) & \text{any} \quad p_\mu \sim \pm\frac{\pi}{a} \end{cases}$$

➠ Doublers receive divergent $\mathcal{O}(a^{-1})$ mass

INTERACTING THEORY

- We rescale to dimensionless fermion fields $a^{3/2}\Psi \to \Psi$
- Include gluon interaction: Connect fermions by gauge links

$$S_F^W = \sum_{x,\mu} \bar{\Psi}(x)\Big(-(r-\gamma_\mu)U_\mu(x)\Psi(x+e_\mu) -(r+\gamma_\mu)U_\mu^\dagger(x-e_\mu)\Psi(x-e_\mu) +(am+4r)\Psi(x)\Big)$$

✓ All doublers removed

✓ Crucial: $\gamma_5 M = M^\dagger \gamma_5$

✗ Chiral symmetry broken

- Mass gets additively renormalized
- Unwanted operator mixing
- Bad scaling: $S_F^W = S_F + \mathcal{O}(a)$

- Widely used for spectroscopy
- Broken chiral symmetry renders physical point difficult

CLOVER IMPROVEMENT

Kill leading $\mathcal{O}(a)$ discretization terms:

$$S_F^C = S_F^W - \underbrace{\frac{iacr}{4}\sum_x \bar{\Psi}(x)\sigma_{\mu\nu}F_{\mu\nu}(x)\Psi(x)}_{\text{clover term}} \qquad \sigma_{\mu\nu} = \frac{i}{4}[\gamma_\mu, \gamma_\nu]$$

with the symmetrically discretized field strength

$$F_{\mu\nu}(x) = \frac{1}{4}\mathrm{Im}\Big(P_{\mu\nu}(x) + P_{\mu\nu}(x-e_\mu) + P_{\mu\nu}(x-e_\nu) + P_{\mu\nu}(x-e_\mu-e_\nu)\Big)$$

Scaling improved:

$$S_F^C = S_F + \underbrace{\mathcal{O}(a^2)}_{\text{classical}} + \underbrace{\mathcal{O}(g^2 a)}_{\text{quantum corrections}}$$

Attention: observables need to be improved, too!

STAGGERED FERMIONS

The naive discretization

$$\bar{\Psi}(x)\gamma_\mu \frac{U_\mu(x)\Psi(x+e_\mu) - U_{-\mu}(x)\Psi(x-e_\mu)}{2a} + m\,\bar{\Psi}(x)\Psi(x)$$

has a 4-fold degeneracy that can be exposed by

$$\bar{\Psi}(x) \to \bar{\chi}(x)\gamma_3^{\frac{x_3}{a}}\gamma_2^{\frac{x_2}{a}}\gamma_1^{\frac{x_1}{a}}\gamma_0^{\frac{x_0}{a}} \qquad \Psi(x) \to \gamma_0^{\frac{x_0}{a}}\gamma_1^{\frac{x_1}{a}}\gamma_2^{\frac{x_2}{a}}\gamma_3^{\frac{x_3}{a}}\chi(x)$$

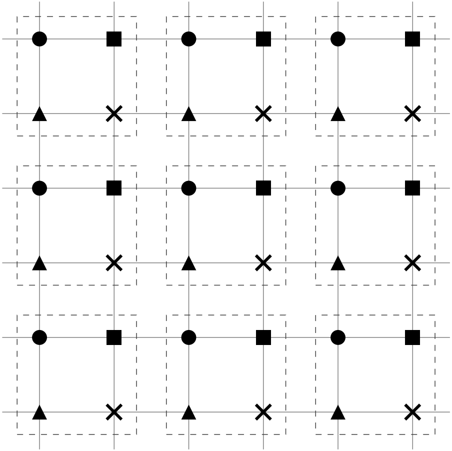
and we obtain the staggered fermion operator

$$\bar{\chi}(x)\eta_\mu(x)\frac{U_\mu(x)\chi(x+e_\mu) - U_{-\mu}(x)\chi(x-e_\mu)}{2a} + m\,\bar{\chi}(x)\chi(x)$$

with the purely numerical factor

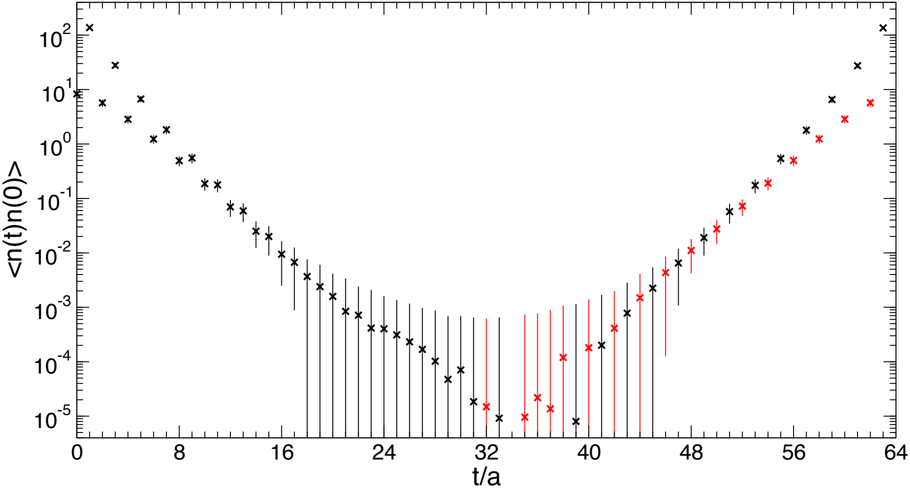
$$\eta_\mu(x) = (-1)^{\sum_{\nu<\mu} x_\nu}$$

STAGGERED FERMIONS (ctd.)



- 2^D components per hypercube
- describe $2^{D/2}$ flavors (“tastes”)
- $2^{D/2}$ components per spinor
- Taste decomposition exact in free theory only ➛ taste breaking
- γ_μ are not ultralocal!
- Spin structure not ultralocal with severe consequences for spectroscopy!

STAGGERED NUCLEON PROPAGATOR



STAGGERED FERMION SUMMARY

Live with some doublers: staggered fermions

- ☞ Naive action has exact $2^{d/2}$-fold degeneracy
- ☞ Lift $2^{d/2}$ degeneracy ➠ $2^{d/2}-1$ doublers remain

✓ Remnant chiral symmetry
- ➠ No additive mass renormalization
- ➠ Scaling: $S_F^S = S_F + \mathcal{O}(a^2)$

✓ Cheap (degeneracy removed)

✓ Crucial: $\eta_5 M = M^\dagger \eta_5$

✗ Some doublers remain

✗ Remaining doublers mix

➠ Delicate continuum limit

- ☞ Widely used because of low cost
- ☞ Ofen used as sea quarks in hybrid calculations
  - ➠ Valence fermions with full spin structure

OTHER FERMION DISCRETIZATIONS

Redefine lattice chiral symmetry: overlap/domain wall fermions

- ☞ Exact chiral symmetry:

$$\gamma_5 D + D\hat{\gamma}_5 = 0 \qquad \text{with} \qquad \hat{\gamma}_5 = \gamma_5 \left(1 - \frac{a}{\rho} D\right)$$

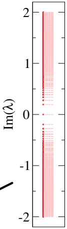
✓ Full chiral symmetry at finite a

- ➠ No additive mass renormalization
- ➠ Scaling: $S_F^S = S_F + \mathcal{O}(a^2)$

✗ D is expensive to construct

Many other variants/hybrids exist (minimally doubled, chirally improved, staggered overlap, etc), but none of them are used much

EIGENVALUE SPECTRA



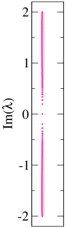
Naive fermions

$D_\mathrm{N} = \gamma_\mu D_\mu$

16 species

remove 4-fold degeneracy

add Wilson term



Staggered fermions

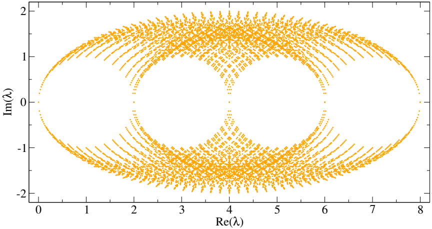
$D_\mathrm{st} = \eta_\mu D_\mu$

4 species

Wilson fermions

$D_\mathrm{W} = \gamma_\mu D_\mu + rW$

1+4+6+4+1 species

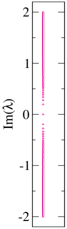


CHIRAL SYMMETRY

Wilson fermions D_W

1+4+6+4+1 species

↓



Staggered fermions

$D_{st} = \eta_\mu D_\mu$

4 species, anomaly hidden

$U(1)_\epsilon : \{D_{st}, \epsilon\} = 0$

$\epsilon = (-1)^{x_1+x_2+x_3+x_4}$

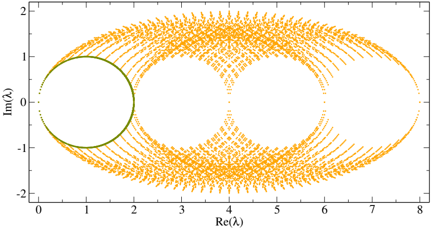
$\sim (\gamma_5 \otimes \xi_5)$

Overlap fermions

$D_{ov} = \rho\,(1 + \gamma_5 \text{sign}\,(\gamma_5\,(D_W - \rho)))$

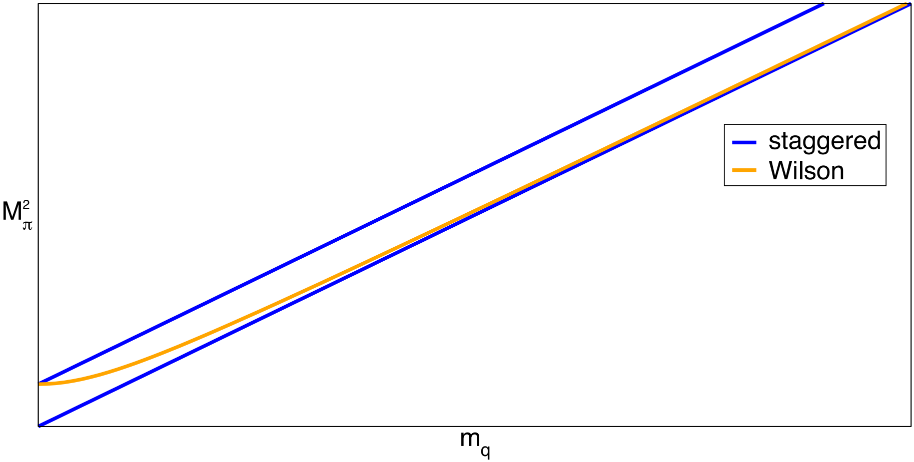
1 species, correct anomaly

Full $SU(N_f)$ chiral Symetry



HOW CHIRAL?

Breakdown pattern at low m_q for different fermions at fixed a:



TREATING UV MODES

UV modes (close to cutoff) pose a huge problem:

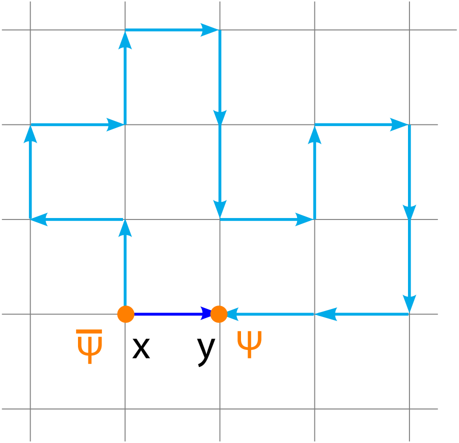
- UV modes are unphysical (huge cutoff effects)
- Their fluctuations may dominate observables
- Wilson type fermions: large chiral symmetry breaking
  - Large additive renormalization constants
- Staggered type fermions: mixes different "tastes"
  - Taste splitting

Removing UV modes:

- Damp UV modes by continuum irrelevant modification

UV FILTERING

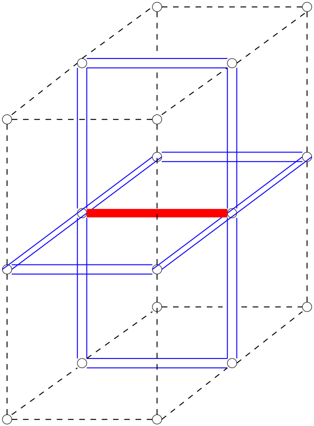
Parallel transports $U(x \to y)$ appear in fermion action

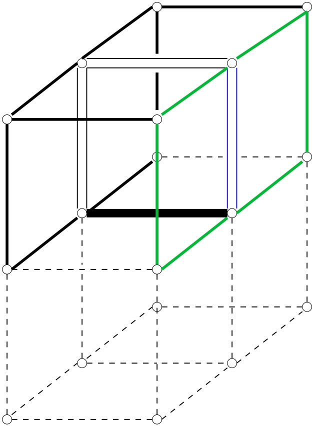


- $U(x \to y)$ not uniquely determined
- In principle any path may be chosen
- Filter UV modes by taking averages (Albanese et. al. (APE) 1987)
- Can be iterated
- Various recipes

(Hasenfratz, Knechtli 2001; Morningstar, Peardon 2003; Dürr CH 2006)

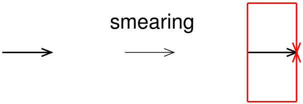
HYP SMEARING





(Hasenfratz, Knechtli 2001)

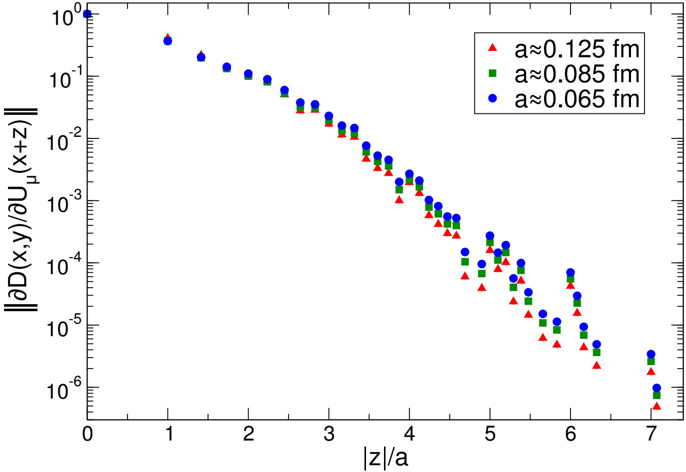
LOCALITY PROPERTIES



- locality in position space:
  $|D(x,y)| < \text{const}\, e^{-\lambda|x-y|}$ with $\lambda = O(a^{-1})$ for all couplings.
  E.g. "6 stout": $D(x,y) = 0$ as soon as $|x-y| > 1$
  (despite smearing)
- locality of gauge field coupling:
  $|\delta D(x,y)/\delta A(z)| < \text{const}\, e^{-\lambda|(x+y)/2-z|}$ with $\lambda = O(a^{-1})$ for all couplings.
  E.g. "6 stout": $\delta D(x,x)/\delta A(z) < \text{const}\, e^{-\lambda|x-z|}$ with $\lambda \simeq 2.2a^{-1}$ for $2 \leq |x-z| \leq 6$

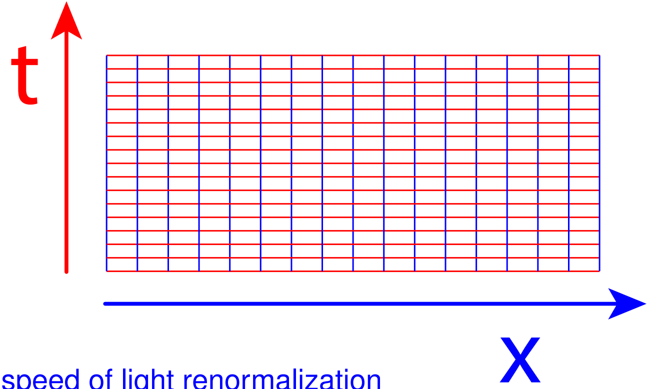
GAUGE FIELD COUPLING LOCALITY

6-stout case:



ANISOTROPIC LATTICES

For excited states we need large volume and fine time resolution



Difficulty: speed of light renormalization

- Has to be matched separately for fermions and gauge fileds

STOCHASTIC INTEGRATION

We want to compute stochastically (on a finite lattice)

$$\langle 0|\mathcal{O}|0\rangle = \frac{\sum_U \mathcal{O}_U e^{-S_U}}{\sum_U e^{-S_U}} \qquad \text{with} \qquad S_U = S_G - \ln\det(M[U])$$

Naive prescription:

- Randomly produce gauge configuration U
- Compute sums with weight e^{-S_U}

Most contributions are exponentially small ➠very inefficient

Importance sampling:

- produce configuration U_i weighted by e^{-S_U}
- Compute the sum $\langle 0|\mathcal{O}|0\rangle = \frac{1}{N}\sum_i \mathcal{O}_i$

NUMERICAL INTEGRATION

For each step we need to compute:

$$\exp(-\Delta S_g)\frac{\det(M(U_{k+1}))}{\det(M(U_k))}$$

- Gauge part: trace of 3×3 matrices
  - Local update possible
  - Low computational cost
- Fermionic part: det of large, usually sparse matrices
  - Only global update possible
  - Size of matrix: $\sim 10^6 \times 10^6 - 10^9 \times 10^9$
    - Dimension of M: 3(color) $\times$ 4(spin) $\times N_x \times N_y \times N_z \times N_t$
    - Number of lattice points: $N_\mu = L_\mu / a$
      $a \lesssim 0.1$fm to resolve a proton
      $N_\mu \gg 1$fm to fit a proton
  - Ignored in mean field approximation: Quenched approximation

STAGGERED ROOTING

For staggered fermions, $\det(M(U_k))$ represents 4 quark flavours that are non-degenerate in the interacting theory

What to do?

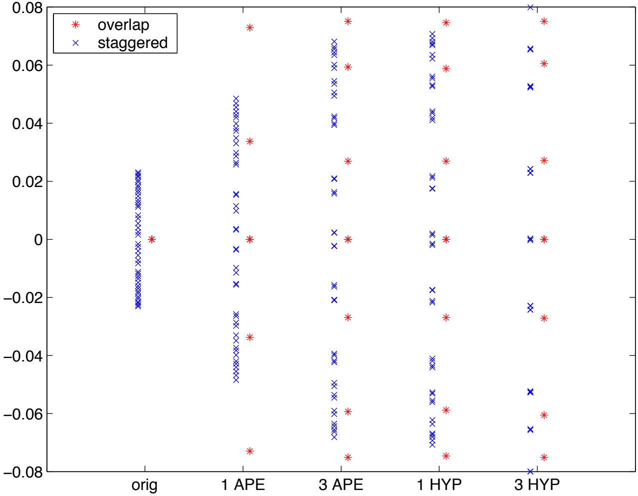
Take $\det(M(U_k))^{1/4}$ instead

Is this allowed?

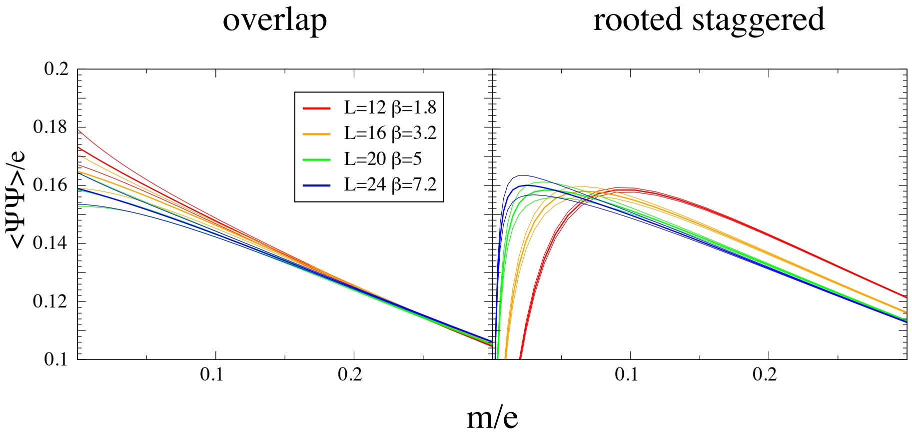
- ✓ Yes for the free theory (Adams 2006)
- ✓ Good numerical evidence if order of limits is observed (Durr, CH 2003-06)

(Creutz 2003-09; Bernard, Golterman, Sharpe 2003-8)

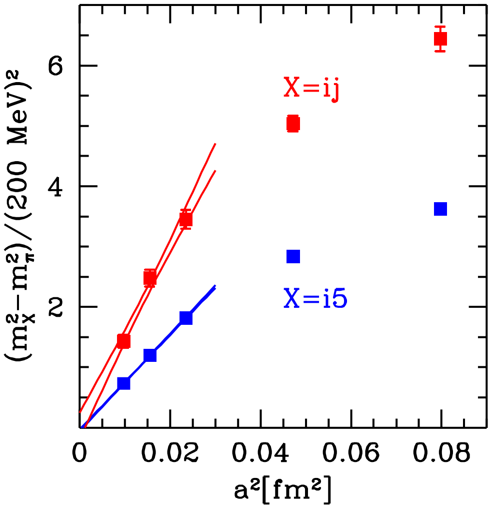
STAGGERED OPERATOR EIGENMODES



STAGGERED CONDENSATE

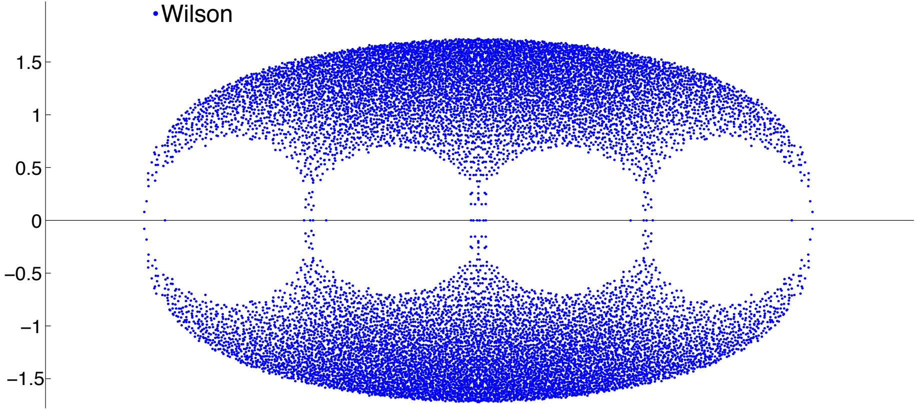


STAGGERED TASTE SPLITTING



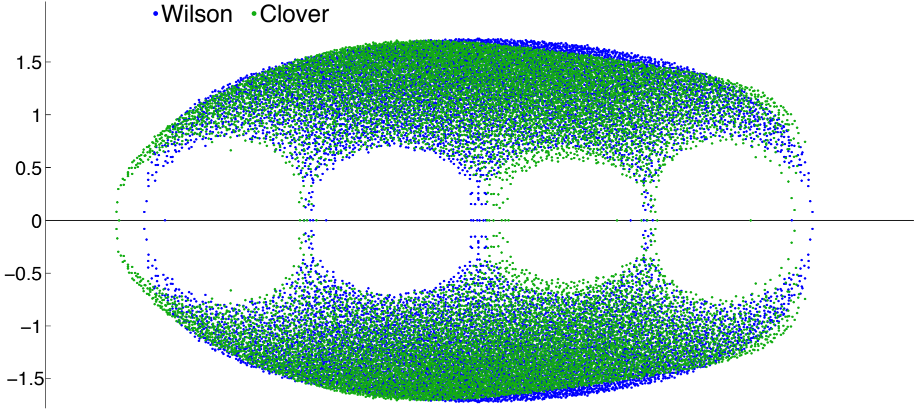
- Vanishes $O(a^2)$
- Sizeable: $\Delta m_\pi^2 \gtrsim (200\ \text{MeV})^2$

