Lattice QCD for hadron and nuclear physics: understanding discrete QCD

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Plan

- A short recap of this morning.
- A look at results from different lattice formulations.
- Extracting physics - energy from correlation functions.
- Discretising QCD - what the consequences (and compromises) for physics.
- Making progress - two routes and how to use and/or understand the resulting lattice data.

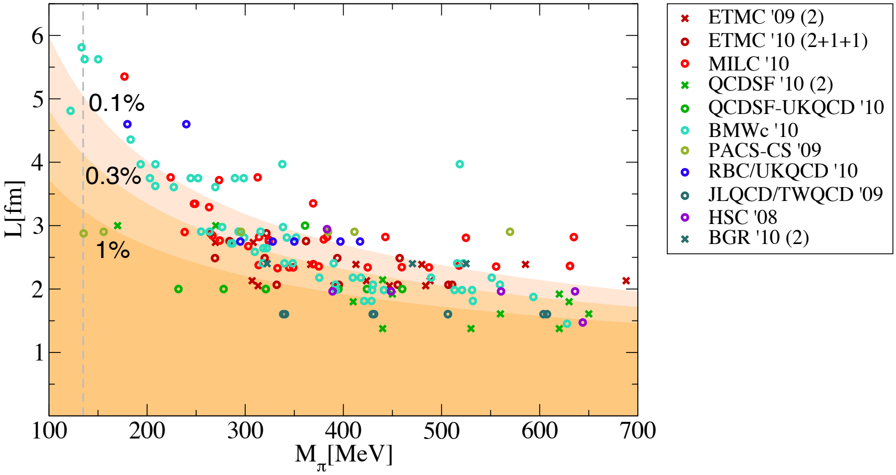
Recap

- QCD - a theory of the strong interaction that is confining and asymptotically free.
- Lattice QCD - a formulation of the theory on a 4-dimensional space-time lattice.
  - provides a regulator for the theory
  - facilitates numerical simulations via Monte Carlo evaluation of path integrals in the Euclideanised theory.
- Fermions “live” on lattice sites and gluons on the links. There is no unique discretisation framework but the continuum theory should be recoverable in a formal way.

Validation:
can we reproduce known results and make verified predictions?

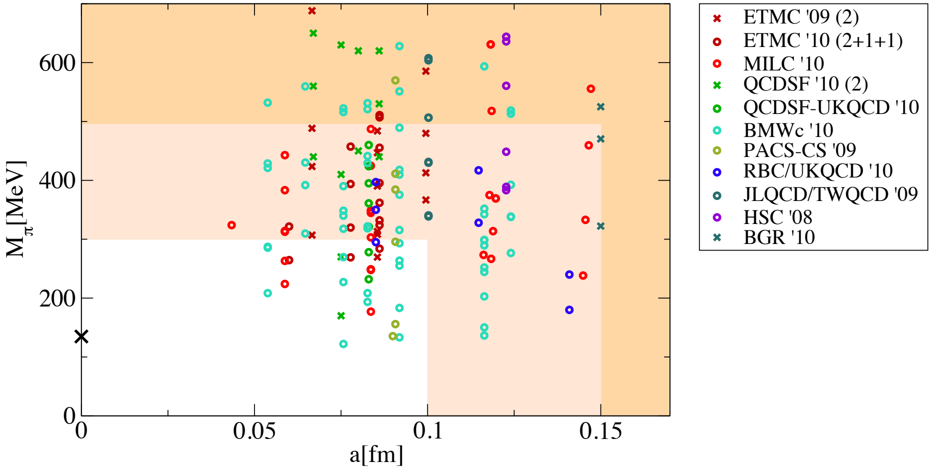
How are we doing?

C. Hoelbling, arXiV.1102.0410



How are we doing (2)?

