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Lattice QCD for hadron and nuclear physics: new (and old) ideas for better measurements

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Lecture Plan

- Key ideas to enable current and future physics programmes
  - Smearing - an (old) and good idea
  - Distillation - for quark propagation
  - Spin identification - as discussed earlier
- Recent results

The traditional idea - point propagators

Quark propagation from orgin to all sites on the lattice.

For better simulations of hadronic quantities look again at the building blocks: the quark propagators

Point propagator pros

- doesn't require vast computing resources

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

Point propagator cons

- restricts the accessible physics
    - flavour singlets and condenstates impossible: quark loops need props w sources everywhere in space
- restricts the interpolating basis used
    - a new inversion needed for every operator that is not restricted to a single lattice point
- entangles propagator calculation and operator construction
- throws away information encoded in configurations

Solutions?

- Improve the determination point props to access the physics of interest: smearing
- Compute all elements of the quark propagator: all-to-all propagators. Problem It's expensive - needs an unrealistic number of inversions.
- Work around: Use stochastic estimators (with variance reduction). *[I won't talk about it here but see refs for details]*
- *or* Rethink the problem: combine smearing and propagation ie distillation

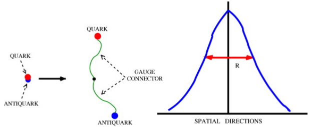
I am picking a few methods to focus on.
See references at the end of this lecture for full descriptions of these and other methods.

Smearing

Smearing techniques

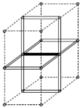
- Hadrons are extended objects ($\mathcal{O}(1) fm$).
- So far the propagator and interpolating fields (operators) are point sources
  - they can have small overlap with the state of interest: quantified by $\mathcal{Z}_n$: ($\langle n | O_M | 0 \rangle$).
  - optimise the projection onto the state we want to study
- Gauge-invariant smearing of quark fields:

$$\Psi(\vec{x}, t) = \sum_{\vec{y}} F(\vec{x}, \vec{y}, U(t)) \Psi(\vec{y}, t)$$



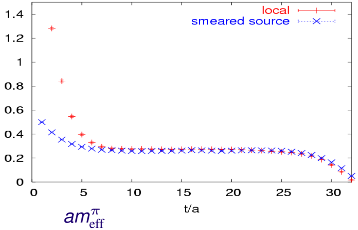
- Gaussian smearing: $F(\vec{x}, \vec{y}, U(t)) = (1 + \kappa_s H)^{n_\sigma}$ and H is the lattice realisation of the covariant Laplacian in 3d
- Variations on a theme: Jacobi, Wuppertal ...
- More improvements to gauge noise by smearing the U fields in F:

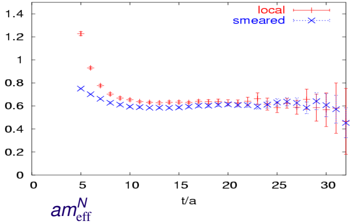
APE, HYP, Stout



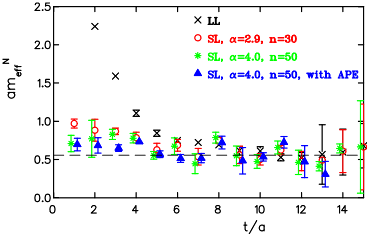
Examples of effective mass plots

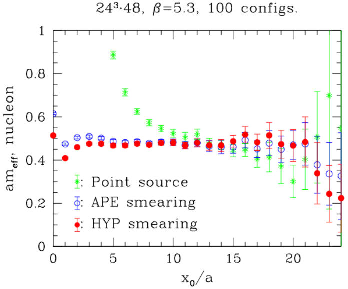
- Quenched at about 550 MeV pions:





- Reduce gauge noise by using APE, hypercubic or stout smearing on the links U that enter the smearing function $F(\vec{x}, \vec{y}, U(t))$.
- $N_F = 2$





Smearing

- **Smeared field:** $\tilde{\psi}$ from ψ, the "raw" quark field in the path-integral:

$$\tilde{\psi}(t) = \square[U(t)] \;\; \psi(t)$$

- Extract the essential degrees-of-freedom.
- Smearing should preserve symmetries of quarks.
- Now form creation operator (e.g. a meson):

$$O_M(t) = \bar{\tilde{\psi}}(t)\Gamma\tilde{\psi}(t)$$

- Γ: operator in $\{\underline{s}, \sigma, c\} \equiv \{\text{position,spin,colour}\}$
- Smearing: overlap $\langle n|O_M|0\rangle$ is large for low-lying eigenstate $|n\rangle$

Can redefining smearing help?

- Computing quark propagation in configuration generation and observable measurement is expensive.
- Objective: extract as much information from correlation functions as possible.

Two problems:

1. Most correlators: signal-to-noise falls exponentially
2. Making measurements can be costly:
   - Variational bases
   - Exotic states using more sophisticated creation operators
   - Isoscalar mesons
   - **Multi-hadron states**

- Good operators are **smeared**; helps with problem 1, can it help with problem 2?