WILSON EIGENMODES



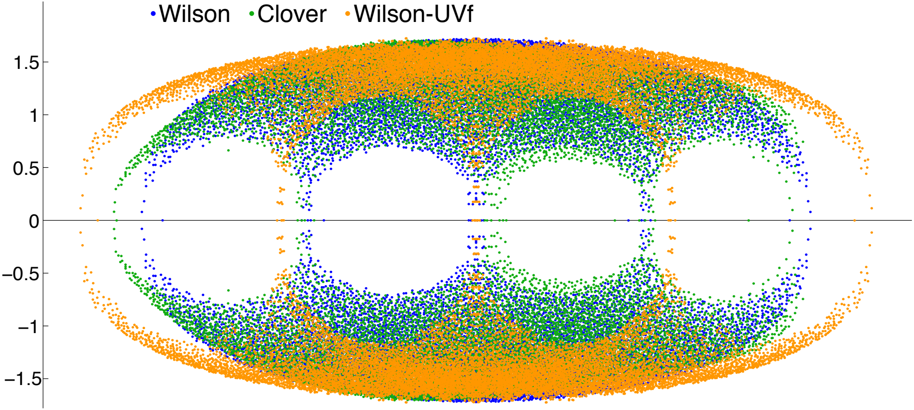
(Dürr, 2012-2014)

WILSON EIGENMODES



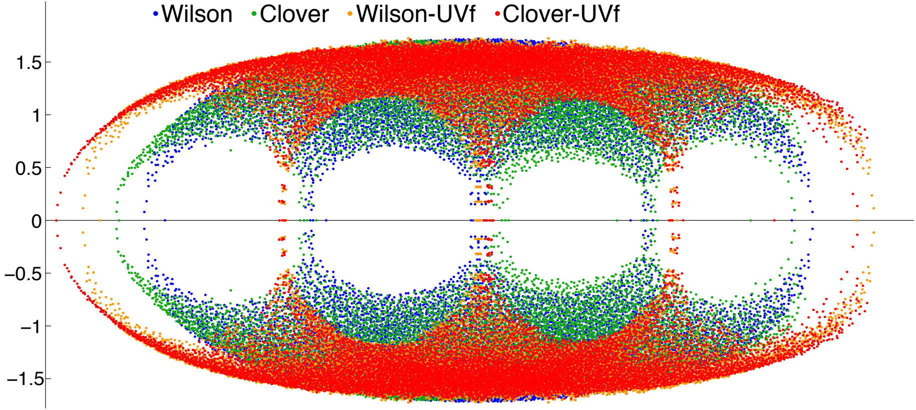
(Dürr, 2012-2014)

WILSON EIGENMODES



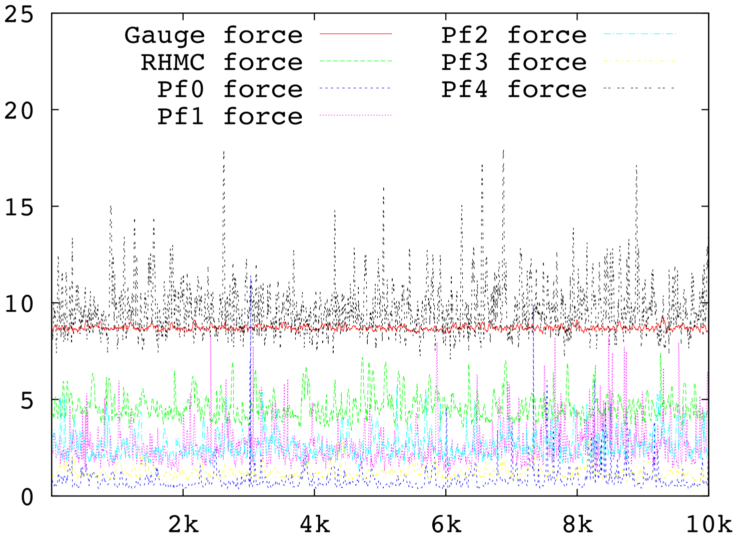
(Dürr, 2012-2014)

WILSON EIGENMODES

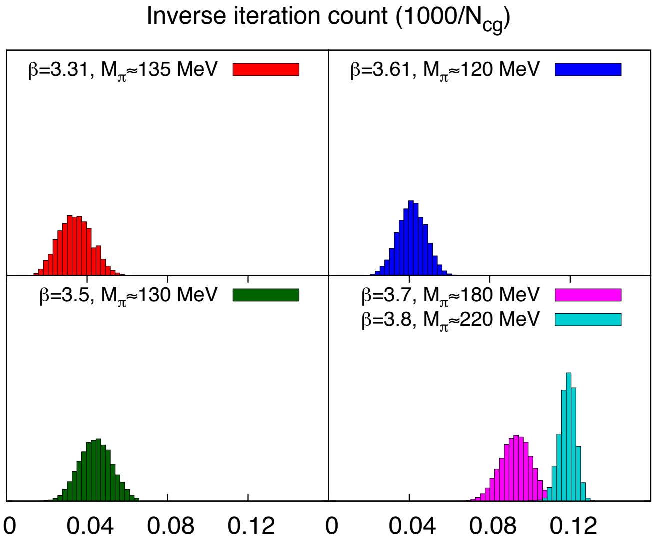


(Dürr, 2012-2014)

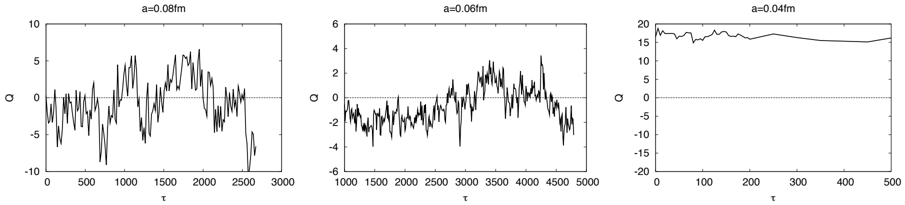
WILSON ALGORITHM STABILITY



WILSON EXCEPTIONAL CONFIGURATIONS

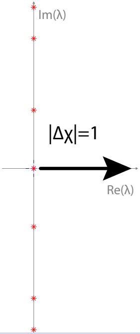


WILSON TOPOLOGY



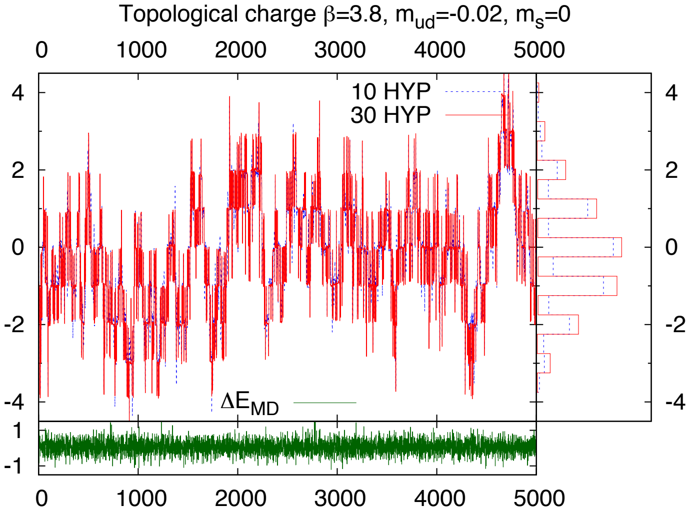
(Schäfer et. al. 2009)

- Huge autocorrelations as lattice gets finer
- Depending on action, algorithm, BC
- To some extend, this is "physical"
  - Discontinuity between top. sectors in continuum
  - This shows up as lattice gets more chiral ($a \to 0$)
  - Topological 0-modes jump



TOPOLOGICAL SECTOR SAMPLING

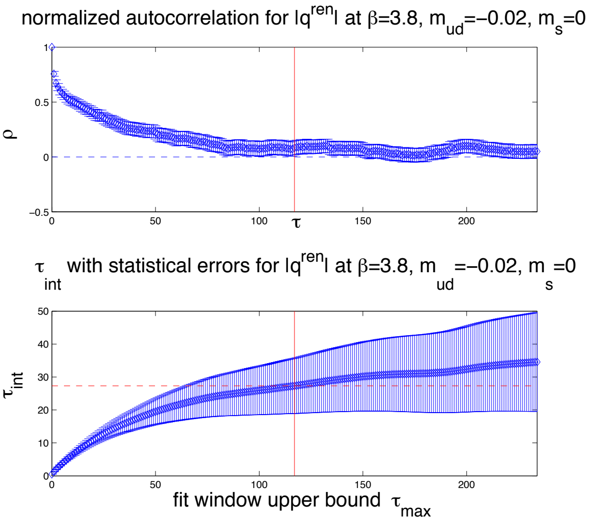
6-stout clover



AUTOCORRELATION TIME

$\tau_{\text{int}} = 27.3(7.4)$

(MATLAB code from Wolff, 2004-7)



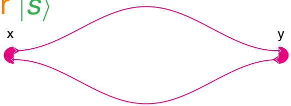
EFFICIENT PROPAGATOR COMPUTATION

For a minimal meson propagator, we need to compute:

$$G(x,y) = \mathrm{Tr}_{c,s}\left(\Gamma_1 M^{-1}_{x,y}(U)\Gamma_2^\dagger M^{-1}_{y,x}(U)\right)$$

Numerically, we get the inverse on a source vector $|s\rangle$

$$M^{-1}(U)|s\rangle$$



With $|s\rangle(z) = \delta_{z,x}$ we obtain the propagator from x to any point

- Additional inversions per sink point y required
- Use $\gamma_5 M = M^\dagger \gamma_5 \rightarrow M^{-1}_{y,x} = \gamma_5 M^{-1*}_{x,y}\gamma_5$

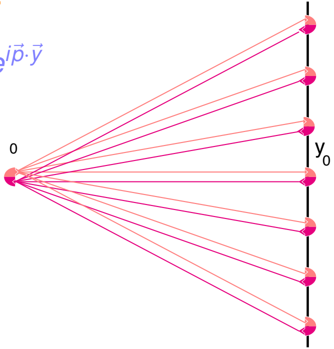
$$G(x,y) = \mathrm{Tr}_{c,s}\left(\gamma_5\Gamma_1 M^{-1}_{x,y}\Gamma_2^\dagger\gamma_5 M^{-1*}_{x,y}\right)$$

- Propagator to arbitrary sink point without further inversions

MOMENTUM PROJECTION

Cheap summation over sink point is possible:

$$G(\vec{p}, y_0) = \sum_{\vec{y}} G(0, y) e^{i\vec{p}\cdot\vec{y}}$$



- Increased statistics from volume sum
  - Independent subvolumes $\sim 1/M_\pi^3$
- Projection on total final state momentum
  - Typically $\vec{p} = 0$ for spectroscopy
  - Eliminates (momentum) excited states
- Sink operator not point-spread ("δ wave function")

SOURCE SIDE VOLUME AVERAGE

Source side volume averaging would increase statistics:

- Requires additional inversions for additional sources
- Only independent regions $V_4 \sim 1/M_\pi^4$ relevant
  - Typical $M_\pi L \sim 4$, $T = 2L$ has ~ 500 independent subvolumes

Strategies to efficiently take the source side sum:

- Stochastic estimators
- Low mode preconditioning (deflation)
- Preconditioning by multilevel-algorithms
- Multi RHS inverters
- Inexact inversions

STOCHASTIC ESTIMATORS

Basic idea: insert stochastic unit matrix $\mathbb{1} = \sum_i |\xi_i\rangle\langle\xi_i|$

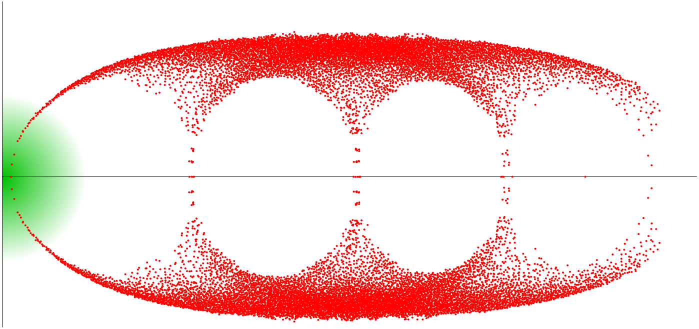
- Construction of $|\xi_i\rangle$:
  independent $U(1)$ or $\mathcal{Z}_2$ random variable per component
- Reconstruct full propagator by $M^{-1} = \sum_i M^{-1}|\xi_i\rangle\langle\xi_i|$
- Trade source point sum for a stochastic sum, e.g.:

$$\sum_U \sum_x \mathrm{Tr}\left(\Gamma M^{-1}_{x,x}(U)\right) = \sum_U \sum_i \langle\xi_i|\Gamma M^{-1}|\xi_i\rangle$$

- Ensemble, stochastic sums commute: balance for optimal signal
- Keeping parts of the unit matrix exact (partitioning, dilution):
  - More inversions but lower noise
  - Typical: spin structure, time slices
  - Essential when signal strongly suppressed (e.g. propagator)

LOW MODE PRECONDITIONING

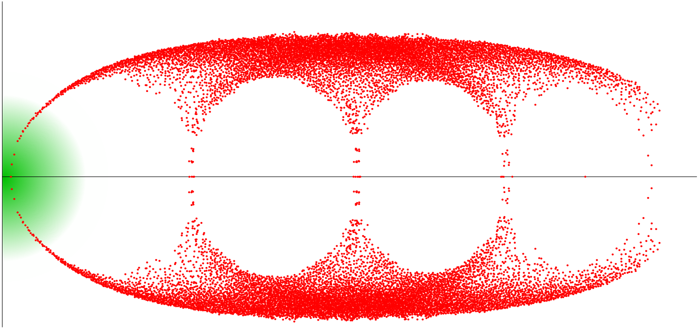
Only IR modes are physical ➛ treat them preferentially



- Classical low mode treatment:
  - Invert exactly on low modes
  - May use stochastic techniques on the complement
- Inexact deflation:
  - Invert on low modes to low precision
  - Use as preconditioner for many inversions

MULTILEVEL ALGORITHMS

IR modes well approximated on coarse lattice



- Construct effective action on coarse lattice (Babich et. al., 2010; Frommer et. al., 2013)
  - Invert fully on coarse lattice
  - Use as preconditioner for many inversions
  - Setup time comparable to single inversion
  - Subsequent inversions 1-2 orders cheaper

COVARIANT APPROXIMATION AVERAGING

Exploit cheap, inexact inversions by using symmetries: (Blum et. al., 2013)

- Perform one exact measurement per config: $\mathcal{O}(U)$
- Identify ensemble symmetry $g \in G$ (e.g. translation)
- Construct symmetry averaged observable

$$\mathcal{O}^G(U) := \sum_{g \in G} \mathcal{O}(U)$$

- Compute $\mathcal{O}^G(U)$ fast with low precision $\tilde{\mathcal{O}}^G(U)$
- Correct with the one exact measurement

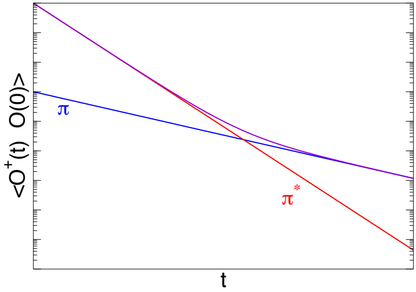
$$\tilde{\mathcal{O}}^{G,\text{improved}}(U) = \tilde{\mathcal{O}}^G(U) + \mathcal{O}(U) - \tilde{\mathcal{O}}(U)$$

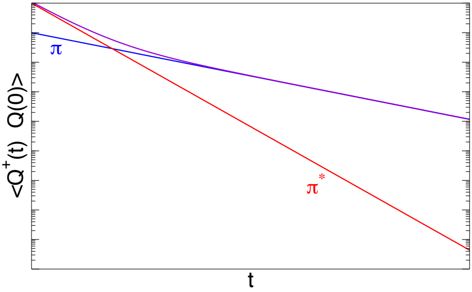
SOURCE AND SINK OPERATORS

Operators can be more general than a sum over point operators

- Overlap with operator decides which states dominate

$$G(t,0) = \sum_n \frac{\langle 0|\mathcal{O}_2^\dagger|n\rangle\langle n|\mathcal{O}_1|0\rangle}{2E_n} e^{-E_n t}$$





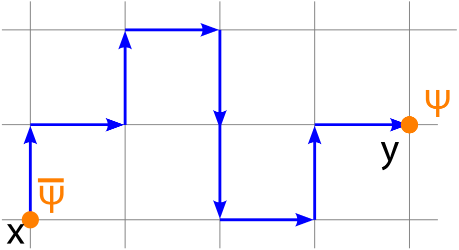
EXTENDED OPERATORS

For a quark-antiquark operator, we can generically write

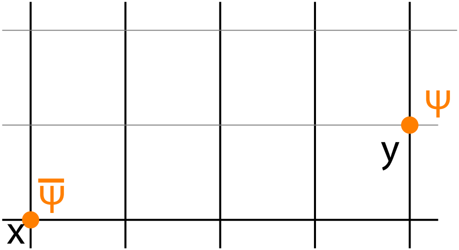
$$\mathcal{O}(t) = \sum_{\vec{x},\vec{y}} \bar{\Psi}(t,\vec{x})\Gamma G(\vec{x},\vec{y})\Psi(t,\vec{y})$$

- Smearing kernel $G \sim$ wave function
- Nonlocal terms in G generically vanish on gauge averaging

➛ covariant terms only



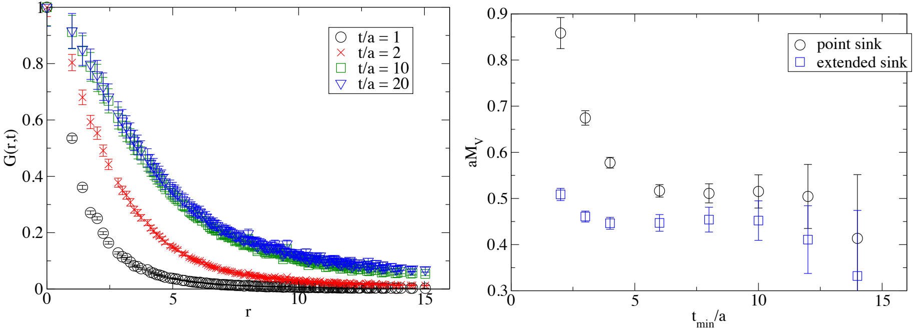
➛ gauge fixing



OPTIMISING OPERATORS

Ideally, the operator has exclusive overlap with target state

- Different gauge fixed kernels: wall, gaussian, sphere, ...
  - Keep constant in physical units across ensembles
- Ground state form can be extracted on the sink side



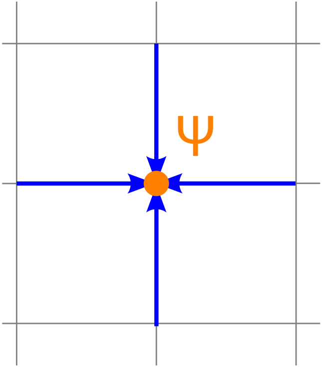
(Babich et. al. 2007)

WUPPERTAL SMEARING

Gauge invariant version of Gaussian kernel (Güsken et. al., 1990)

$$G = \left(\mathbb{1} + \alpha \sum_{i=1}^{3} \left(V_i + V_i^\dagger \right) \right)^N \qquad V_\mu(x,y) = U_\mu(x)\delta_{x+\hat{\mu},y}$$

- Repeated application of gauge invariant Laplacian
- Smearing parameter α
- Number of iterations N
- Gaussian as $\alpha \to 0$
  αN constant
- Smeared links U may be used



LAPH SMEARING

Use eigenmodes of covariant Laplacian (Peardon et. al., 2009)

- Extract eigenmodes $|\lambda_i\rangle$ of gauge invariant Laplacian
- Invert fermion matrix on subspace $\mathcal{P}$ of lowest N eigenmodes
- Good overlap with physical (IR) modes

Stochastic estimators to cover larger subspace

- Construct random sources in subspace $\xi_j \in \mathcal{P}$
- Invert on some $|\hat{\lambda}_j\rangle = \sum_i |\lambda_i\rangle \xi_j(i)$

BARYON OPERATORS

Baryon operators may be constructed along the same lines

- Simplest octet nucleon operator with good overlap

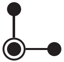
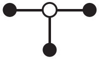
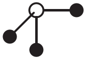
$$\mathcal{O} = \epsilon_{abc} \left(\Psi_a^T \gamma_1 \gamma_3 \Psi_b \right) \Psi_c$$

- Simplest decuplet nucleon operator

$$\mathcal{O} = \epsilon_{abc} \left(\Psi_a^T \gamma_0 \gamma_2 \gamma_\mu \Psi_b \right) \Psi_c$$

  - Has octet component that in principle has to be projected out
- More complex, nonlocal operators possible

UTILISING LATTICE SYMMETRIES

Operator type	Displacement indices
 single-site	$i = j = k = 0$
 singly-displaced	$i = j = 0,\ k \neq 0$
 doubly-displaced-I	$i = 0,\ j = -k,\ k \neq 0$
 doubly-displaced-L	$i = 0,\ \lvert j\rvert \neq \lvert k\rvert,\ jk \neq 0$
 triply-displaced-T	$i = -j,\ \lvert j\rvert \neq \lvert k\rvert,\ jk \neq 0$
 triply-displaced-O	$\lvert i\rvert \neq \lvert j\rvert \neq \lvert k\rvert,\ ijk \neq 0$

(Basak et. al., 2006)

- Choice of basis essential
- Many possible choices
- Use symmetry effectively
- E.g.: irreps of lattice (hyper)cubic symmetry

✎ Caution: Lattice irrep contains many continuum irreps

ROTATIONAL SYMMETRY

On the lattice, $SU(2)$ is broken to discrete octahedral group O

- In the continuum, states are categorised in irreps J of $SU(2)$
- Irreps J of $SU(2)$ are reducible under O
- Number of occurences of irreps of O differ per J

E.g. for fermions:

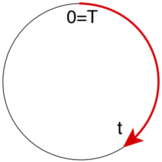
J	$n^J_{G_{1g}}$	$n^J_{G_{2g}}$	$n^J_{H_g}$	J	$n^J_{G_{1g}}$	$n^J_{G_{2g}}$	$n^J_{H_g}$
$\frac{1}{2}$	1	0	0	$\frac{9}{2}$	1	0	2
$\frac{3}{2}$	0	0	1	$\frac{11}{2}$	1	1	2
$\frac{5}{2}$	0	1	1	$\frac{13}{2}$	1	2	2
$\frac{7}{2}$	1	1	1	$\frac{15}{2}$	1	1	3