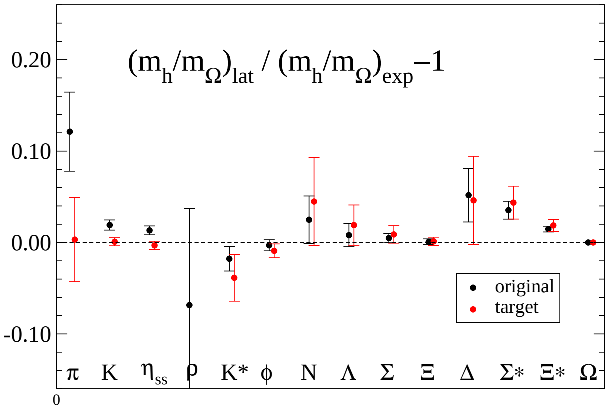
C. Hoelbling, arXiV.1102.0410



$N_f = 2 + 1$ SIMULATIONS AT THE PHYSICAL POINT

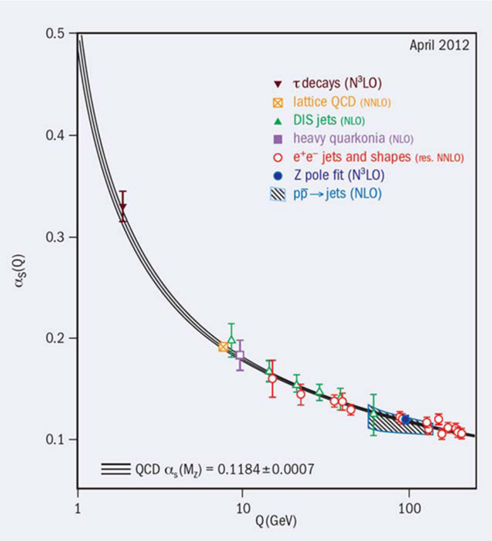
- First $N_f = 2 + 1$ simulations at physical quark mass.
- PACS-CS computer, U Tsukuba. 14.3 Tflops peak
- Lattice spacing: $a = 0.08995(40)\text{fm}$ (from m_Ω).

PACS-CS Collaboration [arXiv:0911.2561]

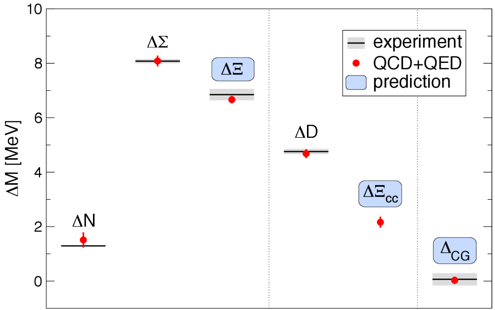


Validation

The running coupling, α_s



Baryon electromagnetic mass splittings

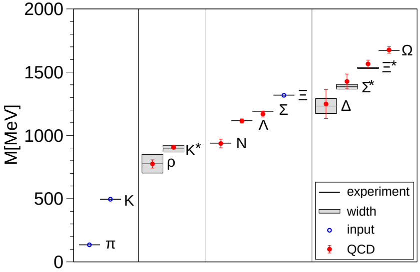


QED + QCD

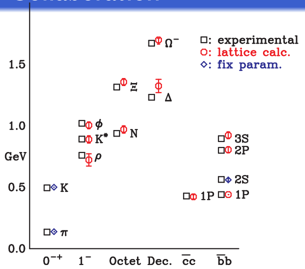
BMW Collab. Science 347 (2015) 1452

Convergence through universality

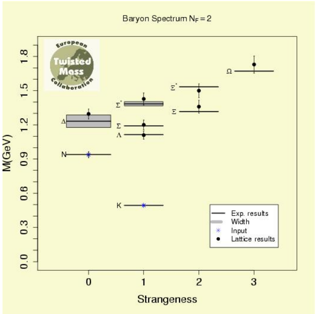
BMW Collaboration



MILC Collaboration



ETMC Collaboration



- **BMW:** SW-Wilson

[Science 322:1224-1227,2008.]

- **ETMC:** Twisted Mass

[arXiv:0910.2419,0803.3190]

- **MILC:** Staggered

[arXiv:0903.3598]

The QCD spectrum

- Goal is to extract the energy of (colourless) states of **QCD** .
- This information is encoded in the 2-point correlation functions

$$C(t) = \langle \phi_i(t) | \phi_i^\dagger(0) \rangle$$

where $\phi^\dagger$ and $\mathcal{O}$ are operators acting on the quark fields to create a state at $t = 0$ and annihilate at $t = t$.