(Basak et. al., 2006)

PROPAGATOR FIT FORMS

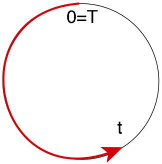
Single state, propagating forward:

$$c_f(t) = c_f^0 e^{-mt}$$



The backward contribution:

$$c_b(t) = c_b^0 e^{-m(T-t)}$$

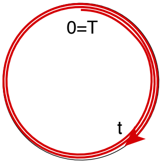


Include contributions warping around the lattice (tiny):

$$c_f(t) = c_f^0 \left(e^{-mt} + e^{-m(T+t)} + \dots \right)$$

$$= c_f^0 e^{-mt} \times \sum_{n=0}^{\infty} e^{-nmT}$$

$$= c_f^0 e^{-mt} \frac{1}{1 - e^{-mT}}$$



SYMMETRIC FIT FORMS

For T (P) symmetric ($c^0 = c^0_f = c^0_b$)

resp. antisymmetric ($c^0 = c^0_f = -c^0_b$):

$$c_t = \frac{c^0}{1 - e^{-mT}} \left(e^{-mt} \pm e^{-m(T-t)} \right)$$

$$= \frac{c^0}{1 - e^{-mT}} e^{-m\frac{T}{2}} \times \begin{cases} cosh\left(m\left(\frac{T}{2} - t\right)\right) \\ sinh\left(m\left(\frac{T}{2} - t\right)\right) \end{cases}$$

Effective mass $M_{t+\frac{1}{2}}$ from numerical solution of:

$$\frac{c_{t+1}}{c_t} = \frac{cosh\left(M_{t+\frac{1}{2}}\left(\frac{T}{2} - t - 1\right)\right)}{cosh\left(M_{t+\frac{1}{2}}\left(\frac{T}{2} - t\right)\right)}$$

SYMMETRIC FIT FORMS

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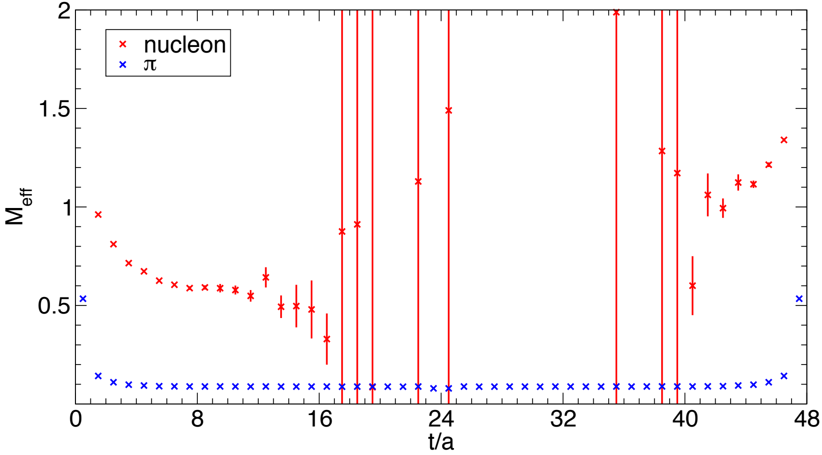
MASS PLATEAUS



Identify plausible fit ranges from mass plateaux

MASS FIT

After identifying plateau range, we fit the propagators with

$$p_t = \frac{c^0}{1 - e^{-mT}} \left(e^{-mt} \pm e^{-m(T-t)} \right)$$

where m and c^0 are fit parameters
Maximum likelihood fit assuming normal error distribution[1]:

$$\chi^2 = (c - p)_s (\Sigma^{-1})_{st} (c - p)_t \to \text{min}$$

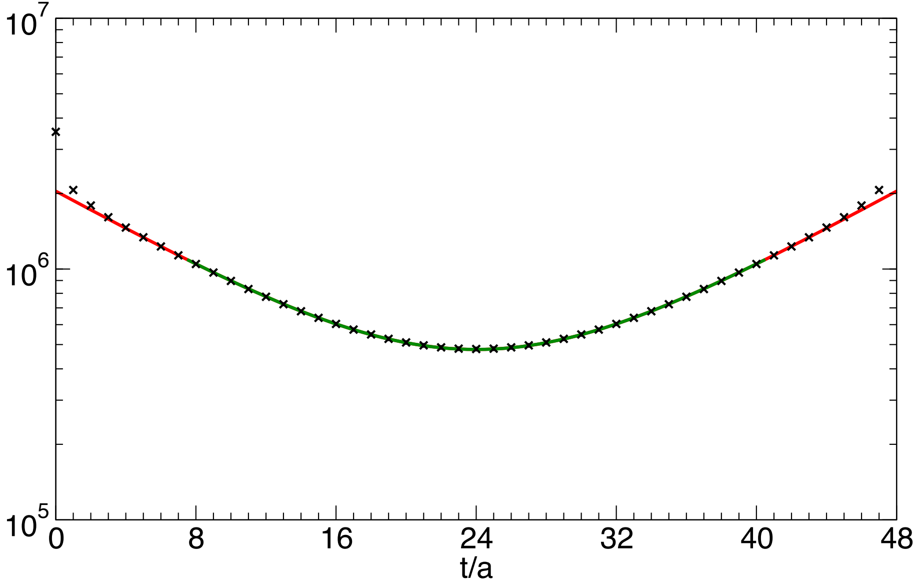
Data points c, fit function p and covariance matrix Σ

$$\Sigma_{st} = \langle (c_s - \langle c_s \rangle)(c_t - \langle c_t \rangle) \rangle$$

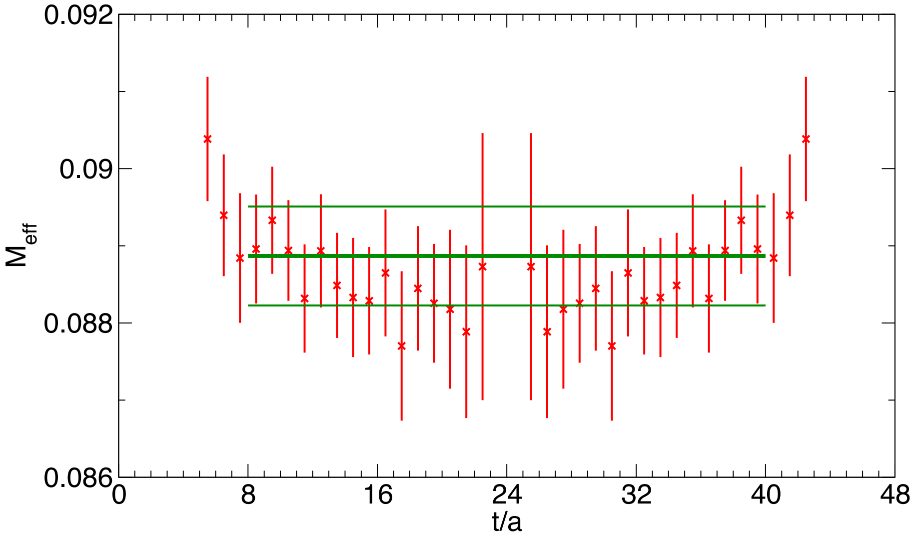
Usual variance in diagonal elements $\Sigma_{tt} = \sigma(c_t)^2$

[1] Not strictly fulfilled, but can be ignored (Endres et. al., 2011)

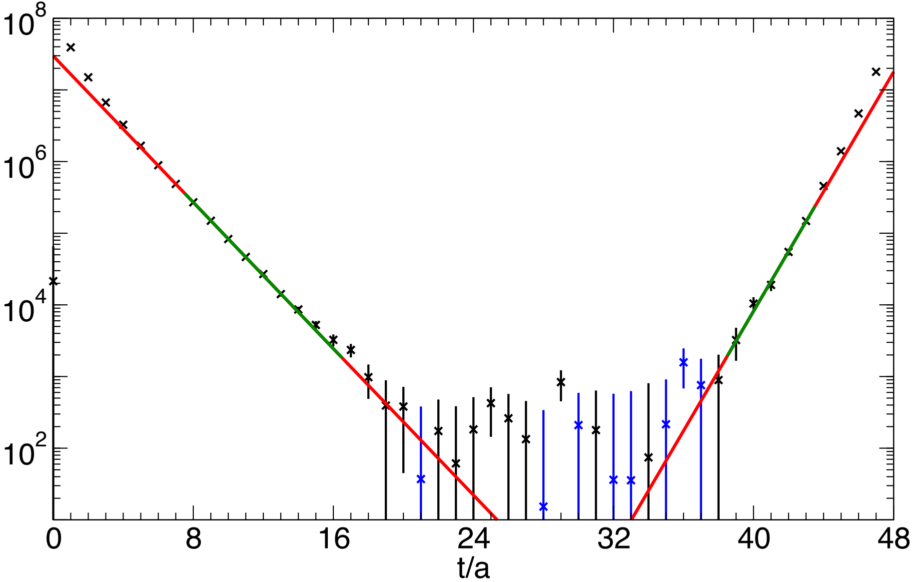
EXAMPLE PION FIT



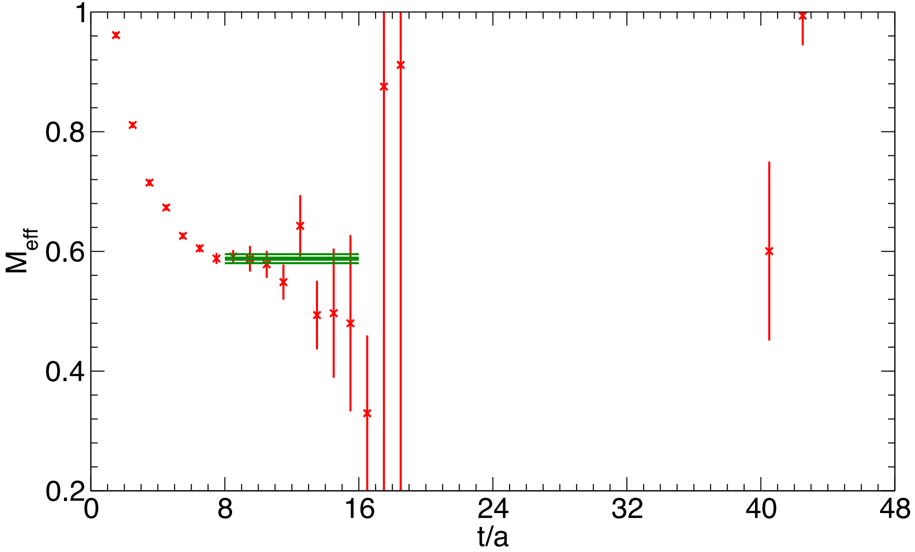
EXAMPLE PION FIT



EXAMPLE NUCLEON FIT



EXAMPLE NUCLEON FIT



FIT RESULTS

From a fit we in principle get 3 things:

✓ The most likely value of the fit parameters

- Values of the parameters at $\chi^2 \to \min$

✓ Standard errors of the parameters
(more generally, confidence regions)

- Contours of constant $\Delta\chi^2 = \chi^2 - \chi^2_{\min}$

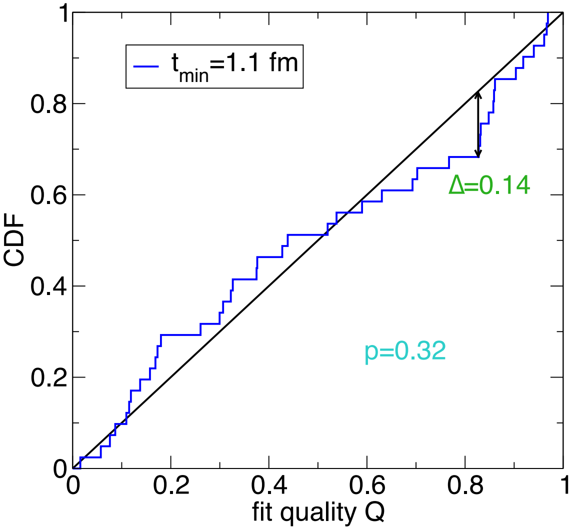
✓ The quality of the fit

- From $Q = \frac{\Gamma(\frac{n}{2}, \frac{\chi^2}{2})}{\Gamma(\frac{n}{2})} = \frac{\int_{\frac{\chi^2}{2}}^{\infty} t^{\frac{n}{2}-1} e^{-t} dt}{\int_0^{\infty} t^{\frac{n}{2}-1} e^{-t} dt}$

- Q: probability that - given the model - the data are at least as far off the prediction as the real data

☞ Q should be a flat random value $\in [0, 1]$

EXAMPLE Q DISTRIBUTION



- Need many ensembles
- Plot CDF
- KS test flat distribution

$P(\Delta > \text{observed})$:

$$p(\Delta(\sqrt{N} + 0.12 + \frac{0.11}{\sqrt{N}}))$$

with

$$p(x) = \sum_j \frac{(-)^{j-1}2}{e^{-2j^2x^3}}$$

CORRELATIONS

For uncorrelated data, Σ is diagonal

$$C_{st} = \frac{\Sigma_{st}}{\sigma(c_s)\sigma(c_t)}$$

Typical (estimated) normalized covariance C for a correlator:

1.0000	0.9963	0.9840	0.9746	0.9509
0.9963	1.0000	0.9912	0.9801	0.9595
0.9840	0.9912	1.0000	0.9934	0.9846
0.9746	0.9801	0.9934	1.0000	0.9912
0.9509	0.9595	0.9846	0.9912	1.0000

Eigenvalues:

4.9224	0.0661	0.0059	0.0041	0.0014

PROBLEMS WITH CORRELATIONS

The structure of the covariance matrix can be problematic

- Covariance matrix determined statistically
- In C^{-1}, small modes dominate
- Smallest modes have large errors

One can:

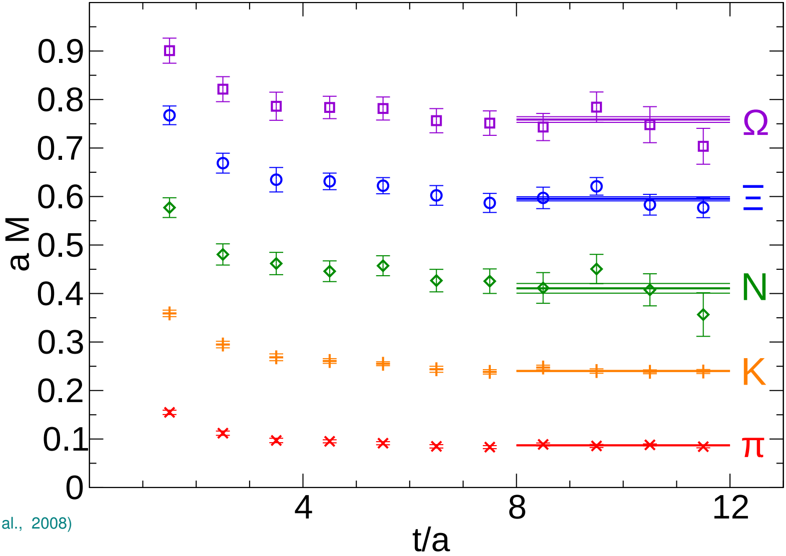
- Do an uncorrelated fit: Σ diagonal
- Truncate small eigenmodes
  - Truncate them (optionally correct diagonal)
  - Average them (Michael, Mc Kerrell, 1994)

Problem: Q and parameter errors useless

➢ Need to be determined in some other way

The structure of the covariance matrix can be problematic

MASS PLATEAUS AND FITS

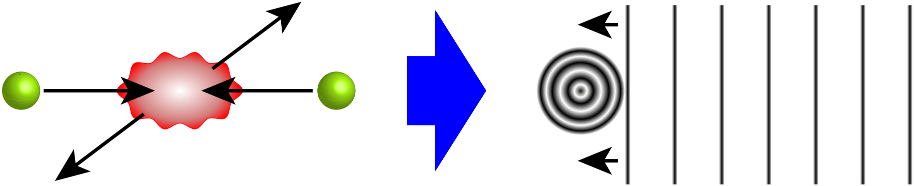


(Durr et. al., 2008)

RESONANCES

Resonances are complex poles in a continuos spectrum

- Simplest case: resonances in 2-particle elastic scattering
- Can be treated as a scattering problem



- Finite volume: discrete eigenstates
- How to relate to infinite volume scattering?

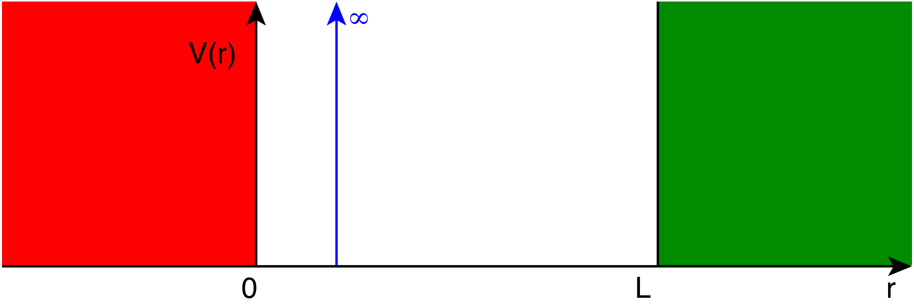
A SIMPLE QM MODEL

As a simple example, consider 1D QM scattering

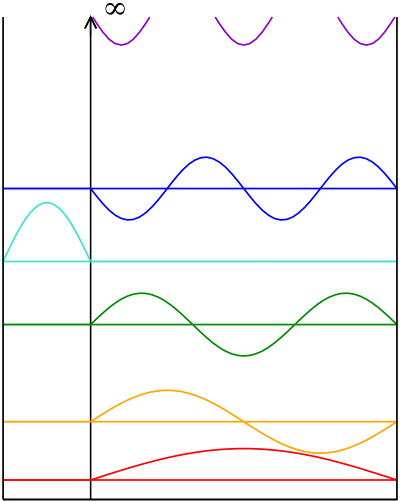
- Resonance $\sim$ metastable bound state

$$V(x) = K\delta(a) \qquad \text{with} \qquad r > 0 \quad r < L$$

- Coupling of resonance $\sim 1/K$
- Restricted to finite size L

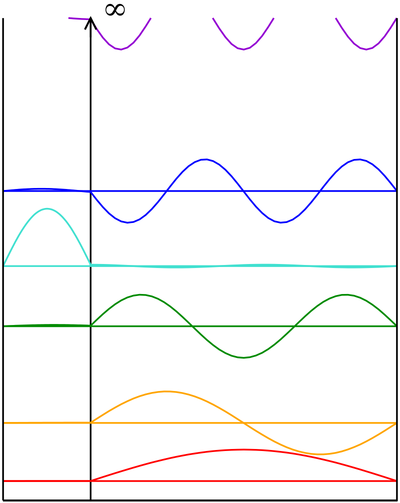


A QM MODEL



- Scattering as QM problem
- Essence from double well
- No mixing (stable state)
- Level repulsion with coupling
- Larger coupling
  ➛ larger repulsion

A QM MODEL



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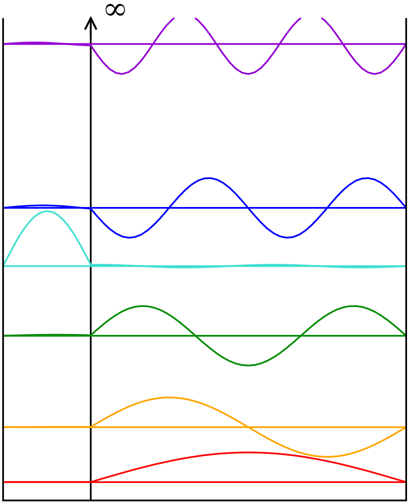

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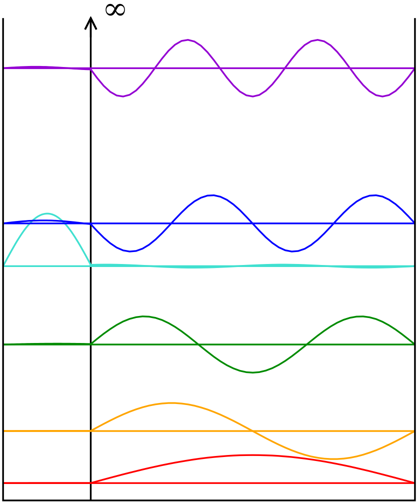

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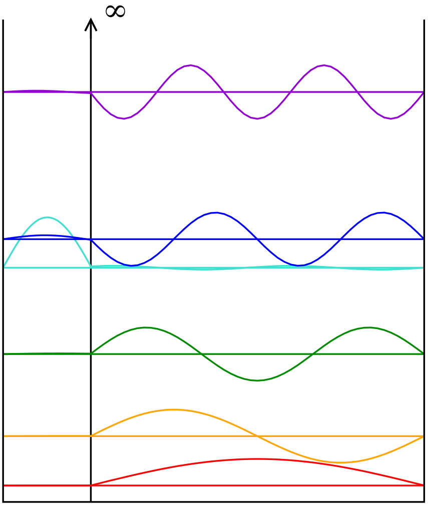

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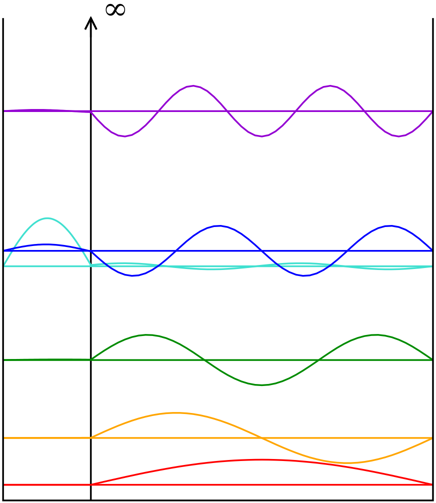

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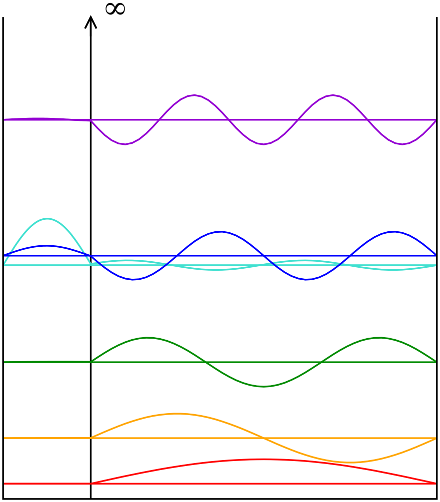

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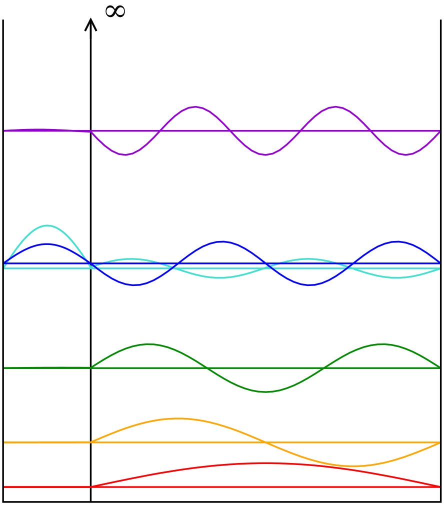