- Euclidean time evolution: $\phi(t) = e^{Ht} \phi e^{-Ht}$ and inserting a complete set of states $1 = \sum_n |n\rangle\langle n|$ gives

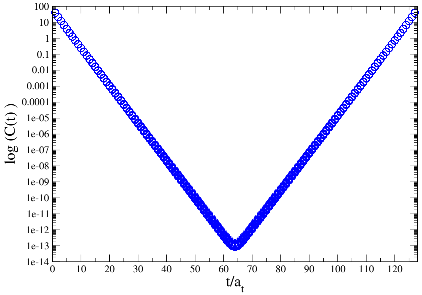
$$C(t) = \sum_{n=0}^{\infty} \frac{|\langle \phi | n \rangle|^2}{2m_n} e^{-E_n t}$$

we work in the low-temp limit ie $\beta = 1/kT = L_t$ large.

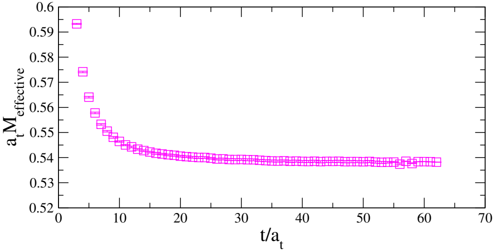
- Now as $t \to \infty C(t) = Ze^{-E_0 t}$
- At large times the exponential fall off of $C(t)$ gives the ground state energy.

From correlators to energies

- In general works well for extracting ground states
- Higher excitation energies hard to extract by just fitting to exponentials.



$$a_t m_{effective} = -ln\left(\frac{C(t)}{C(t-1)}\right)$$



- The correlator and effective mass of the J/Ψ meson.
- For $\mathcal{O}_i = \mathcal{O}_j$ the correlation function is positive definite and $a_t m_{effective}$ converges monotonically from above.

The QCD spectrum (2)

- The lattice has finite extent - impose (anti)-periodic boundary conditions. Then meson correlators are symmetric about the midpoint of the lattice i.e. $e^{-mt} \longrightarrow e^{-mt} + e^{-m(T-t)}$ where T is the time extent.
- Want to optimise $\mathcal{O}$ to get a large overlap with the wavefunction of the state of interest i.e. make

$$\mathcal{Z}_n(\vec{p}) \equiv \frac{|\langle 0|\mathcal{O}_i|n\rangle|^2}{2E_n(\vec{p})}$$

  the spectral weight of the n^{th} state large for state of interest and small for the rest.

What about excitations?

One approach: variational method

If we can measure $C_{ij}(t) = \langle 0|\phi_i(t)\phi_j^\dagger(0)|0\rangle$ for all i, j and solve generalised eigenvalue problem:

$$\mathbf{C}(t)\,\underline{v} = \lambda \mathbf{C}(t_0)\,\underline{v},$$

then

$$\lim_{t-t_0\to\infty} \lambda_k = e^{-E_k t} + \mathcal{O}\left(e^{-\Delta E_n t}\right)$$

For this to be practical, we need:

- a 'good' basis set that **resembles the states** of interest.
- **all elements** of this correlation matrix measured.

[see Blossier et.al. JHEP 0904 (2009) 094]

Extracting Energies
aka
The Dark Art of Fitting Data

The effective mass

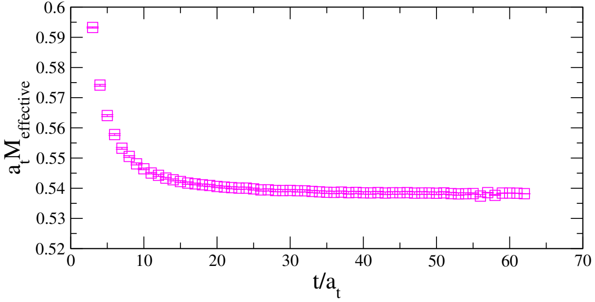
A useful quantity is the effective mass

$$a_t M_{\text{eff}}(t) = \ln\left(\frac{C(t)}{C(t+1)}\right)$$

- A useful quantity to see ground state dominance: $a_t m_{eff} \to$ constant - the plateau
- The onset and length of the plateau depends on $\mathcal{O}$
- The hadron mass is extracted from a fit to correlator data in the plateau region
- statistical errors grow exponentially with t, except for the pion

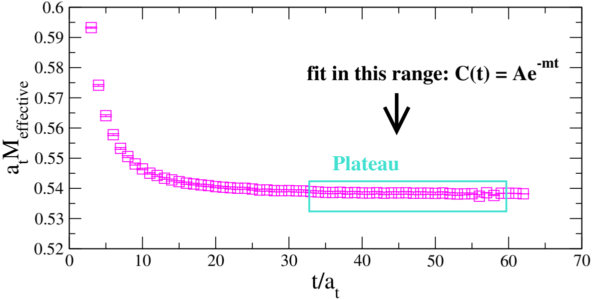
An effective mass plot

At large times, effective mass converges to the ground state energy - see a plateau in the effective mass plot as a function of time.



An effective mass plot (2)

At large times, effective mass converges to the ground state energy - see a plateau in the effective mass plot as a function of time.



- The correlator data is fitted to the expected $C(t) = Ae^{-E_0 t}$ form. Eg using a χ^2 minimisation algorithm with A and E_0 free parameters and for some “reasonable” choice of time range.
- Errors are estimated by bootstrap or jackknife.

Resampling techniques

- Two methods: Bootstrap and Jackknife
  - Jackknife from Quenouille (1956) and Tukey (1957)
  - Consider N measurements, remove the first leaving a jackknifed set of $N-1$ "resampled" measurements.
  - Repeat analysis (fits) on this reduced set, giving parameters $\alpha_{J^{(1)}}$.
  - Repeat resampling, throwing out 2nd measurement etc to get α_{J^i}, $i = 1, \ldots, N$.
  - Then

$$\sigma_J^2 = \frac{(N-1)}{N} \sum_{i=1}^{N} (\alpha_{J^{(i)}} - \alpha)^2$$

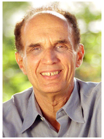
where α is the result from fitting the full dataset.

John Tukey: also gave us FFT and box plots!

Resampling techniques (2): bootstrap

Bootstrap from Efron (late '70s). See Numerical Recipes and Efron's book An Introduction to the Bootstrap

- A resampling technique.
- Create a new dataset by drawing N datapoints with replacement from the original dataset, size N.
- Replacement means you do not get the original set each time - but a set with a random fraction of the original points.
- As for jackknife repeat analysis on each new set.



Bradley Efron

Numerical Recipes in C says

Offered the choice between mastery of a five-foot shelf of analytical statistics books and middling ability at performing statistical Monte Carlo simulations, we would surely choose to have the latter skill.

How to choose a fit range

When fitting the correlator data we are looking for:

- a good $\chi^2/N_{d.o.f.}$
- a "reasonable" range in t
- a "reasonable" fit error
- a fit that is stable with respect to the choice of t. In particular with respect to small changes in t_{min} the minimum timeslice included in the fit.

Common quantities to look at

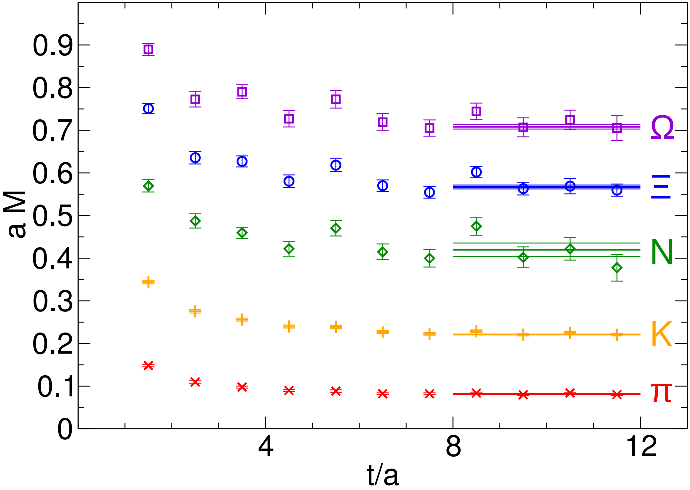
- a sliding window: plot the fitted mass as a function of t_{min}
- a fit-histogram: plot $QN_{dof}/(\Delta m)$ for each (t_{min}, t_{max}) and $Q = \Gamma[(interval - N_{param})/2, \chi^2/2]$. Choose the (t_{min}, t_{max}) that maximises this quantity.
- A good idea to check your fit range looks reasonable on the effective mass plot

Homework

Have some fun with data! See homework exercise on web page.