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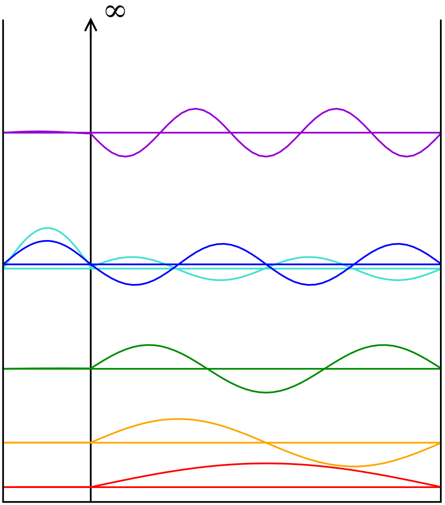

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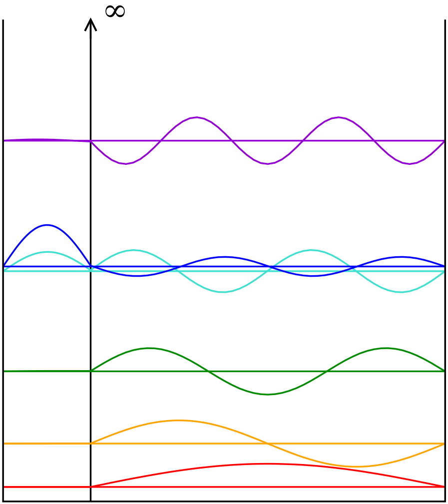

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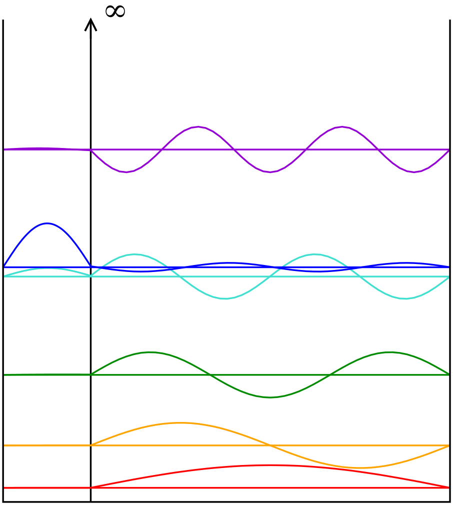

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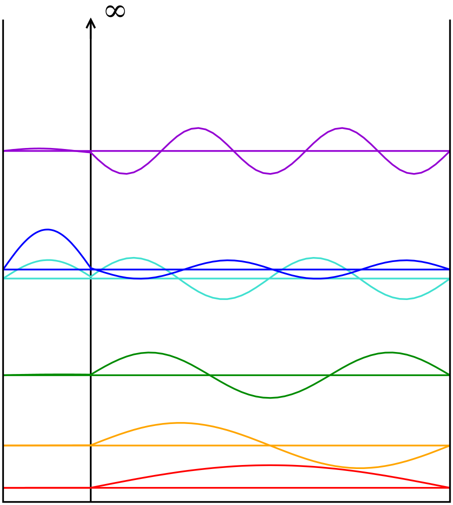

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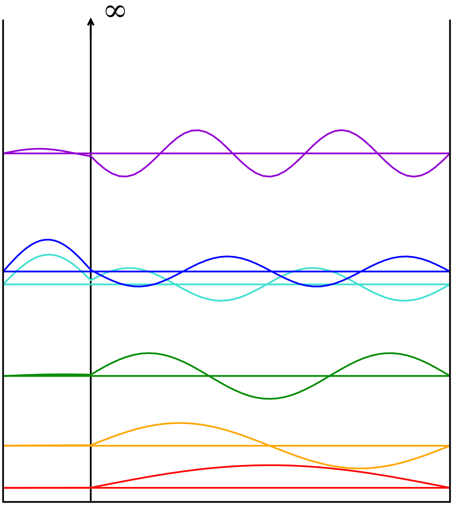

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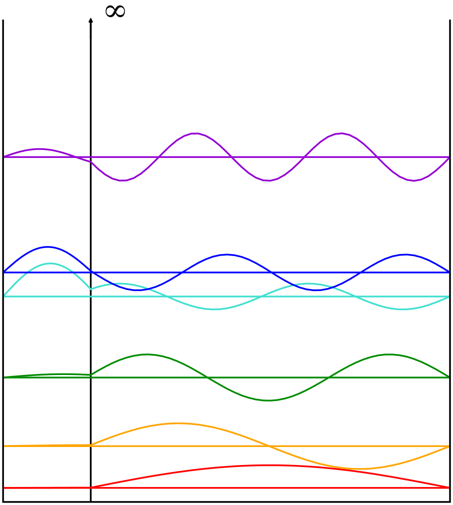

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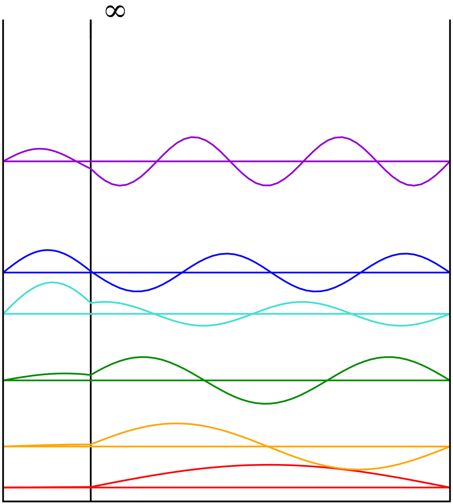

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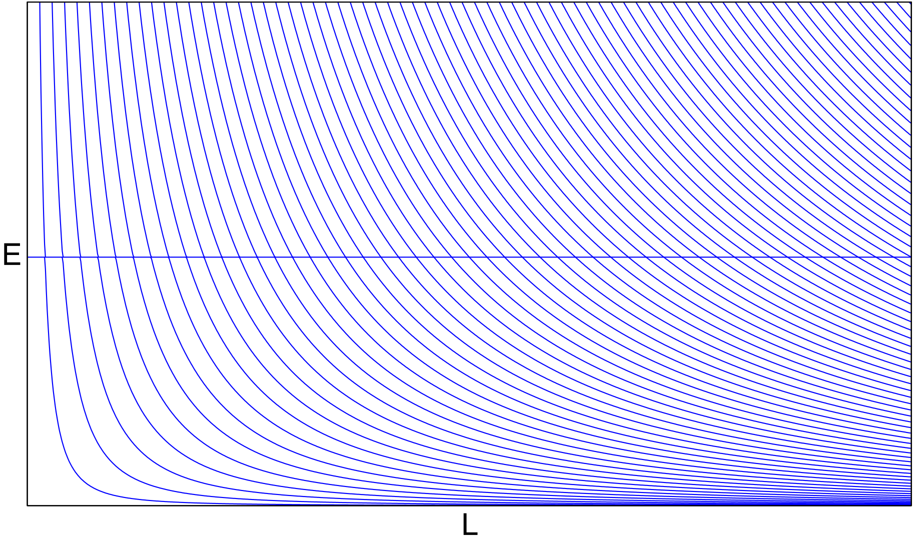
VOLUME DEPENDENCE OF ENERGY LEVELS



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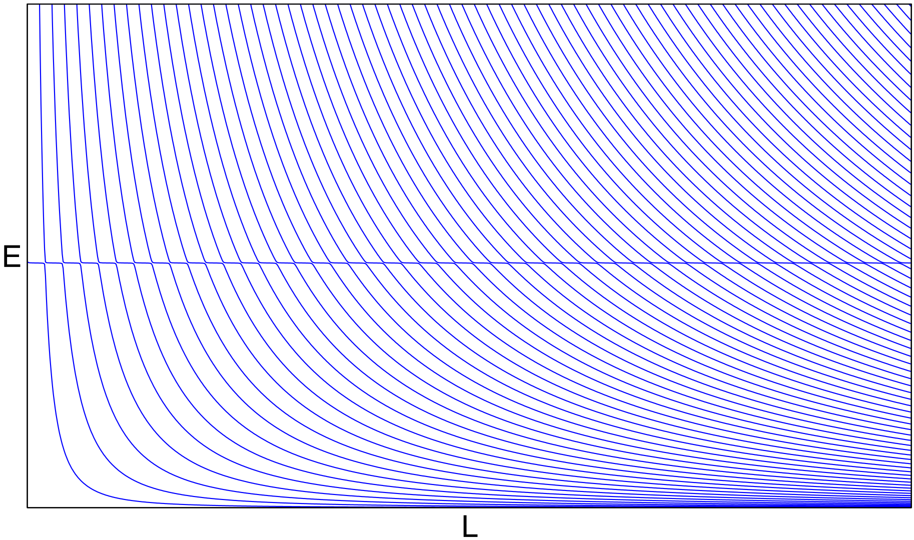

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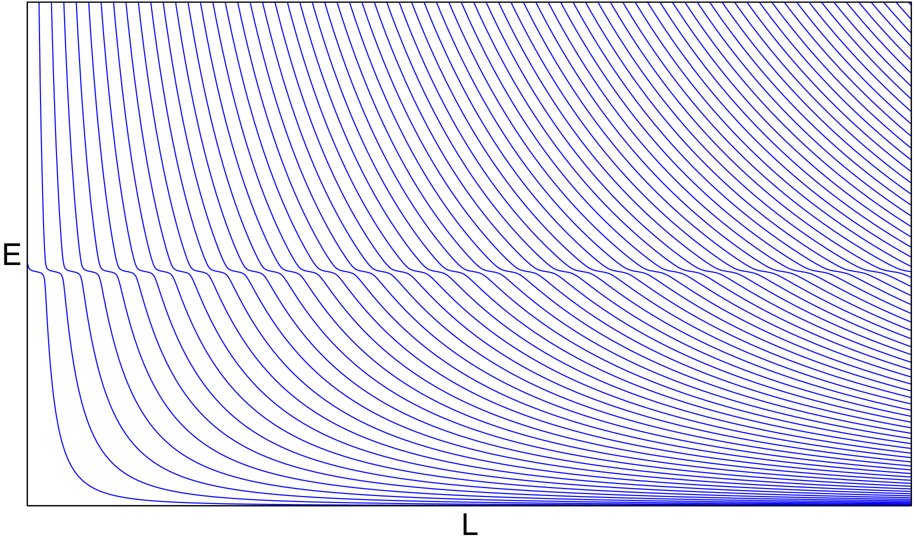

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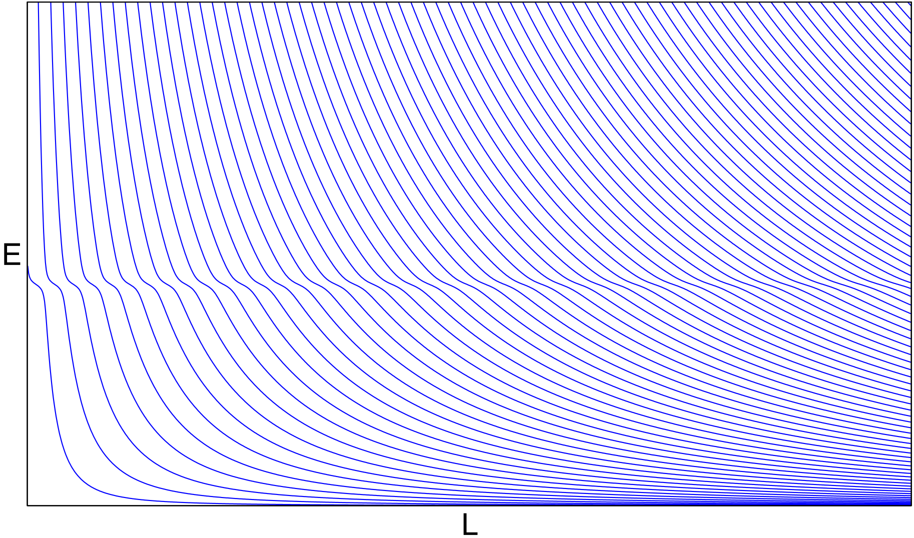

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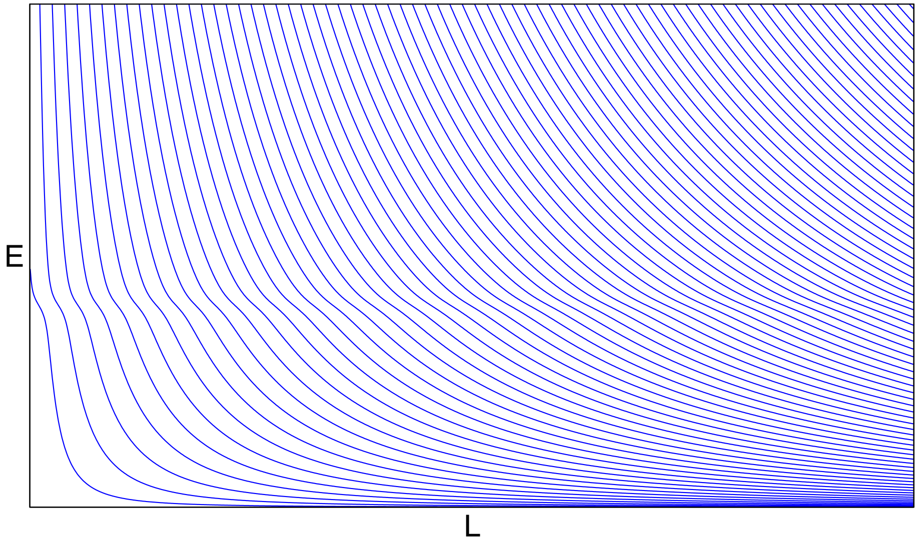

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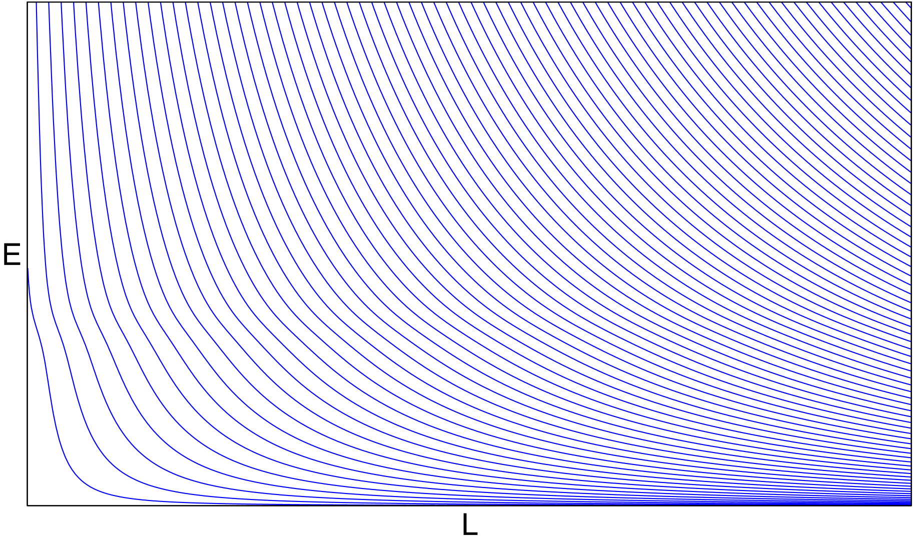

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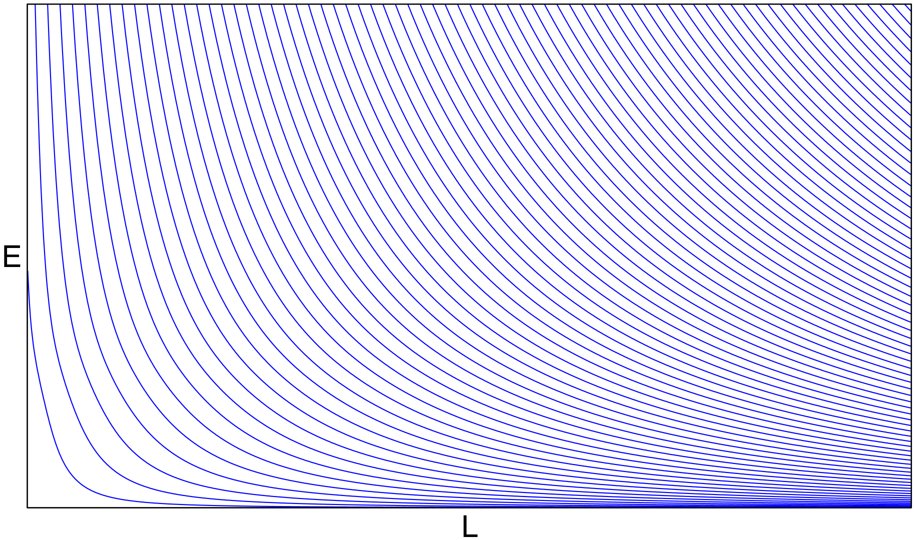
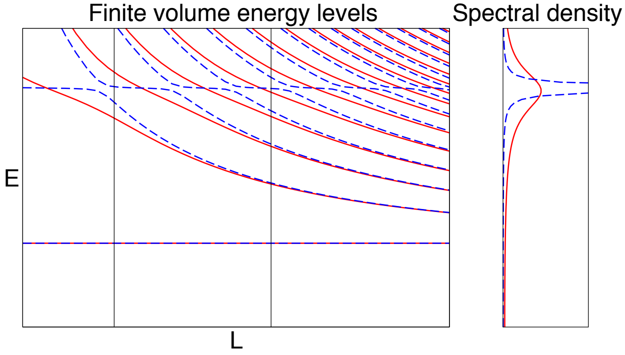


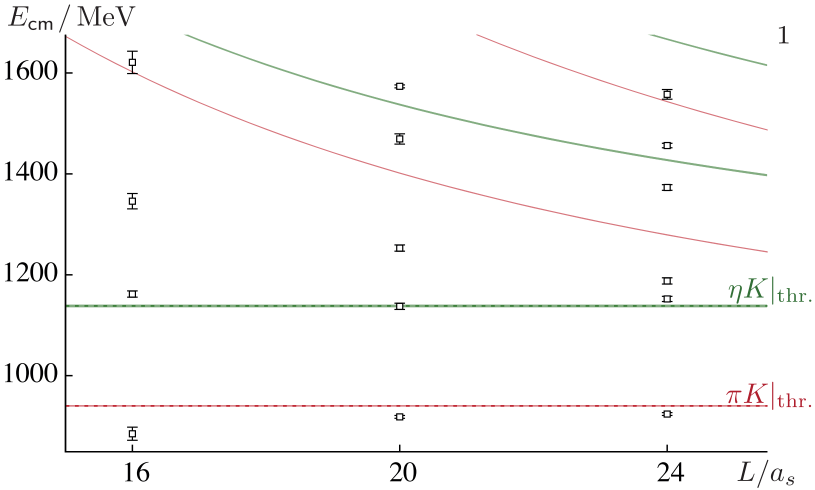
EXTRACTION OF EXCITED STATES MASSES

Extracting excited states is much tougher:

- Extraction of energy levels is harder:
  Die out at large t ➠ need to use small t correlators
- Once extracted, relation to $V \to \infty$ is nontrivial:
  Disentangle resonances and scattering states at finite volume



COUPLED CHANNEL SCATTERING



(Dudek et. al., 2014)

EXTRACTION OF EXCITED STATES MASSES

First problem: Extraction of energy levels:

- Fit single channel with two (or more) exponentials

$$C(t) \propto a_0 e^{-E_0 t} + a_1 e^{-E_1 t}$$

  ☞ Unstable fits, accuracy limited

- Variational method: use different sources $\mathcal{O}_i$

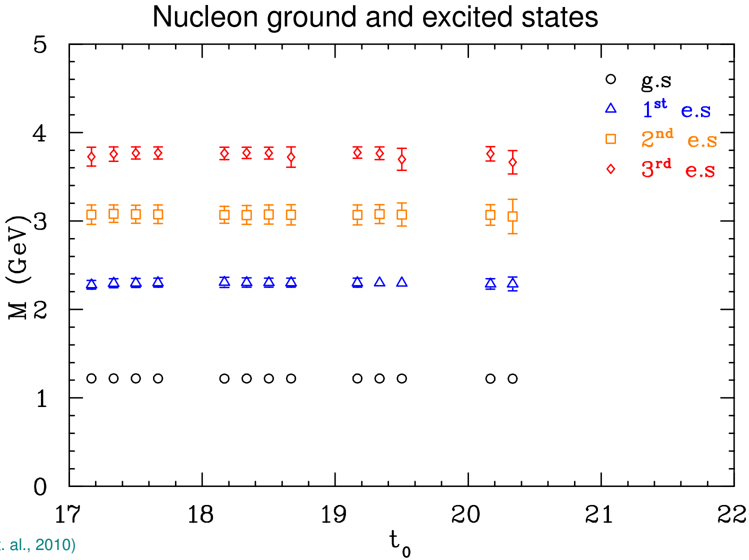
$$C_{ij}(t) = \langle 0|\mathcal{O}_i^\dagger(t)\mathcal{O}_j(0)|0\rangle \qquad M(t,t_0) = C(t)C^{-1}(t_0)$$

➠ Eigenvalues of $M(t,t_0)$:

$$\lambda_n = e^{-E_n(t-t_0)}$$

  ☞ Choice of operator basis $\mathcal{O}_i$: good coupling to all states

VARIATIONAL METHOD



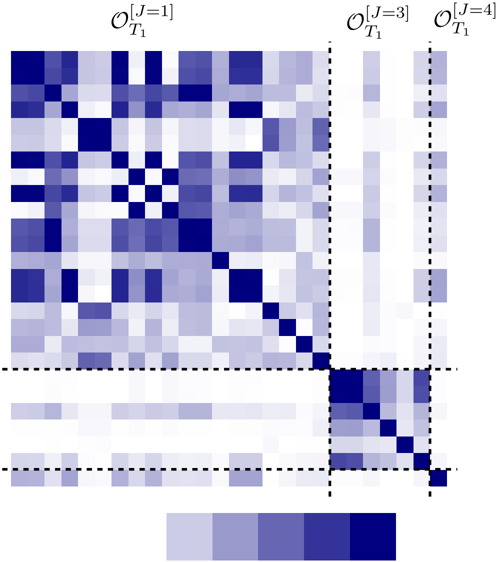
(Mahbub et. al., 2010)

OPERATOR BASIS

Λ	Λ^{-+}	Λ^{--}	Λ^{++}	Λ^{+-}
A_1	12	6	13	5
A_2	4	6	5	5
T_1	18	26	22	22
T_2	18	18	22	14
E	14	12	17	9

(HSC:Dudek et. al., 2012)