Effective mass plots

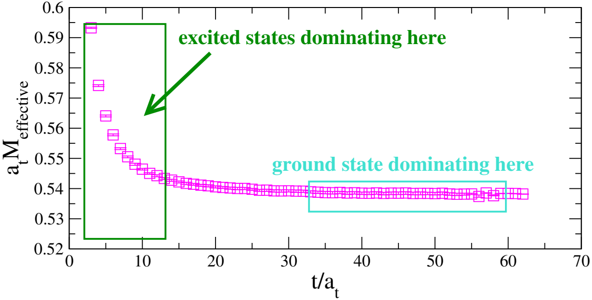
BMW Collaboration (Dürr et al) 0906.3599v1



- $L/a = 48$, $a = 0.085fm$, $m_\pi = 190\text{MeV}$

The effective mass (again)

At large times, effective mass converges to the ground state energy - see a plateau in the effective mass plot as a function of time.



- How can we determine excited state energies?
- First guess: fit to 2 exponentials - $C(t) = Ae^{-E_0 t} + Be^{-E_1 t}$, where A, B, E_0, E_1 are fit parameters.
- Since the regions where E_0 and E_1 are relevant are different: fit for E_0 and freeze its value in a fit for E_1.
- Notoriously unstable fits.
- Different approach needed

Extracting excited state energies

There are a number of ideas on the market

- Bayesian analysis
- χ^2-histogram analysis
- Variational analysis
- $\vdots$

Variational analysis - the most successful method

- Consider a basis of operators $\mathcal{O}_i$, $i = 1, \ldots, N$ in a given lattice irrep.
- Form a matrix of correlators

$$C_{ij}(t) = \langle \mathcal{O}_i(t) \mathcal{O}_j^\dagger(0) \rangle$$

- Treat as a generalised eigenvalue problem (GEVP):

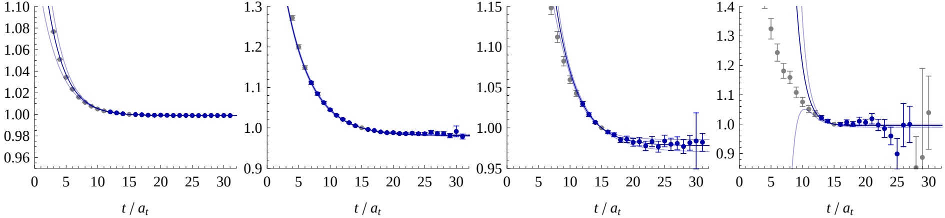
$$C(t) v_n(t, t_0) = \lambda_n(t, t_0) C(t_0) v_n(t, t_0)$$

  where t_0 is a refence timeslice (you choose)
- The vectors v_n diagonalise $C(t)$
- For finite N one can prove [Lüscher & Wolff 1990]

$$E_n^{eff}(t, t_0) = -\partial_t \log \lambda_n(t, t_0) = E_n + O(e^{-\Delta E_n t})$$

Fitting principal correlators

- Typical fits for a set of excited states in the T_1^{--} irrep in charmonium (26 operators!) are



- plotting $\lambda_n(t) \cdot e^{m_n(t_1 - t_0)}$ with $t_0 = 15$.
- Expect a plateau at 1.0 if single-exp dominates.

Improving resolution: anisotropic lattices

Improving resolution - the anisotropic lattice

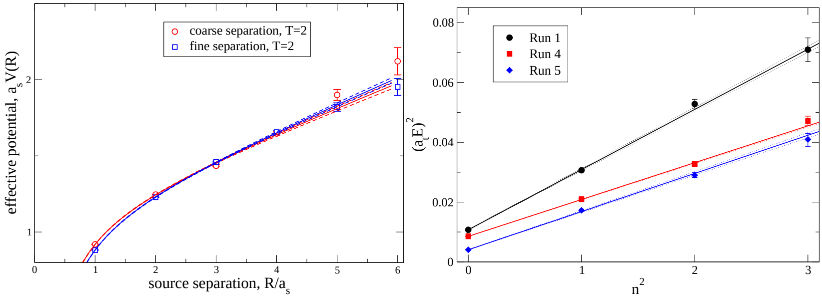
- If we can build a good basis of operators, we can extract energies of low-lying states from the correlator at short distances.
- The lattice correlator can only be sampled at discrete values of t and signal falls quickly for a massive state, while the statistical noise does not. Reducing the lattice spacing is extremely computationally expensive
- Mitigate this cost by reducing just the temporal lattice spacing, keeping the spatial mesh coarser; the anisotropic lattice.
- Unfortunately this reduces the symmetries of the theory from the hypercubic to the cubic point group. The dimension four operators on the lattice now split;

$$\begin{aligned} \mathrm{Tr}\, F_{\mu\nu} F_{\mu\nu} &\rightarrow \left\{ \mathrm{Tr}\, F_{ij} F_{ij}, \mathrm{Tr}\, F_{i0} F_{i0} \right\} \\ \bar{\psi} \gamma_\mu D_\mu \psi &\rightarrow \left\{ \bar{\psi} \gamma_i D_i \psi, \bar{\psi} \gamma_0 D_0 \psi \right\} \end{aligned}$$

- On $3 \oplus 1$ anisotropic lattices, spatial symmetries unchanged.