IDENTIFICATION OF CONTINUUM SPIN

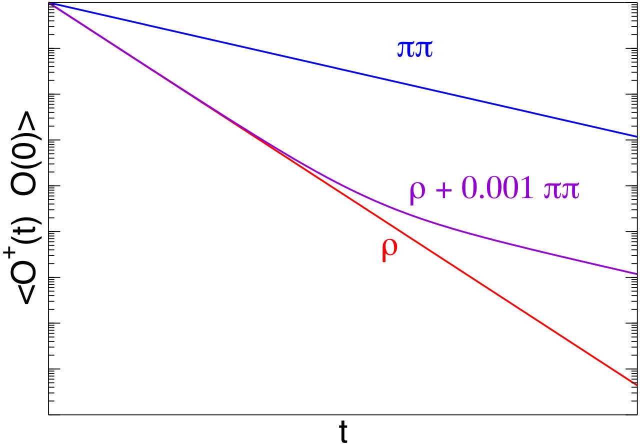


- Before diagonalization
- Approx. block diagonal
- Extract continuum spin

(HSC:Dudek et. al., 2012)

GROUND STATE EXTRACTION

Problematic: Operator coupling to ground state suppressed

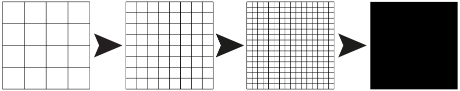


✎ Often happens on valence quark mismatch: e.g. $\pi\pi|\bar{q}q\rangle \ll \rho|\bar{q}q\rangle$

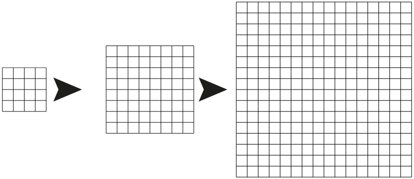
LATTICE

Lattice QCD=QCD when

- Cutoff removed (continuum limit)



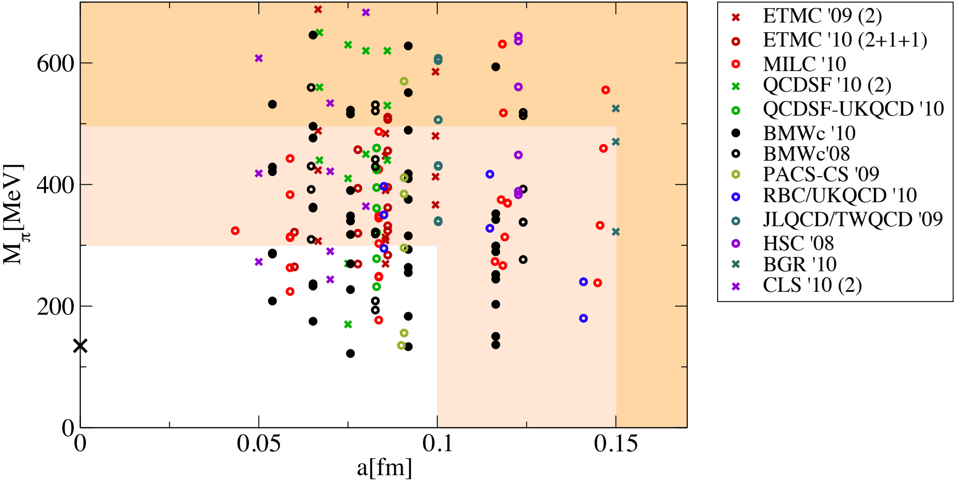
- Infinite volume limit taken



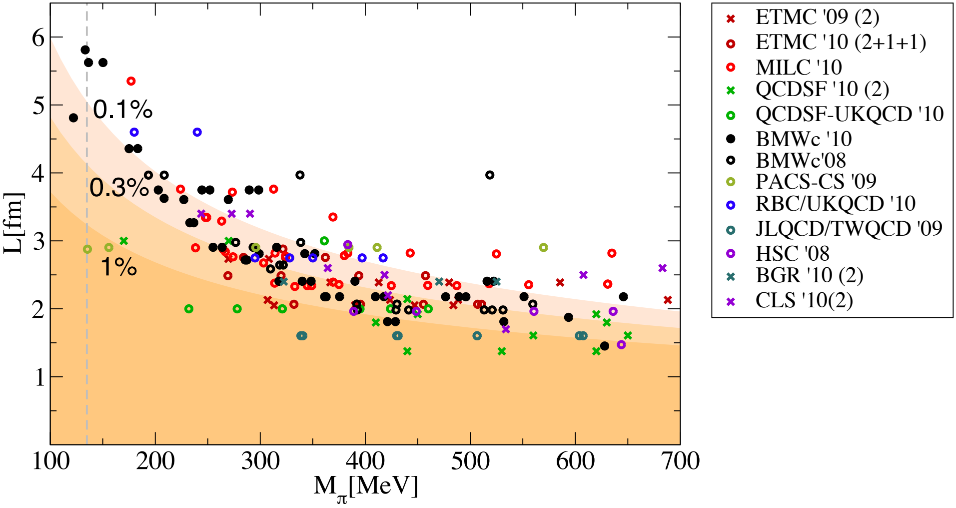
- At physical hadron masses (Especially π)
  - Numerically challenging to reach light quark masses

Statistical error from stochastic estimate of the path integral

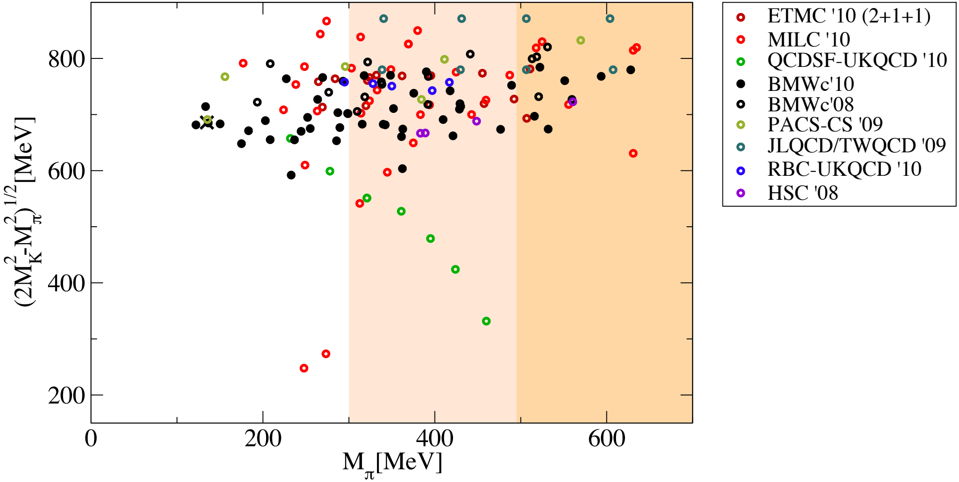
Landscape M_π vs. a



Landscape L vs. M_π

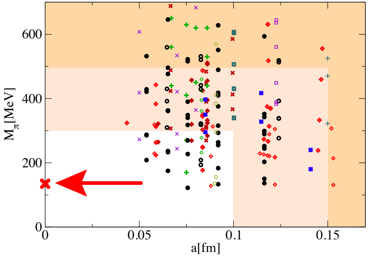


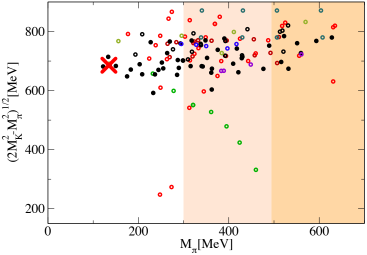
Landscape M_K vs. M_π

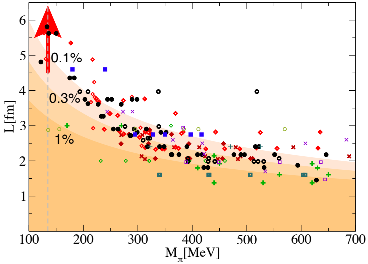


SKELETON OF A LATTICE CALCULATION

- Compute target observable
- Identify physical point
- Extrapolate to physical point
- (Renormalize if necessary)







SCALE SETTING

Goal:

- Set a reference scale on the lattice
  - Input quantities not physically measurable
  - Reference length (energy) has to be measured

Method:

- Pick one dimensionful reference observable
  - Experimentally well known
  - Easy to measure on the lattice
  - Small dependence on m_π
- Express all dimensionful quantities in terms of this reference observable
  - "Mass independent": one scale per coupling
  - "Mass dependent": scale can depend on quark masses, too

In a consistent theory, all methods continuum equivalent

SCALE SETTING OBSERVABLES

Spectral quantities ((M_ρ), M_Ω, M_Ξ):

- Directly observable (no intermediate step)
- Require measuring the baryon operators

Weak decay constants (F_K, F_π):

- "Almost" directly observable (CKM)
- Require mesonic operators only

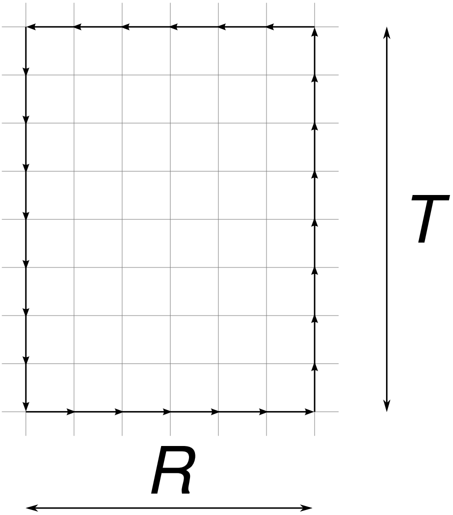
QCD string based quantities ($\sqrt{\sigma}$, $r_{0/1}$):

- Not observable, need to be determined
- No hadronic measurement involved

Purely gluonic (flow based) (t_0, w_0):

- Not observable, need to be determined
- Purely gluonic

QCD STRING



Static quark potential:

$$V(R) = -\lim_{T\to\infty} \frac{\ln W_{R,T}}{T}$$

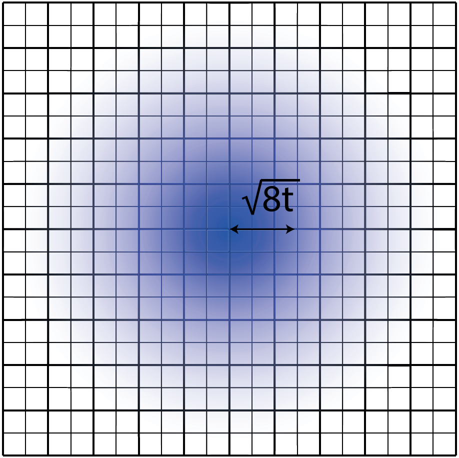
String tension:

$$\sigma = \lim_{R\to\infty} \frac{dV(R)}{dR}$$

Sommer scale r_0:

$$R^2 \left.\frac{dV(R)}{dR}\right|_{R=r_{0/1}} = 1.65/1$$

GRADIENT FLOW



Flow equation (smearing):

$$\dot{\Phi} := \frac{\partial \Phi}{\partial t} = -\frac{\delta S[\Phi]}{\delta \Phi}$$

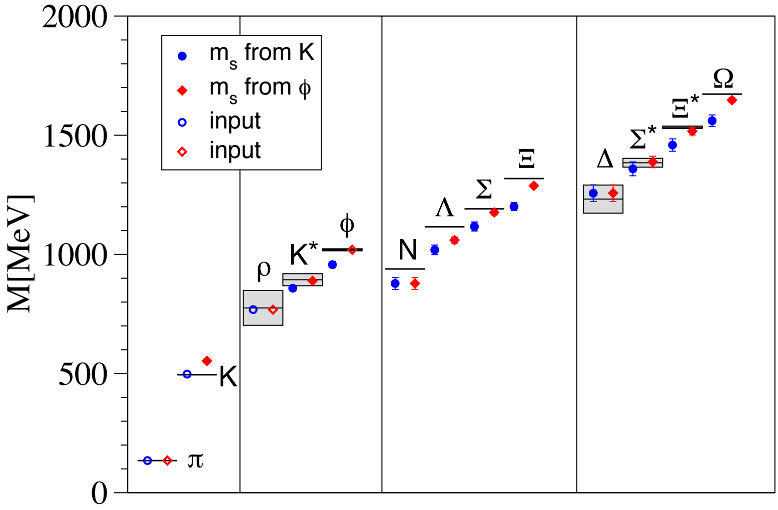
Scale from smeared gluon field:

$$t_0^2 \langle E(t_0) \rangle = 0.3, \quad E = -\frac{G_{\mu\nu}^2}{4}$$

More stable:

$$t \frac{d}{dt} t^2 \langle E(t) \rangle \Big|_{t=w_0^2} = 0.3$$

NEVER USE A RESONANCE FOR SCALESETTING



(CP-PACS 2000)

PHYSICAL POINT EXTRAPOLATION

Second stage of the analysis:

- We have collected data at different bare quark masses
- We want to make a prediction at the physical point (for simplicity we ignore continuum and infinite volume)

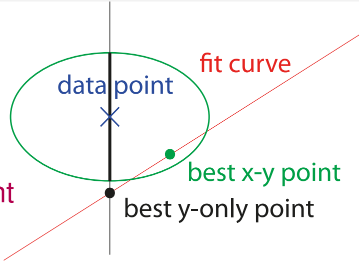
How do we proceed?

- Define the physical point (e.g. in M_π, M_K)
- Extra/interpolate target observable there

M_π is not a parameter!

- Fit to data with “x-errors”
- Potentially problematic large correlation matrices

X-ERRORS



Fitting data with errors in the x-axis:

- ➢ add each x-value as a fit parameter
- ➢ constrain each x-value with measurement

Uncorrelated case:

$$\chi^2 \to \chi^2 + \sum_i (x_i - p_i)^2 / \sigma_{x_i}^2$$

Generalization with full covariance matrix

✎ Big covariance matrices lead to uncontrolled fits

Mandatory to eliminate spurious correlations

CORRELATED ERRORS

Special case: x_i, y_i correlated, but uncorrelated with x_j, y_j $i \neq j$

- ➢ Appears naturally in fit of independent ensembles
- ➢ Covariance matrix reduces to block diagonal form

Contribution to χ^2:

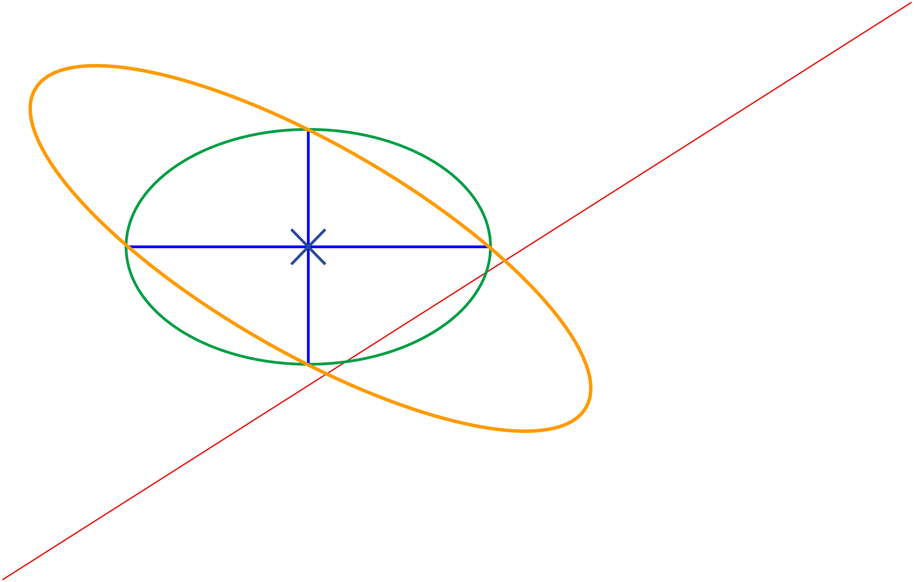
$$\chi^2 \supset \chi_i^2 \begin{pmatrix} \Delta x & \Delta y \end{pmatrix} \begin{pmatrix} \Sigma_{xx}^{-1} & \Sigma_{xy}^{-1} \\ \Sigma_{xy}^{-1} & \Sigma_{yy}^{-1} \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix}$$

- χ_i^2 constant along an ellipse
- Covariance Σ_{xy}^{-1} tilts the axis

✓ Including x-errors can never increase χ_i^2

✓ Including x-errors does not change n (d.o.f.)

ERROR ELLIPSES



CONTINUUM-CHIRAL FIT

How to treat input from mass independent scale setting:

- Subsets of data points are correlated
- 3 independent ensembles at each of 3 lattice spacings
- A measurement of each of the 3 lattice spacings a_i

How do you extrapolate the observable M to the continuum?

- Form $M = M_{\text{lat}}/a_i$ for each ensemble
- Error on $M = M_{\text{lat}}/a_i$ is combination of errors on M_{lat} and a_i
- ✗ Introduces correlations between independent ensembles

CONTINUUM-CHIRAL FIT

How to treat input from mass independent scale setting:

- Subsets of data points are correlated
- 3 independent ensembles at each of 3 lattice spacings
- A measurement of each of the 3 lattice spacings a_i

How do you extrapolate the observable M to the continuum?

- Form $M = M_{\text{lat}}/a_i$ for each ensemble
- Error on $M = M_{\text{lat}}/a_i$ is error on M_{lat}, ignore a_i

✗ Lattice spacing error not accounted for

CONTINUUM-CHIRAL FIT

How to treat input from mass independent scale setting:

- Subsets of data points are correlated
- 3 independent ensembles at each of 3 lattice spacings
- A measurement of each of the 3 lattice spacings a_i

How do you extrapolate the observable M to the continuum?

- Introduce a fit parameter $\hat{a}_i$ for each lattice spacing
- Constrain $\hat{a}_i$ with measurement
- Fit $M_{\text{lat}} = M\hat{a}_i$ for each ensemble

THE GLOBAL FIT

When doing your continuum/chiral/infinite volume fit

- Data points are results of fits themselves
- How do you compute the quality of cascaded fits?

Theoretical ideal (not feasible):

- Do one big fit

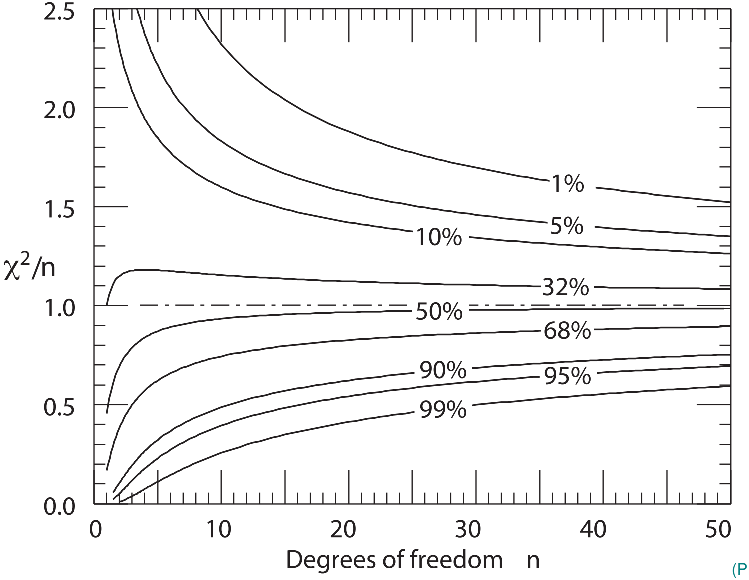
All original fits worked fully correlated:

- Assume gaussian error distribution of 1st stage fit results
- Carry over covariance of results (e.g. bootstrap)
- Sum χ^2 and d.o.f. of all fits ➛ Q

Original fits not fully correlated:

- Treat data points as input, just compute Q of final fit
- Don't worry, this increases the systematic error estimate

FIT QUALITY



(PDG, 2012)

SYSTEMATICS

One conservative strategy for systematics:

- Identify all higher order effects you have to neglect
- For each of them:
  - Repeat the entire analysis treating this one effect differently
  - Add the spread of results to systematics
- Important:
  - Do not do suboptimal analyses
  - Do not double-count analyses
  - Extract all information from data, but not more

make sure there are no unknown unknowns

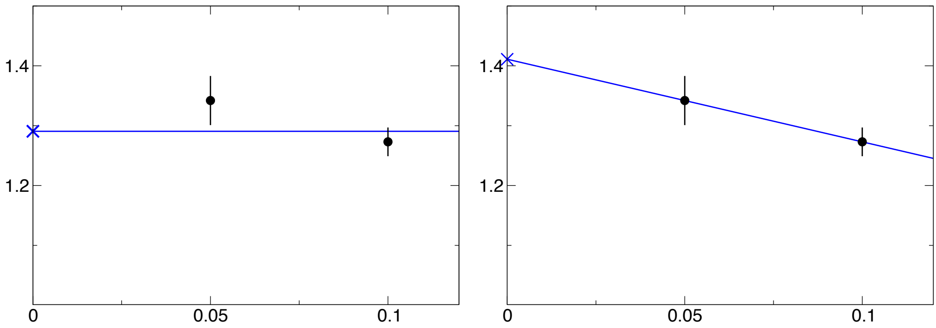
WHICH FIT IS BETTER?

The following slides compare 2 fits each

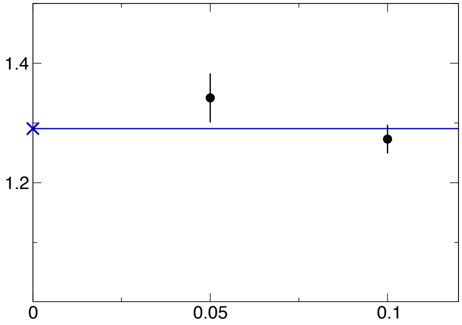
All data are uncorrelated

Which fit can be trusted more?

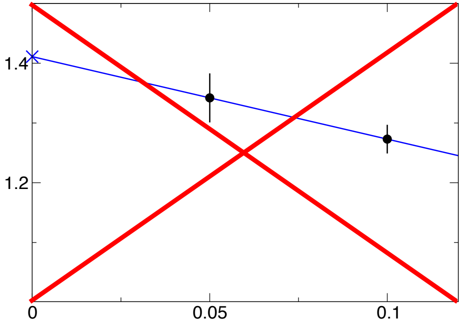
WHICH FIT IS BETTER?



WHICH FIT IS BETTER?



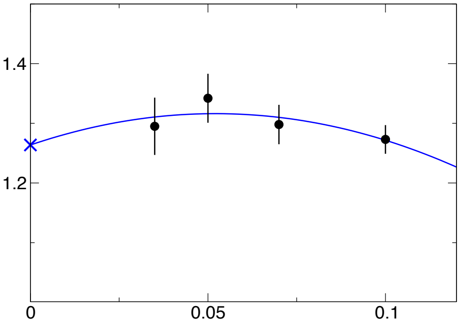
$Q = 0.15$

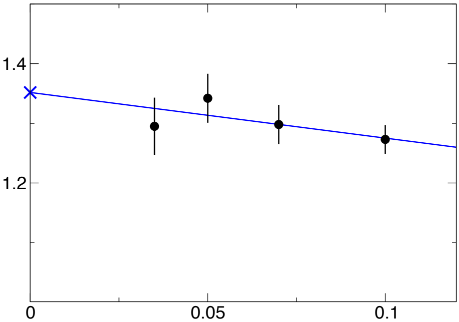


$Q =$????

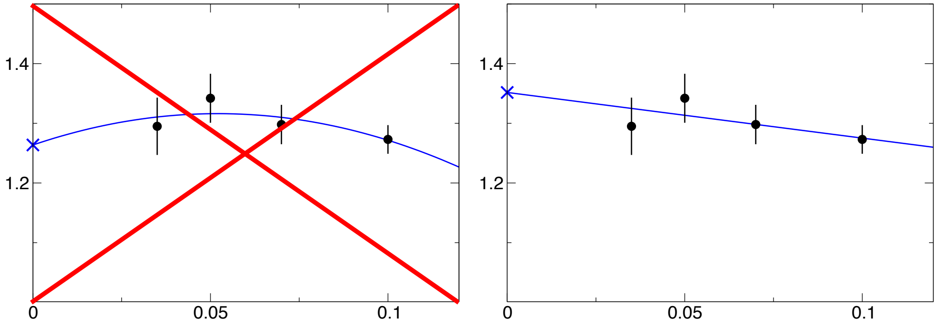
Never leave 0 d.o.f., you loose control over fit quality

WHICH FIT IS BETTER?





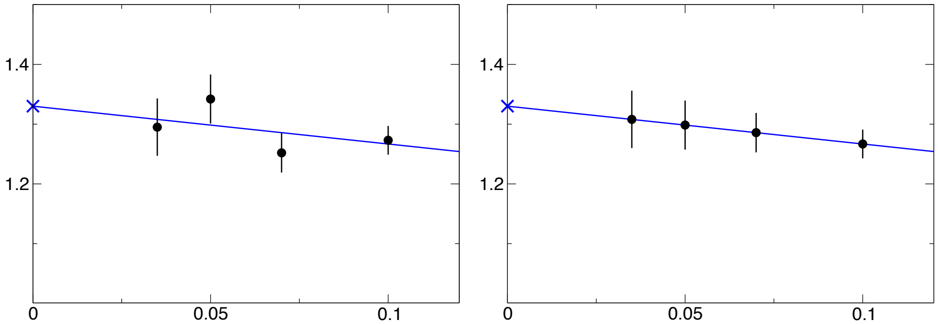
WHICH FIT IS BETTER?



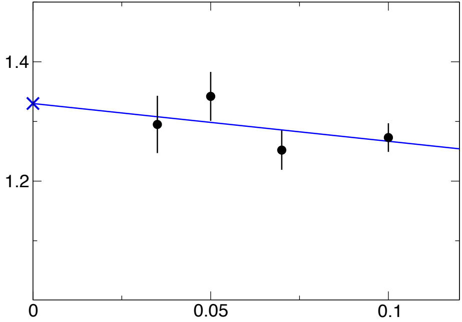
$Q = 0.42$ $\qquad$ $Q = 0.64$

- Do not try to extract too much from the data
- The displayed data have no sensitivity towards a curvature term. It is compatible with 0.

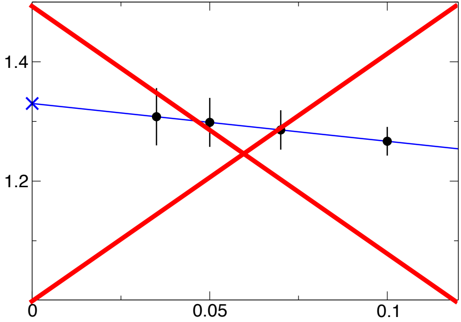
WHICH FIT IS BETTER?



WHICH FIT IS BETTER?



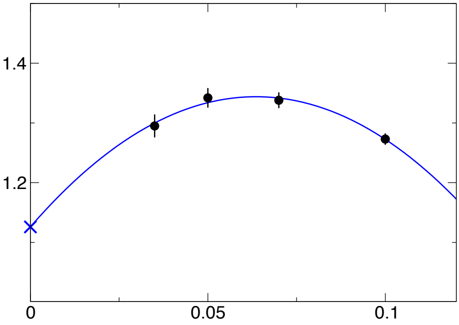
$Q = 0.31$

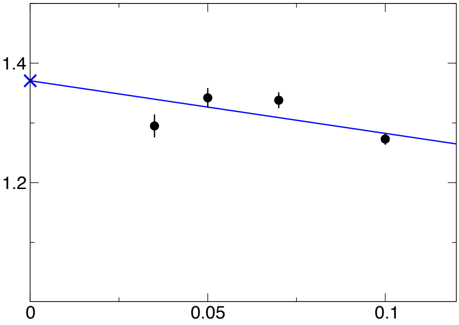


$Q = 1.00$

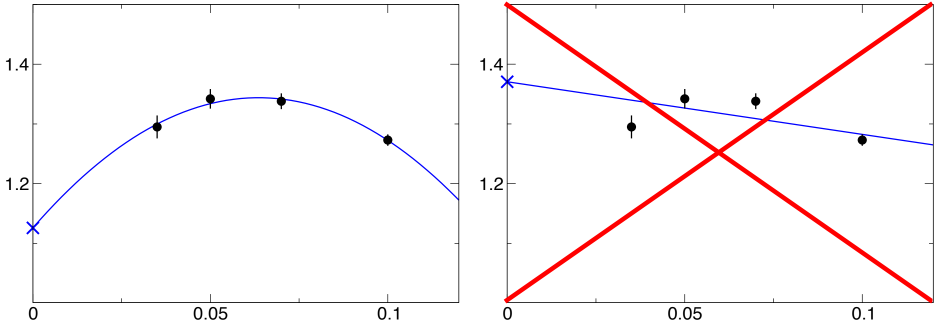
- $1 - Q = 8 \times 10^{-13}$ ➛winning the lottery is more probable than having a result this good by chance
- Data are suspicious (unrecognized correlation)

WHICH FIT IS BETTER?





WHICH FIT IS BETTER?



$Q = 0.54$ $\qquad$ $Q = 0.002$

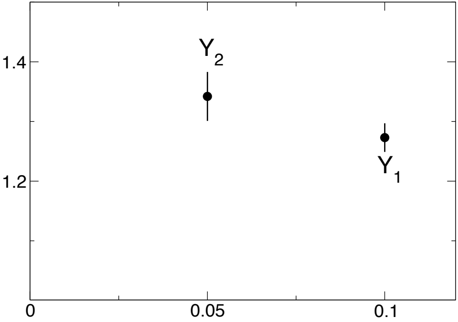
Linear modell is not sufficient for these data

SYSTEMATICS

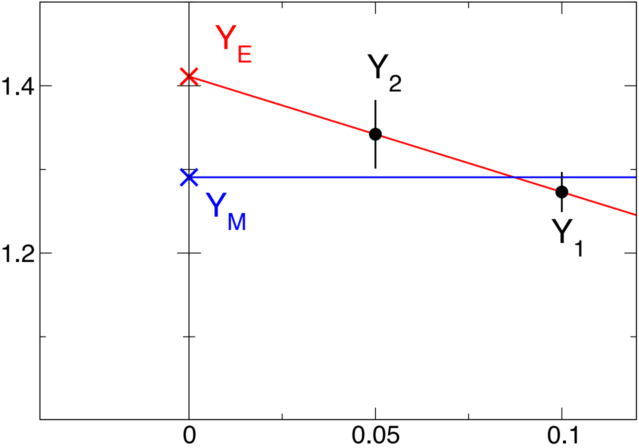
How do we compute the systematic error?

- We don't
- Systematics can only be estimated
- There is no single correct procedure

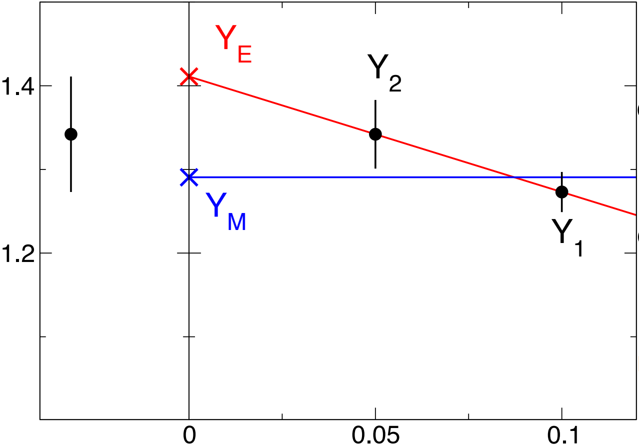
Example: systematic error of $x \to 0$



SIMPLE ESTIMATES



SIMPLE ESTIMATES

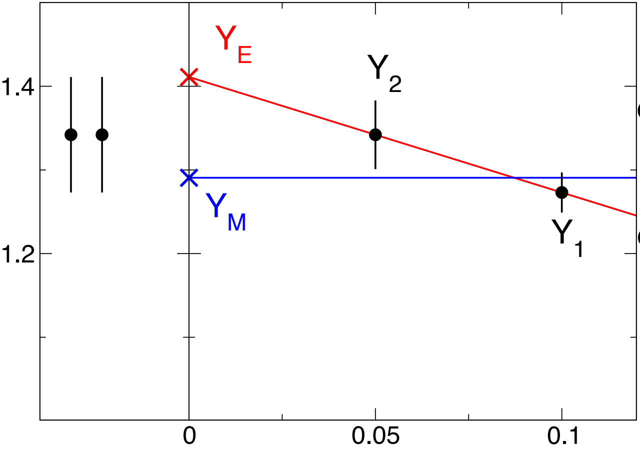


central value Y_2

error $|Y_2 - Y_E|$

no linear fit

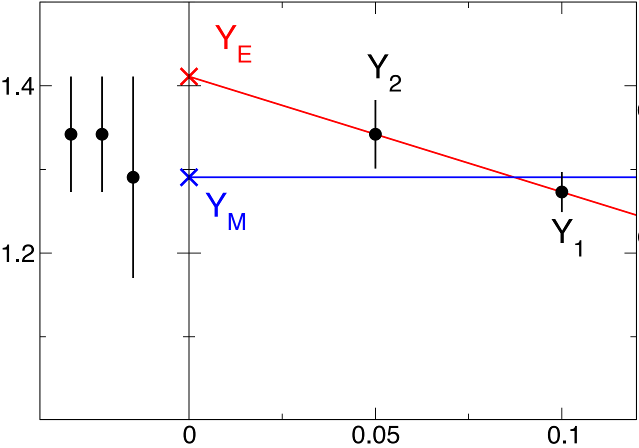
SIMPLE ESTIMATES



central value Y_2

error $|Y_2 - Y_1|$

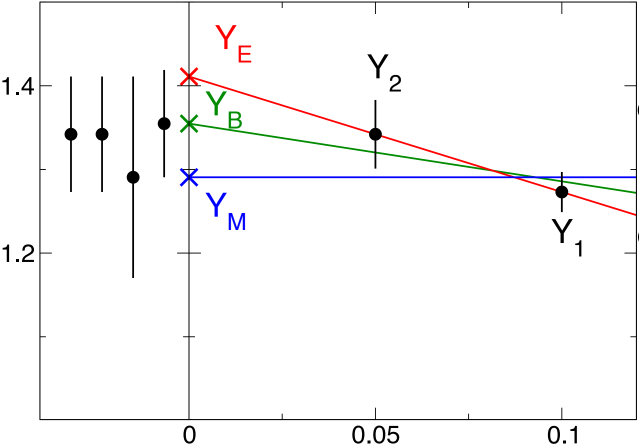
SIMPLE ESTIMATES



central value Y_M

error $|Y_M - Y_E|$

SIMPLE ESTIMATES



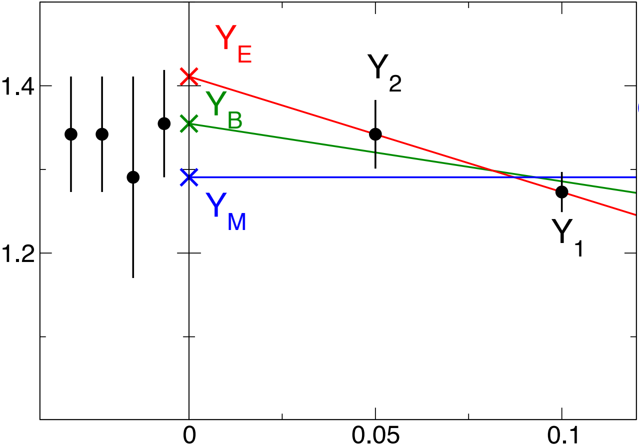
central value Y_B

error $|Y_M - Y_B|$

You can do a linear fit if you have prior knowledge on the slope

☞Constraint on slope is an additional data point

SIMPLE ESTIMATES



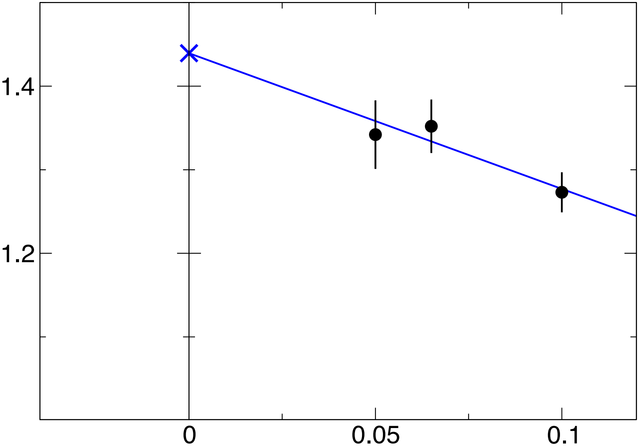
Constant fit reasonable

$Q = 0.15$

These are estimates for what systematics?

☞Neglecting first order (linear) corrections to constant

SIMPLE ESTIMATES



One more data point: error on linear term is now statistical

☞Now we need to estimate systematic due to higher ordes

SYSTEMATIC ERROR TREATMENT

One conservative strategy for systematics:

- Identify all higher order effects you have to neglect
- For each of them:
  - Repeat the entire analysis treating this one effect differently
  - Add the spread of results to systematics
- Important:
  - Do not do suboptimal analyses
  - Do not double-count analyses

make sure there are no unknown unknowns

COMBINING RESULTS

How to determine the spread of results?

- Stdev or 1σ confidence interval of results
- Can weight it with fit quality Q

Information theoretic optimum: Akaike Information Criterion

- Information content of a fit depends on how well data are described per fit parameter
- Information lost wrt. correct fit $\propto$ cross-entropy J
- Compute information cross-entropy J_m of each fit m
- Probability that fit is correct $\propto e^{J_m}$

AKAIKE INFORMATION CRITERION

- N measurments Γ_i from unknown pdf $g(\Gamma)$
- Fit model $f(\Gamma|\Theta)$ with parameters Θ
- Cross-entropy ($\sim$ Kullback-Leibler divergence)

$$J_m = J(g, f_m[\Theta]) = \int d\Gamma g(\Gamma) \ln(f(\Gamma|\Theta))$$

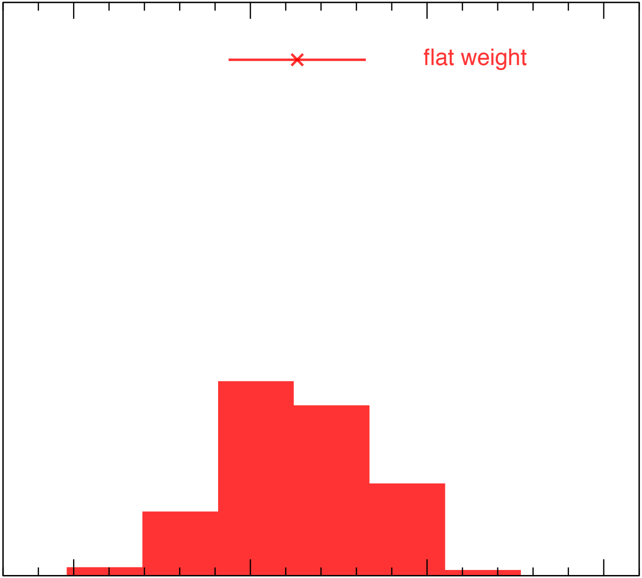
- For $N \to \infty$ and f close to g:

$$J_m = -\frac{\chi^2_m}{2} - p_m$$

where p_m is the number of fit parameters

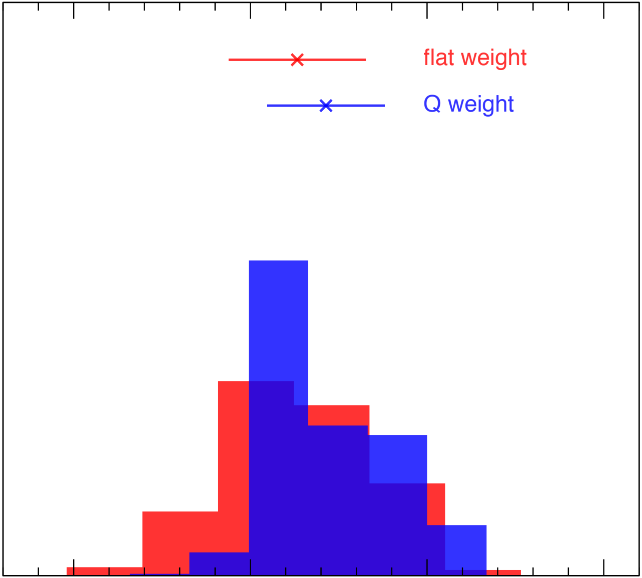
Is this the only correct method?

COMBINING RESULTS



- AIC suppresses strongly
- Other weights more conservative
- Agreement is excellent crosscheck

COMBINING RESULTS



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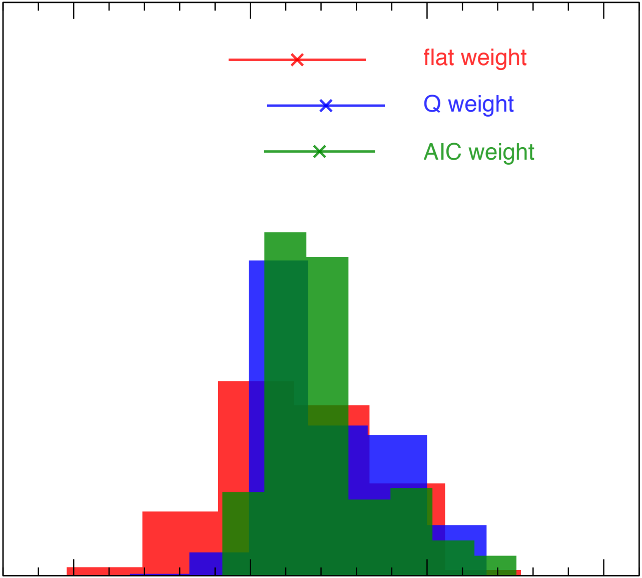
COMBINING RESULTS



- AIC suppresses strongly
- Other weights more conservative
- Agreement is excellent crosscheck

AN EXAMPLE CALCULATION

- Example: light hadron spectrum:(BMWc, Science 322 (2008) 1224)
  - Ground state baryons and vector mesons
- Goal:
  - Extract physical predictions from lattice data
- Challenge:
  - Recover real-world physics
    - Physical quark masses
    - Continuum: $a \to 0$
    - Infinite volume: $V \to \infty$ (treatment of resonant states)
  - Minimize and control all systematics on the way
- Method:
  - UV-filtered clover on tree-level Symanzik improved glue

QUARK MASS DEPENDENCE

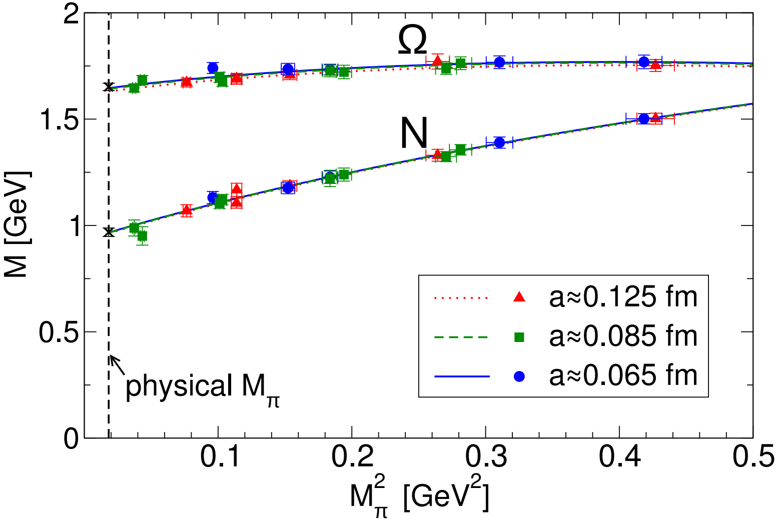
Goal:

- Extra-/Interpolate M_X (baryon/vector meson mass) to physical point (M_π, M_K)

Method:

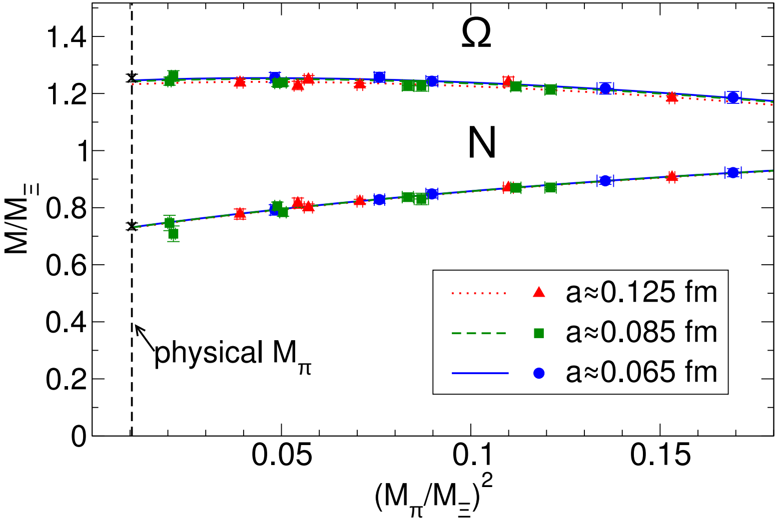
- Fundamental parameters: g, m_s, $m_{ud} = \frac{m_u+m_d}{2}$ (isospin averaged)
  - Experimentally inaccessible (confinement!)
  - Must be set via 3 experimentally accessible quantities
  - Isospin breaking
- Use M_Ξ or M_Ω and M_π, M_K to set parameters
- Variables to parametrize M_π^2 and M_K^2 dependence of M_X:
  - Use bare masses aM_y, $y \in \{X, \pi, K\}$ and a (bootstrapped)
  - Use dimensionless ratios $r_y := \frac{M_y}{M_{\Xi/\Omega}}$ (cancellations)
- Parametrization: $M_X = M_x^{(0)} + \alpha M_\pi^2 + \beta M_K^2 +$ higher orders

CHIRAL FIT



Ω
N
M [GeV]
M_π^2 [GeV^2]
physical M_π
a≈0.125 fm
a≈0.085 fm
a≈0.065 fm
0
0.5
1
1.5
2
0.1
0.2
0.3
0.4
0.5