QCD AND THE ANISOTROPIC LATTICE

- The space-time symmetry breaking in QCD introduces extra bare parameters in the lagrangian, that must be tuned to restore Euclidean rotational invariance in the continuum limit.
- For QCD, both the quarks and gluons must "feel" the same anisotropy; this requires tuning *a priori*.
- Two physical conditions are satisfied simultaneously, derived from the "sideways" potential and the pion dispersion relation.



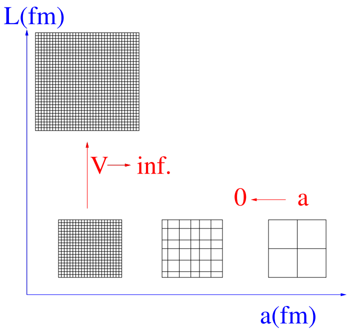
Further thoughts on lattice calculations

Compromises and the Consequences

1. Working in a finite box at finite grid spacing

Further notes on RGE and asymptotic scaling in notes on line.

- Identify a "scaling window" where physics doesn't change/changes weakly with a or V. Recover continuum **QCD** by extrapolation.
- Lattice spacing small enough to resolve structures induced by strong dynamics
- Volume large enough to contain lightest particle in spectrum: $m_\pi L \geq 2\pi$

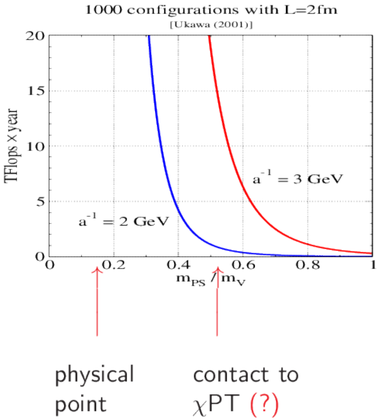


A costly procedure but a regular feature in lattice calculations now

2. Simulating at physical quark masses: light quarks

- Light quarks in gauge generation through fermion determinant M.
- Computational cost grows rapidly with decreasing quark mass $\longrightarrow m_q = m_{u,d}$ costly.

$$C \propto \left(\frac{m_\pi}{m_\rho}\right)^{-6} (L)^5 \, (a)^{-7}$$



- Work horse is Hybrid Monte Carlo (HMC) Duane et al 1987
- Many improvements over the years for all fermion discretisations

- The wall has come down - Physical point can be reached!
- Care needed vis location of decay thresholds and identification of resonances.

2. Simulating at physical quark masses: heavy quarks

- Discretisation errors grow as $\mathcal{O}(am_q)$ becoming large for reasonable a and heavy quarks
- Bottom quarks treated with Effective Field Theories - NRQCD, Fermilab etc
  - Continuum limits and EFTs can be tricky - not always possible e.g. with NRQCD
  - Controlling systematics important for precision CKM physics
- Charm quarks can be handled relativistically
  - Anisotropic lattices useful here: $a_s \neq a_t$ and $a_t m_c < 1$. Care needed to ensure errors $\mathcal{O}(a_s m_c)$ are not large.

Better algorithms for physical light quarks and/or chiral extrapolation. Relativistic m_b is in reach.

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Turn a weakness into a strength by using lattice simulations to study *quark mass dependence*!

3. Breaking symmetry

- Almost all symmetries of **QCD** are preserved. But Lorentz symmetry broken at $a \neq 0$ so $SO(4)$ rotation group broken to discrete rotation group of a hypercube.
- Angular momentum and parity J^P correspond to irreducible representations of the rotation group $O(3)$
- A spatially isotropic lattice breaks $O(3) \to O_h$, the cubic point group.
- Eigenstates of the lattice $\mathcal{H}$ transform under irreps of O_h so states are classified by these irreps and not by J^P.
- Classify states by irreps of O_h and relate by subduction to J values of O_3.
- 5 irreps of $O(3)$ and an infinite number for J^P so values are distributed across lattice irreps.
- Lots of degeneracies in subduction for $J \geq 2$ and physical near-degeneracies. Complicates spin identification.