CHIRAL FIT USING RATIOS



CONTINUUM EXTRAPOLATION

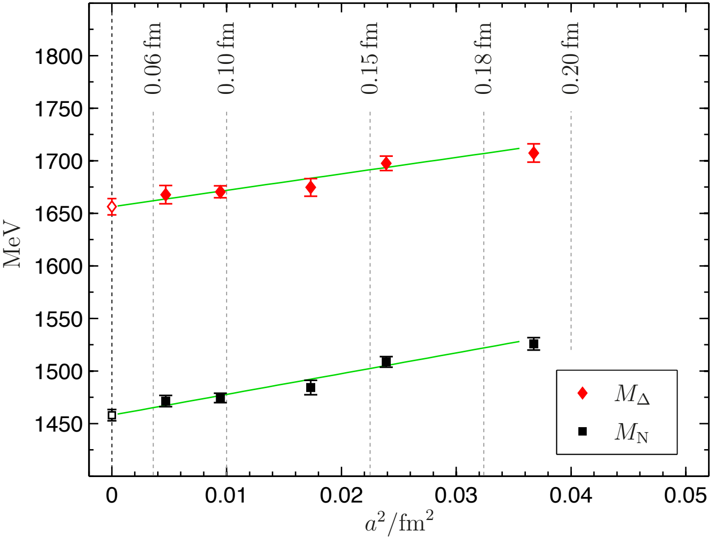
Goal:

- Eliminate discretization effects
  - Strongly dependent on action used

Method:

- Formally leading terms: $O(\alpha_s a)$ and $O(a^2)$
- Extrapolate to continuum
  - Need at least 3 lattice spacings
- Discretization effects depend on scale setting variable
  - Usually small if hadron masses are used to set scale
  - Depends on action, range of lattice spacings
- Typically small in spectroscopy if scale from spectral quantity

CONTINUUM LIMIT



Scaling study (not physical)

$O(\alpha_s a)$, $O(a^2)$ indistinguishable

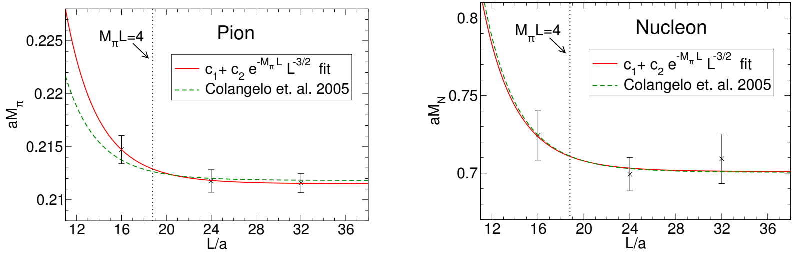
FINITE VOLUME EFFECTS FROM VIRTUAL PIONS

Goal:

- Eliminate virtual pion finite V effects
  - Hadrons see mirror charges
  - Exponential in lightest particle (pion) mass

Method:

- Best practice: use large V
  - Rule of thumb: $M_\pi L \gtrsim 4$
  - Leading effects $\frac{M_X(L)-M_X}{M_X} = cM_\pi^{1/2} L^{-3/2} e^{M_\pi L}$ (Colangelo et. al., 2005)



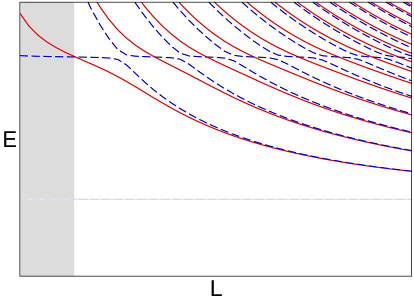
FINITE VOLUME EFFECTS IN RESONANCES

Goal:

- Eliminate spectrum distortions from resonances mixing with scattering states

Method:

- Stay in region where resonance is ground state
  - Otherwise no sensitivity to resonance mass in ground state



- Treatment as scattering problem
  (Lüscher, 1985-1991)
  - Parameters: mass and coupling (width)
  - Alternative approaches suggested

SYSTEMATIC UNCERTAINTIES

Goal:

- Accurately estimate total systematic error

Method:

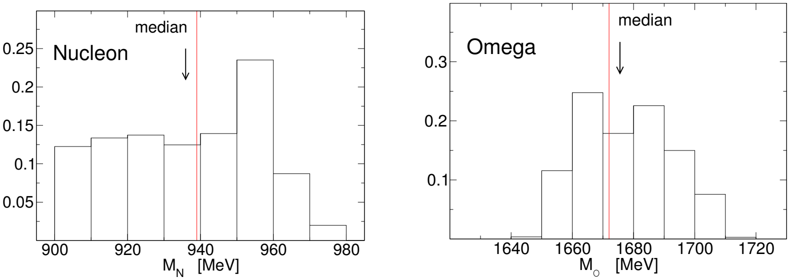
- We account for all the above mentioned effects
- When there are a number of sensible ways to proceed, we take them: Complete analysis for each of
  - 18 fit range combinations
  - ratio/nonratio fits (r_X resp. M_X)
  - $O(a)$ and $O(a^2)$ discretization terms
  - NLO χPT M_π^3 and Taylor M_π^4 chiral fit
  - 3 χ fit ranges for baryons: $M_\pi < 650/550/450$ MeV

  resulting in 432 (144) predictions for each baryon (vector meson) mass with each 2000 bootstrap samples for each Ξ and Ω scale setting

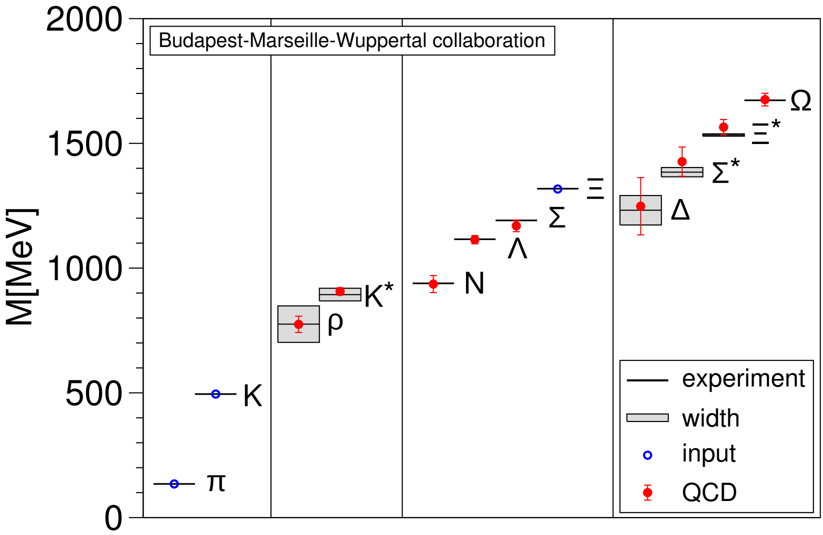
SYSTEMATIC UNCERTAINTIES II

Method (ctd.):

- Weigh each of the 432 (144) central values by fit quality Q
  - Median of this distribution ➛final result
  - Central 68% ➛systematic error
- Statistical error from bootstrap of the medians



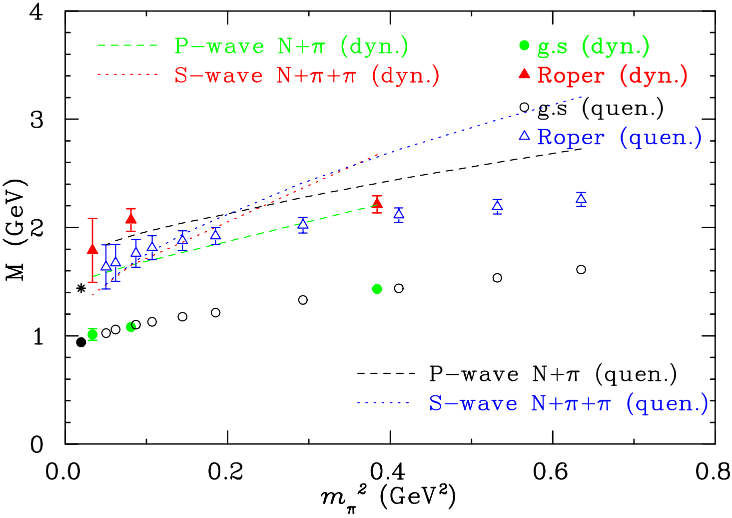
THE LIGHT HADRON SPECTRUM



EXCITED STATE SPECTROSCOPY

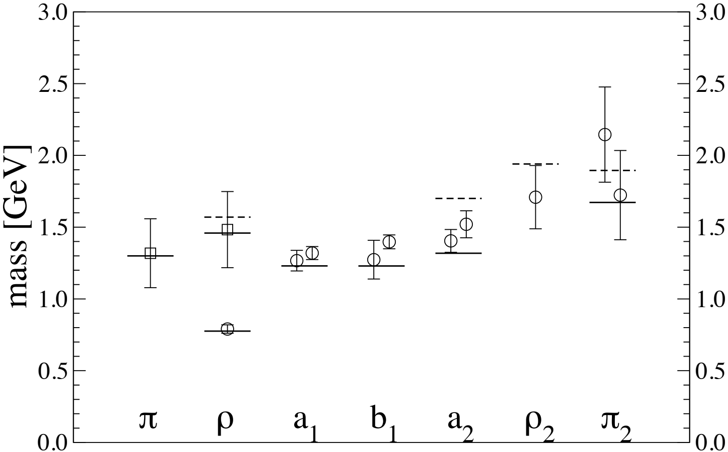
- ✓ Large operator bases
- ✓ Stable signal for many energy levels
- ✓ Sometimes additional tricks: finer time discretization
- ✓ Extrapolation to physical point done sometimes
- ✗ Typically only one lattice spacing
- ✗ No treatment of resonant finite V effects

NUCLEON EXCITATIONS



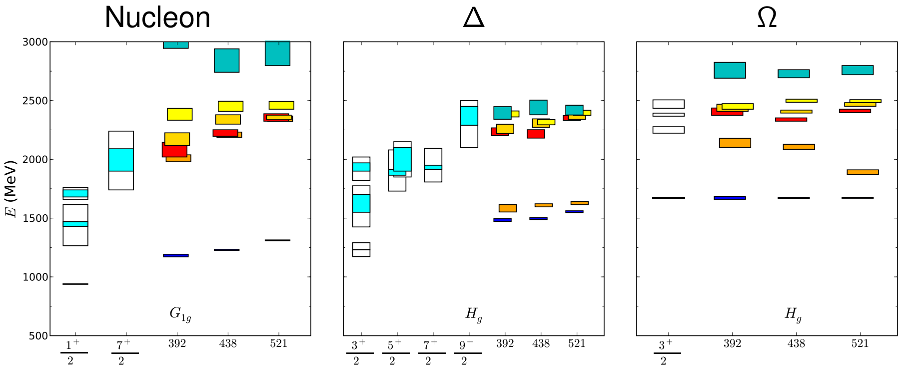
(Mahbub et. al., 2010)

EXCITED MESONS



(Engel et. al., 2010)

HIGH LYING RESONANCES

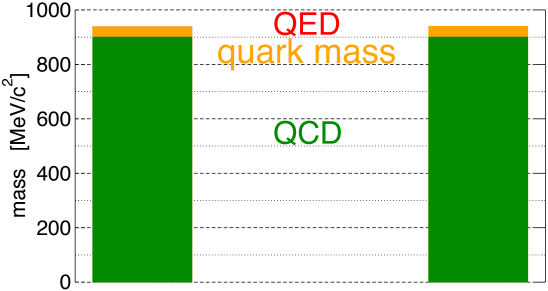


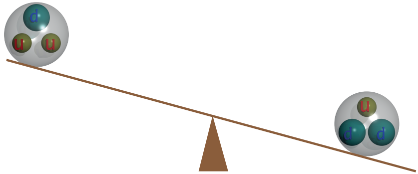
(Bulava, et al., 2010)

✓ Qualitative understanding of experimental spectrum

✗ No extrapolation to physical point, continuum

IS THE FINE STRUCTURE RELEVANT?





Proton Neutron

- Proton, neutron: 3 quarks
- Proton: uud
- Neutron: udd

- $m_u < m_d$: $M_p < M_n$
- $m_u = m_d$: $M_p > M_n$ Proton decays
- $M_p + M_{e^-} \gtrsim M_n$ No hydrogen

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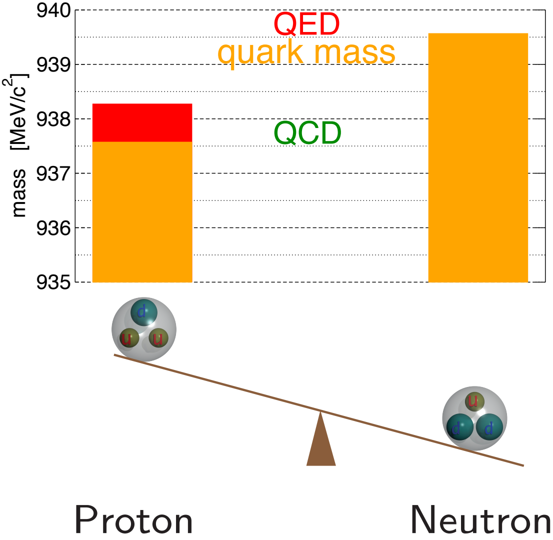

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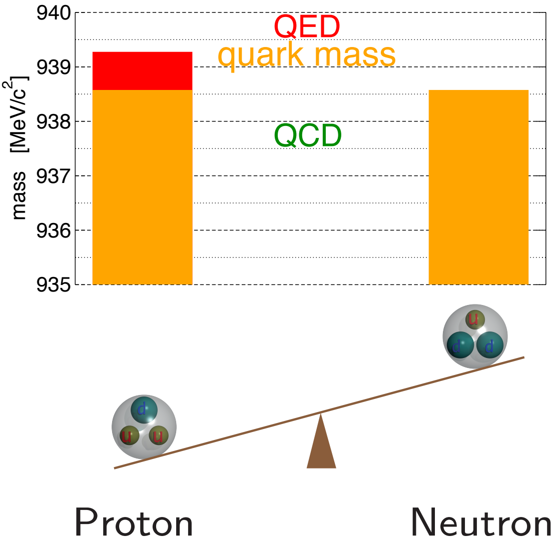

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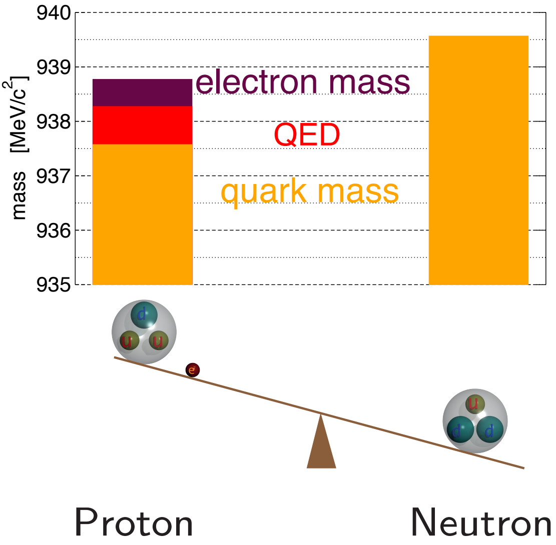

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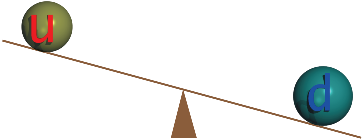
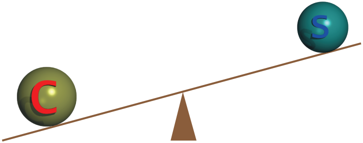
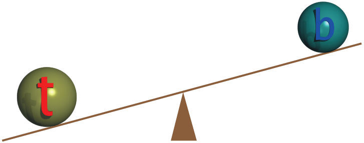
ANTHROPIC PUZZLE? THE LIGHT UP QUARK



1^{st} generation: $m_u < m_d$ Why?

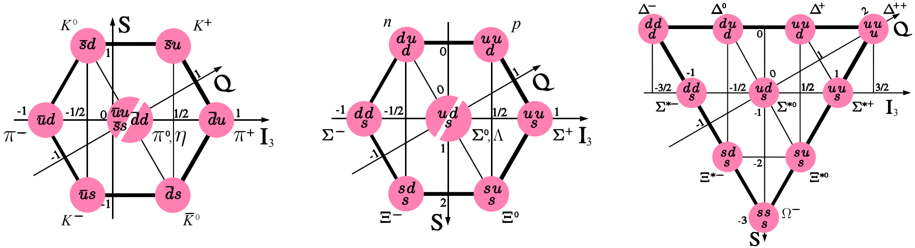


2^{nd} generation: $m_c > m_s$



3^{rd} generation: $m_t > m_b$

SOURCES OF ISOSPIN SPLITTING

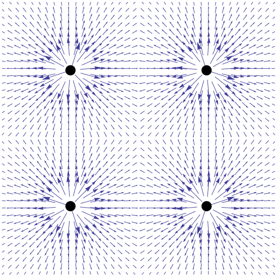


- Two sources of isospin breaking:
  - QCD: $\sim \frac{m_d - m_u}{\Lambda_{QCD}} \sim 1\%$
  - QED: $\sim \alpha(Q_u - Q_d)^2 \sim 1\%$
- On the lattice:
  - Include nondegenerate light quarks $m_u \neq m_d$
  - Include QED

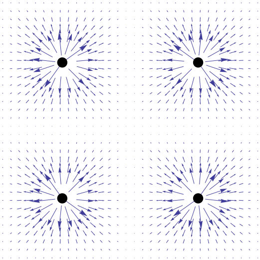
CHALLENGES OF QED SIMULATIONS

- Effective theory only (UV completion unclear)
- π^+, p, etc. no more gauge invariant
- QED (additive) mass renormalization
- Power law FV effects (soft photons)

EM field of a point charge cannot be made periodic & continuous



Remove $\vec{p} = 0$ modes in fixed gauge (Hayakawa, Uno, 2008)



QED ACTION

QED is an Abelian gauge theory with no self-interaction

- Compactifying QED induces spurious self-interaction

➢ Keep it non-compact (no problem with topology in 4D-$U(1)$)

- Need signals for gauge dependent objects

➢ insert gauge links or gauge fixing

$$S_{\text{QED}} = \frac{1}{2V_4} \sum_{\mu,k} |\hat{k}|^2 |A_\mu^k|^2 \quad \text{with} \quad \hat{k}_\mu = \frac{e^{iak_\mu} - 1}{ia}$$

- Momentum modes decouple ➢ quenched theory trivial

MOMENTUM SUBTRACTION

Absence of a mass gap ➛ IR divergences ($1/k^2$ in momentum sum)

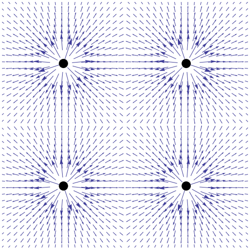
- Removing momentum modes with measure 0 as $V \to \infty$ allowed
- Remove $k = 0$ from momentum sum (QED_{TL})
  - Realised by a constraint term in the action

$$\frac{1}{\xi}\left(\int d^4 x A_\mu(x)\right)^2$$

  - Couples all times ➛ no transfer matrix!
- Remove $\vec{k} = 0$ from momentum sum (QED_L)
  - Realised by a constraint term in the action

$$\int dt \frac{1}{\xi(t)}\left(\int d^3 x A_\mu(x)\right)^2$$

  - Transfer matrix exists



- Corresponds to total charge subtraction in Coulomb gauge

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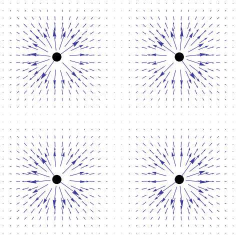
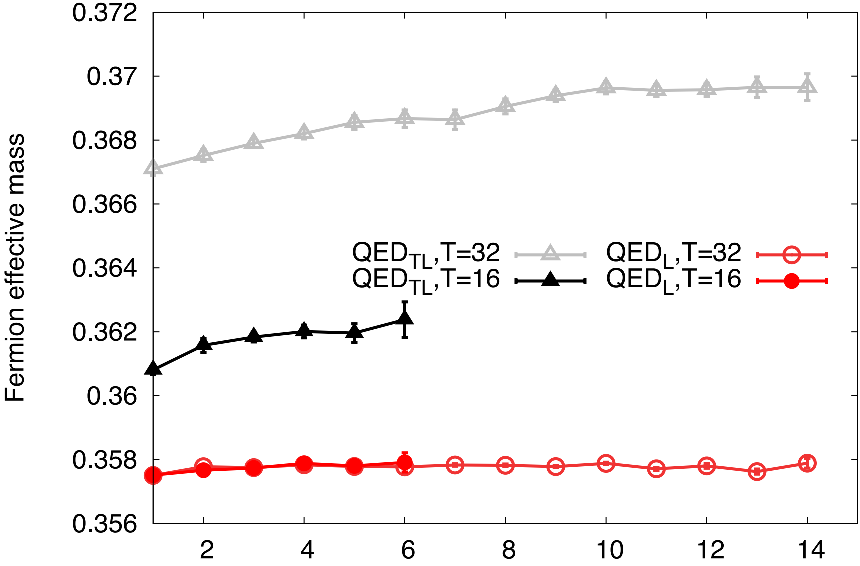


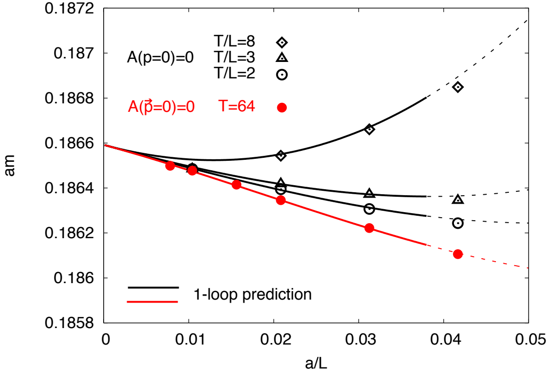
- Corresponds to total charge subtraction in Coulomb gauge

QUENCHED QED FV EFFECTS



FINITE VOLUME SUBTRACTION

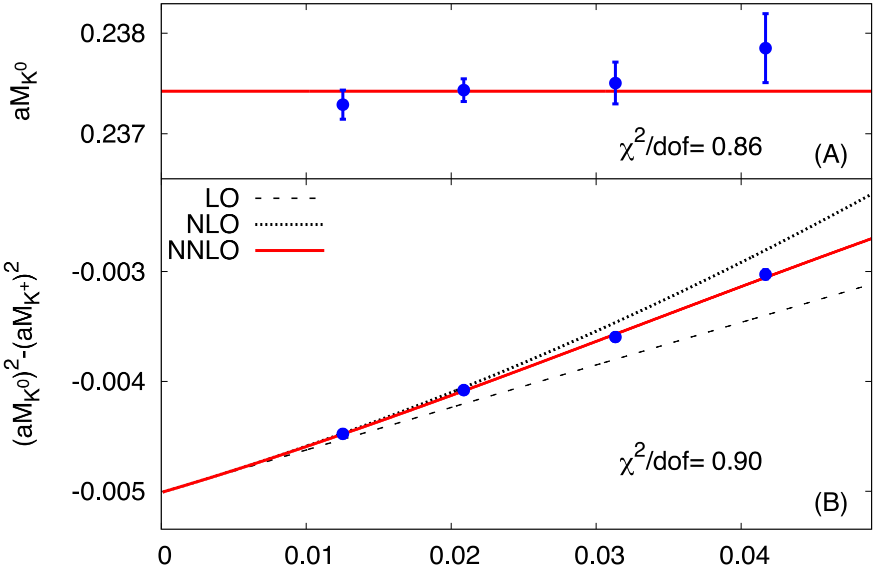
- Universal to $O(1/L^2)$
- Compositmess at $1/L^3$
- Fit $O(1/L^3)$
- Divergent T dependence for $p = 0$ mode subtraction
- No T dependence for $\vec{p} = 0$ mode subtraction