Connecting lattice and continuum groups

	A_1	A_2	E	T_1	T_2
$J=0$	1				
$J=1$				1	
$J=2$			1		1
$J=3$		1		1	1
$J=4$	1		1	1	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

- In principle then to identify a $J=2$ state, results from E and T_2 at finite a should extrapolate to the same result.
- an expensive business(!)
- Even then, is this enough information to disentangle high-spin states eg $4=0\oplus 1\oplus 2$?
- In charmonium a radial excitation of the near-degenerate $(0^{++}, 1^{++}, 2^{++})$ could be close in energy to the 4^{++} ground state.

A solution - Spin identification at finite lattice spacing: 0707.4162, 1204.5425

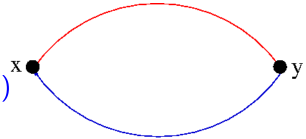
4. Making propagators - Wick revisited

- Recall that to calculate particle properties the fermion matrix M - a large ($\sim 10^8 \times 10^8$) matrix is inverted followed by Wick contractions of quark fields.

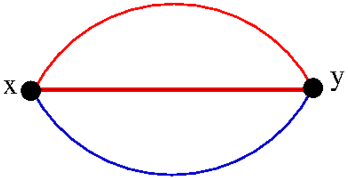
$$C(t, \mathbf{x}) = \langle \mathrm{Tr}(\gamma_5 M_a^{-1}(x,0)^\dagger \gamma_5 \Gamma M_b^{-1}(x,0)\Gamma^\dagger) \rangle$$

Mesons e.g. a pion

$$\langle \bar{u}(x)\gamma_5 d(x)\bar{d}(y)\gamma_5 u(y)\rangle = Tr\{\gamma_5 M_{dd}^{-1}(x,y;U)^\dagger \gamma_5 M_{uu}^{-1}(y,x;U)\Gamma^\dagger)$$



Baryons e.g. a proton:
2 up quarks, 1 down quark. Must keep track of which u quark from x goes to which u quark at y - 2 contractions: $(N_u! \times N_d!)$
Now, for proton-proton scattering have $4! \times 2! = 48$ contractions
For He3 (ppn) $5! \times 4! = 2880$ and for He4 (ppnn) $6! \times 6! = 518400$.



Symmetries reduce the problem and better algorithms

Yamazaki et al, PRD81 2010; Orginos& Detmold PRD87 2013

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5. Making propagators - signal-to-noise

- Particularly severe for nucleons.
- Signal for a proton correlation function $\sim Ze^{-m_N t}\left[1 + \delta Z_n e^{-(E_n - m_N)t}\right]$.
- Signal to noise for a proton is then $\sim \sqrt{N_{cfg}}e^{-(m_N - \frac{3}{2}m_\pi)t}$ with $m_N \sim 939MeV$ and $m_\pi \sim 135MeV$.
- Signal to noise for A nucleons is $\sim \sqrt{N_{cfg}}e^{-A(m_N - \frac{3}{2}m_\pi)t}$

To solve this extract information from the correlators at early Euclidean time i.e. before the noise becomes dominant. Requires "better" operators for nucleons (which also increases the Wick contraction problem!).

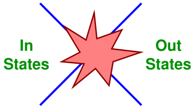
Setting the scale

Lattice quantities are computed in lattice units e.g. am_N. Convert to physical units to compare to experiment/make predictions of physical observables e.g. masses and form factors.

Choose an observable O that is relatively easy to calculate and insensitive to e.g. up and down quark masses (which may not be correct in the simulation) and match to its experimental value to determine a. This quantity is no longer a prediction!

- Stable masses e.g. M_ω, M_K
- Force between static quarks: $F(r) = -\frac{B}{r^2} + \sigma$ and $r_0^2 F(r_0) = 1.65$ with $r_0 \sim 0.5 fm$ from experiment/phenomenology of charmonium bottomonium systems.
- Wilson flow. A new idea that is precisely and easily calculated from the gauge action.

Many reasonable choices and discretisation errors mean there is some uncertainty from this procedure.