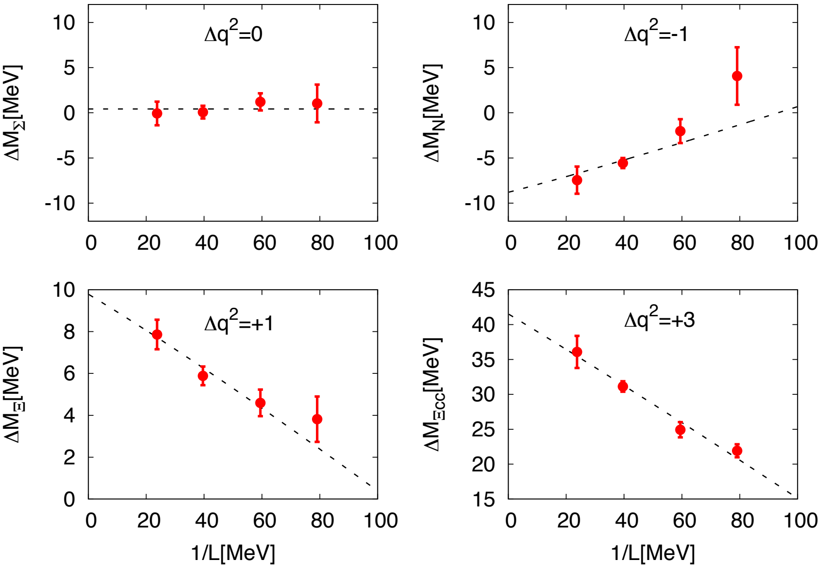
$$\delta m = q^2 \alpha \left(\frac{\kappa}{2mL} \left(1 + \frac{2}{mL} - \frac{3\pi}{(mL)^3} \right) \right)$$

(BMWc, 2014)

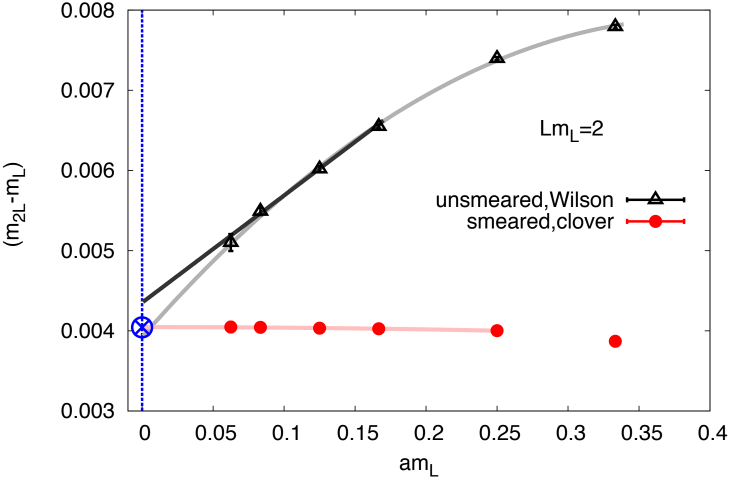
KAON FV IN QCD+QED



BARYON FV IN QCD+QED



UV FILTERING



Moderate smearing (1 stout) improves scaling dramatically

UPDATING PHOTON FIELD

Long range QED interaction ➛ huge autocorrelation in standard HMC

- Solution: HMC in momentum space

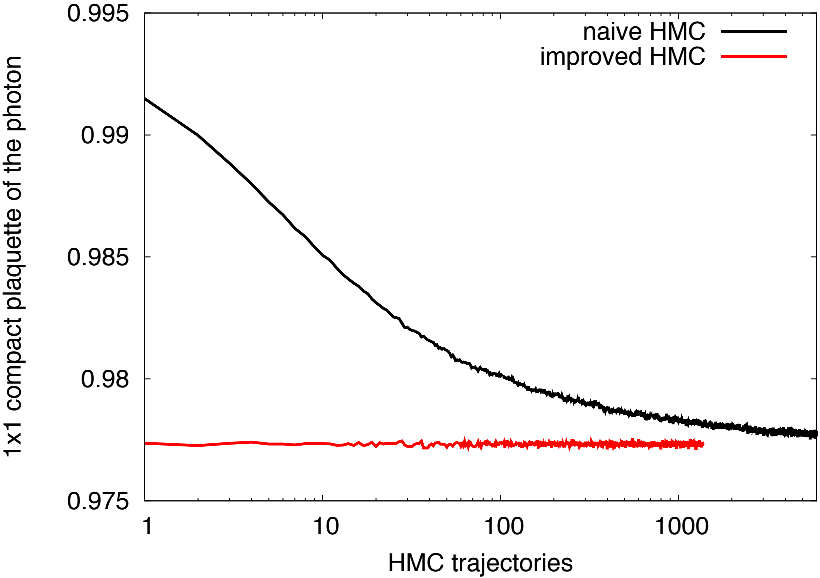
$$\mathcal{H} = \frac{1}{2V_4}\sum_{\mu,k}\left(|\hat{k}|^2|A_\mu^k|^2 + \frac{|\Pi_\mu^k|^2}{m_k}\right)$$

- Use different masses per momentum

$$m_k = \frac{4|\hat{k}|^2}{\pi^2}$$

- Zero mode subtraction trivial
- Coupling to quarks in coordinate space ➛ FFT in every step

HMC FOR PHOTON FIELDS



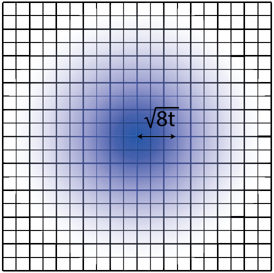
IDENTIFYING THE PHYSICAL POINT

We need to fix 6 parameters: m_u, m_d, m_s, m_c,, α_s and α

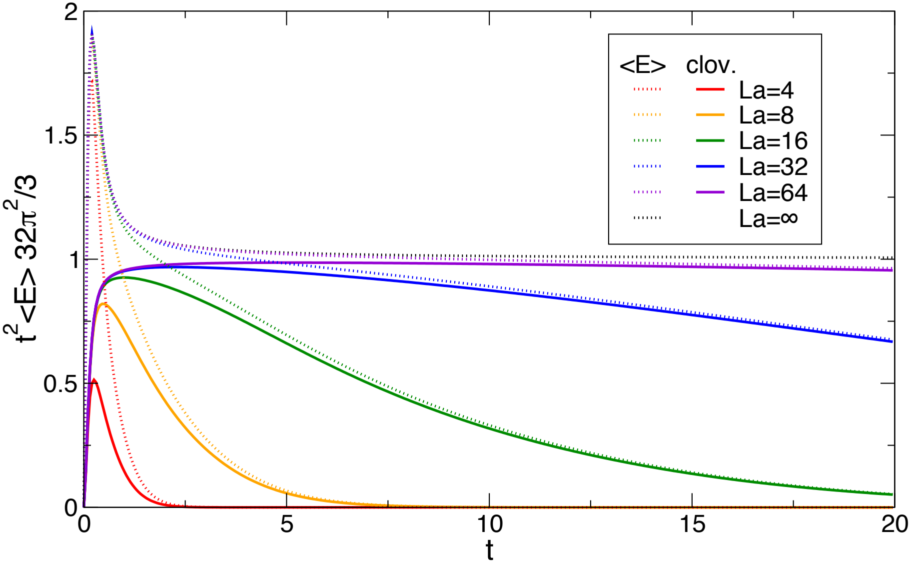
- Requires fixing 5 dimensionless ratios from 6 lattice observables
- 4 "canonical" lattice observables: $M_{\pi^\pm}$, M_{K^+}, M_Ω, M_D
- Strong isospin splitting from $M_{K^\pm} - M_{K^0}$
- what about α?
  - ✗ From $M_{\pi^\pm} - M_{\pi^0}$ ➛ disconnected diagrams, very noisy
  - ✗ From e^- e^- scattering ➛ far too low energy
  - ✗ From $M_{\Sigma^+} - M_{\Sigma^-}$ ➛ baryon has inferior precision
  - ✓ Take renormalized α as input directly
  - ➛ Use the QED gradient flow
    Analytic tree level correction

$$\langle F_{\mu\nu} F_{\mu\nu} \rangle = \frac{6}{V_4} \sum_k e^{-2|\hat{k}|^2 t}$$

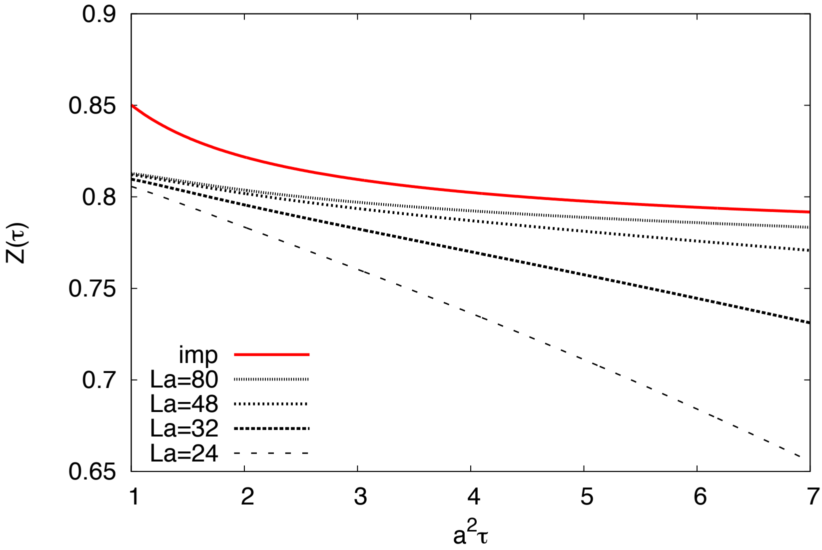
Slightly more complicated for clover plaquette



TREE LEVEL CORRECTION



EFFECT OF TREE LEVEL CORRECTION



SCALING IN RENORMALISED COUPLING

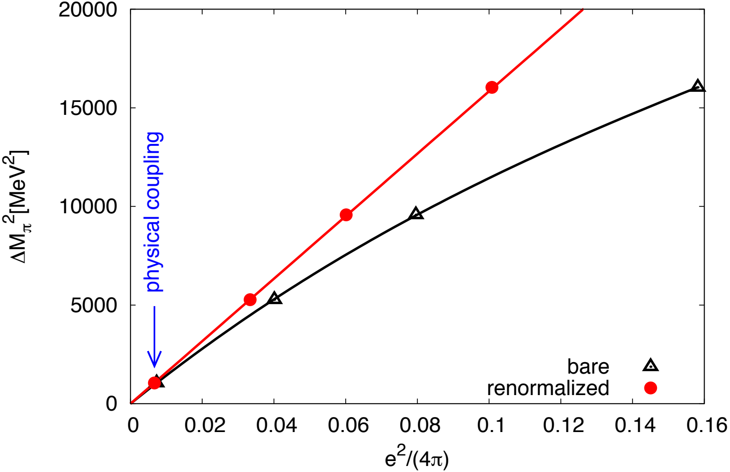
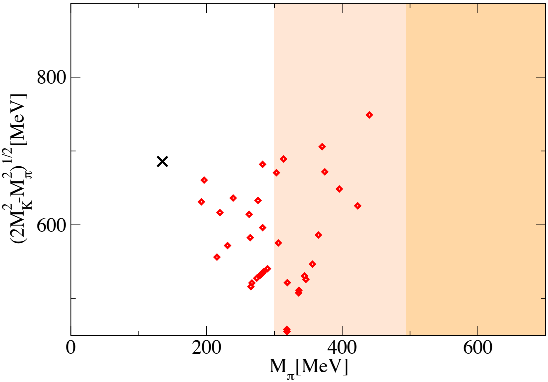


Illustration with precise $\Delta M_\pi^2 = M_{\bar{u}d}^2 - (M_{\bar{u}u}^2 + M_{\bar{d}d}^2)/2$

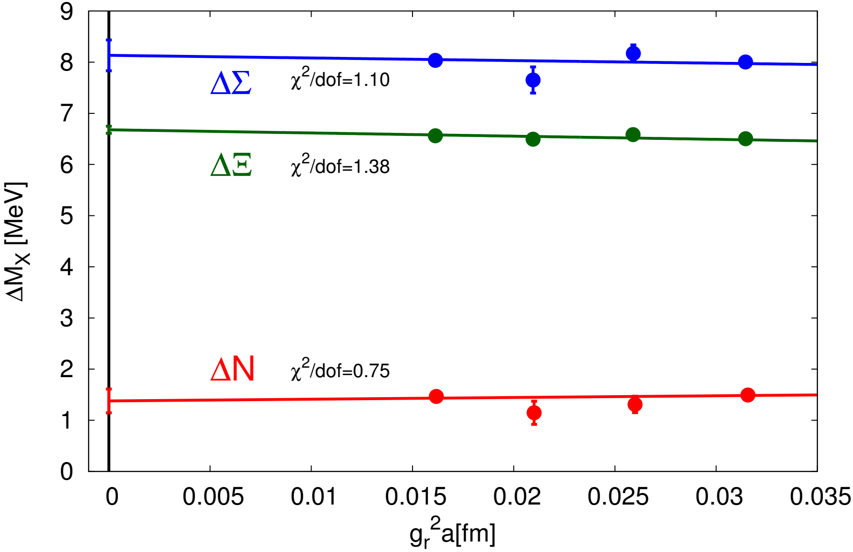
LANDSCAPE



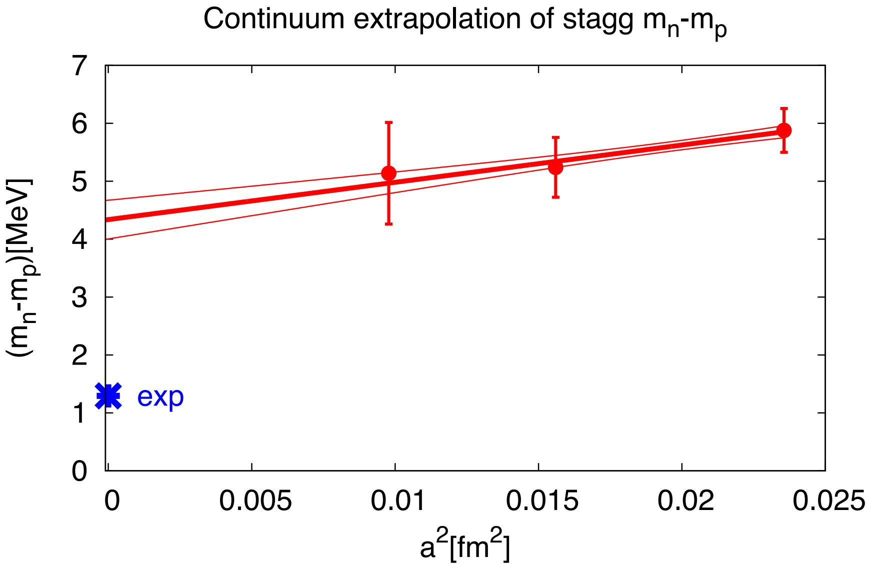
- Small extrapolation to physical point
- Charm mass is physical
- $u - d$ splitting is physical
- Why use $\alpha \gg \alpha^{\text{phys}}$?

- Hadron masses are even in e, so signal $\propto e^2$
- Per configuration fluctuations are not even in e, so noise $\propto e$
- Per configuration cancellation helps in qQED, but not dynamically

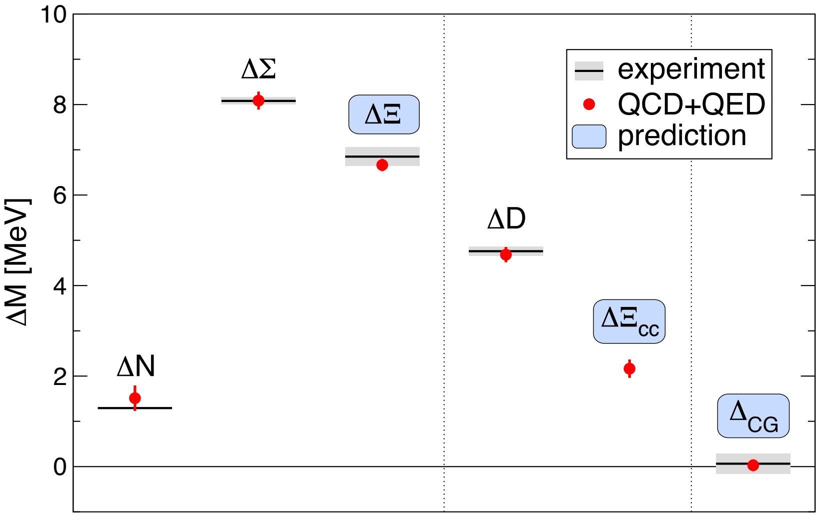
SCALING


ΔΣ
χ²/dof=1.10
ΔΞ
χ²/dof=1.38
ΔN
χ²/dof=0.75
ΔM_X [MeV]
g_r²a[fm]
0
1
2
3
4
5
6
7
8
9
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035

DONT DO THIS STAGGERED



ISOSPIN SPLITTING

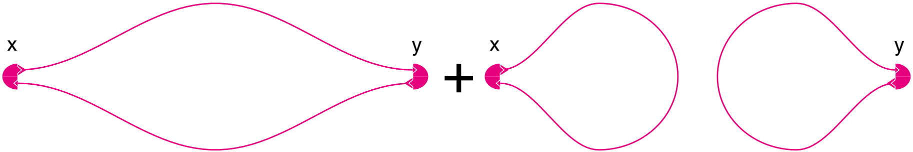


(BMWc 2014)

DISENTANGLING CONTRIBUTIONS

Problem:

- Disentangle QCD and QED contributions
  - Not unique, $O(\alpha^2)$ ambiguities
- Flavor singlet (e.g. π^0) difficult (disconnected diagrams)



Method:

- Use baryonic splitting Σ^+-Σ^- purely QCD
  - Only physical particles
  - Exactly correct for pointlike particle
  - Corrections below the statistical error

ISOSPIN SPLITTINGS NUMERICAL VALUES

	splitting [MeV]	QCD [MeV]	QED [MeV]
$\Delta N = n - p$	1.51(16)(23)	2.52(17)(24)	-1.00(07)(14)
$\Delta\Sigma = \Sigma^- - \Sigma^+$	8.09(16)(11)	8.09(16)(11)	0
$\Delta\Xi = \Xi^- - \Xi^0$	6.66(11)(09)	5.53(17)(17)	1.14(16)(09)
$\Delta D = D^\pm - D^0$	4.68(10)(13)	2.54(08)(10)	2.14(11)(07)
$\Delta\Xi_{cc} = \Xi_{cc}^{++} - \Xi_{cc}^{+}$	2.16(11)(17)	-2.53(11)(06)	4.69(10)(17)
$\Delta_{\mathrm{CG}} = \Delta N - \Delta\Sigma + \Delta\Xi$	0.00(11)(06)	-0.00(13)(05)	0.00(06)(02)

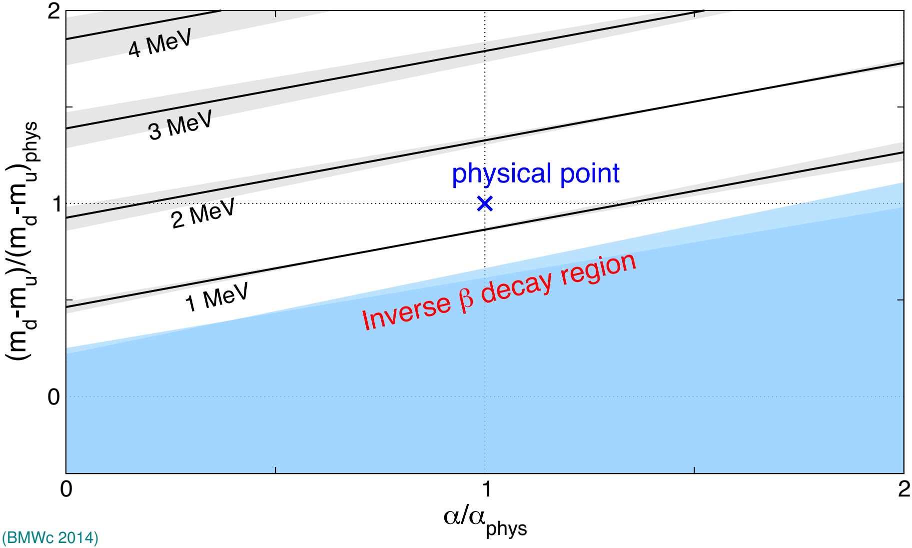
- Quark model relation predicts Δ_{CG} to be small

  (Coleman, Glashow, 1961; Zweig 1961)

$$\Delta_{\mathrm{CG}} = M(udd) + M(uus) + M(dss) - M(uud) - M(dds) - M(uss)$$

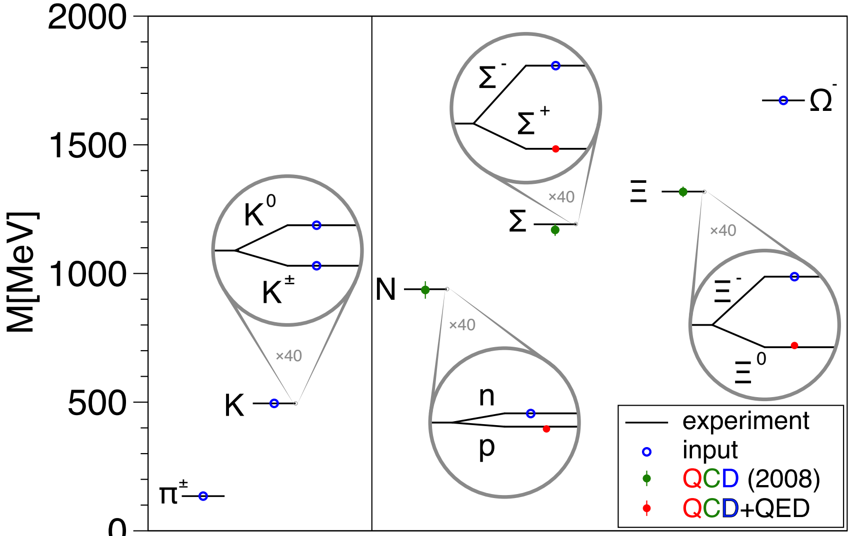
$$\Delta_{\mathrm{CG}} \propto ((m_d - m_u)(m_s - m_u)(m_s - m_d), \alpha(m_s - m_d))$$

NUCLEON SPLITTING QCD AND QED PARTS



(BMWc 2014)

PROGRESS



(BMWc (2013))