7. Working in Euclidean time.

- Scattering matrix elements not directly accessible from Euclidean QFT [*Maiani-Testa theorem*]. Scattering matrix elements: asymptotic $|\text{in}\rangle$, $|\text{out}\rangle$ states: $\langle \text{out}|e^{i\hat{H}t}|\text{in}\rangle \longrightarrow \langle \text{out}|e^{-\hat{H}t}|\text{in}\rangle$. Euclidean metric: project onto ground state. Analytic continuation of numerical correlators an ill-posed problem.

Lüscher and generalisations of: method for indirect access. See more on this later.

8. Quenching

- A computational expedient to set $\det M = 1$ in gauge configuration generation.
- Rarely necessary now, results in a non-unitary theory so not a good approximation of nature.
- Sometimes useful for investigating new methods.

No longer an issue: Simulations with $N_f = 2,\ 2+1,\ 2+1+1$.

Two strategies for progress

In lattice calculations there are complementary efforts

Gold-plated quantities

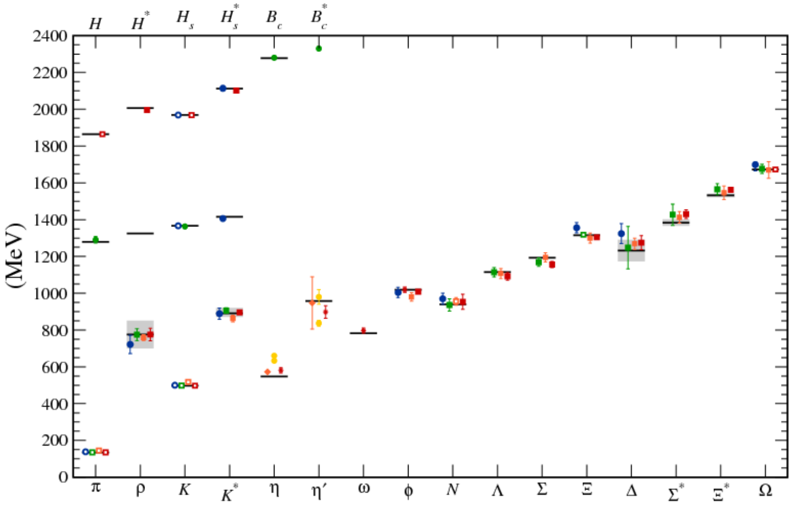
- e.g. single hadron states, or decays below thresholds
- phenomenologically relevant
- incremental progress
- robust/well-tested methods
- careful error budgeting

New directions

- new ideas - theoretical and algorithmic that open new avenues
- recent examples are scattering states, nuclear physics, g-2, ...
- also improves gold-plated
- pioneering, error budgets not yet "robust"

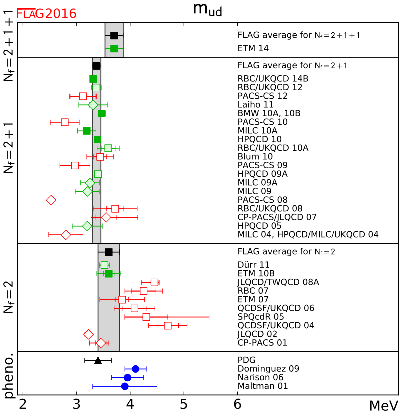
- Look at "gold-plated" results first
- Review new ideas for pioneering calculations next.

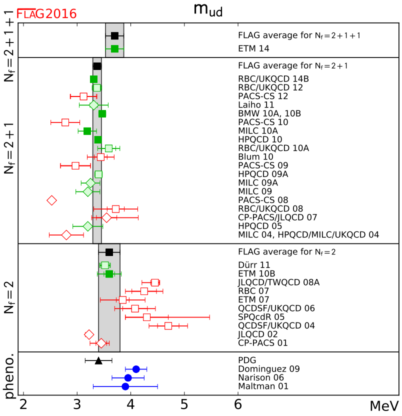
Strategies for progress: gold plated quantities - a selection



A. Kronfeld, Ann.Rev.Nucl.Part.Sci. 62 (2012)

Strategies for progress: gold plated quantities - a selection





FLAG 2013 itpwiki.unibe.ch/flag/

- Stable single-hadron states, below thresholds
- Including continuum extrapolation, realistic quark masses, renormalisation etc

Summary

- Reviewed lattice results showing convergence of results from different methods.
- Understood how to extract information from correlators and some details of fitting.
- Discussed the effects of discretisation and consequences.
- Next: Review new ideas enabling progress and recent results.