Gaussian smearing

- To build an operator that projects effectively onto a low-lying hadronic state need to use **smearing**
- Instead of the creation operator being a direct function applied to the fields in the lagrangian first smooth out the UV modes which contribute little to the IR dynamics directly.
- A popular gauge-covariant smearing algorithm — Gaussian smearing: Apply the linear operator

$$\Box_J = \exp(\sigma \nabla^2)$$

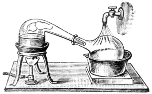
- ∇^2 is a lattice representation of the 3-dimensional gauge-covariant laplace operator on the source time-slice

$$\nabla^2_{x,y} = 6\delta_{x,y} - \sum_{i=1}^{3} U_i(x)\delta_{x+\hat{\imath},y} + U_i^\dagger(x-\hat{\imath})\delta_{x-\hat{\imath},y}$$

- Correlation functions look like $\mathrm{Tr}\ \Box_J M^{-1} \Box_J M^{-1} \Box_J \ldots$

DISTILLATION [0905.2160]

"*distill*: to extract the quintessence of" [OED]



- Distillation: **define** smearing to be explicitly a very low-rank operator. Rank is $N_{\mathcal{D}} (\ll N_s \times N_c)$.

Distillation operator

$$\square(t) = V(t) V^{\dagger}(t)$$

with $V^{a}_{\underline{x},c}(t)$ a $N_{\mathcal{D}} \times (N_s \times N_c)$ matrix

- Example (used to date): $\square_{\triangle}$ the **projection operator into $\mathcal{D}_{\triangle}$, the space spanned by the lowest eigenmodes of the 3-D laplacian**
- Projection operator, so idempotent: $\square_{\triangle}^2 = \square_{\triangle}$
- $\lim_{N_{\mathcal{D}} \to (N_s \times N_c)} \square_{\triangle} = I$
- Eigenvectors of ∇^2 not the only choice...
- Using eigenmodes of the gauge-covariant laplacian preserves lattice symmetries.

Distillation

- Distillation: a redefinition of smearing as **explicitly** a low-rank operator.
- Effect: project out eigenmodes that do not contribute to hadronic physics.
- In the low-rank space M^{-1} can be calculated exactly.

- Consider an isovector meson two-point function with $\{\underline{s}, \sigma, c\}$ for position, spin, colour.

$$C_M(t_1 - t_0) = \langle\langle \bar{u}(t_1)\Box_{t_1}\Gamma_{t_1}\Box_{t_1} d(t_1)\ \bar{d}(t_0)\Box_{t_0}\Gamma_{t_0}\Box_{t_0} u(t_0)\rangle\rangle$$

- Integrating over quark fields yields

$$C_M(t_1 - t_0) = \langle \mathrm{Tr}_{\{\underline{s},\sigma,c\}} \left(\Box_{t_1}\Gamma_{t_1}\Box_{t_1} M^{-1}(t_1, t_0)\Box_{t_0}\Gamma_{t_0}\Box_{t_0} M^{-1}(t_0, t_1)\right)\rangle$$

- Substituting the low-rank distillation operator $\Box$ reduces this to a **much smaller** trace:

$$C_M(t_1 - t_0) = \langle \mathrm{Tr}_{\{\sigma,\mathcal{D}\}} \left[\Phi(t_1)\tau(t_1, t_0)\Phi(t_0)\tau(t_0, t_1)\right]\rangle$$

- $\Phi^{\alpha,a}_{\beta,b}$ and $\tau^{\alpha,a}_{\beta,b}$ are $(N_\sigma \times N_\mathcal{D}) \times (N_\sigma \times N_\mathcal{D})$ matrices.

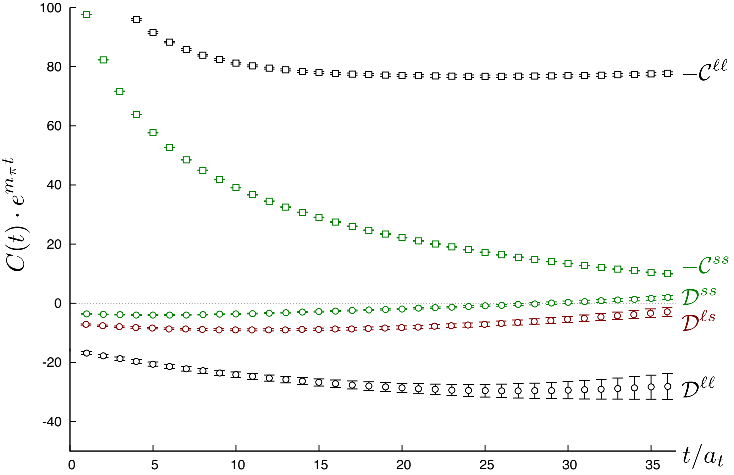
$$\Phi(t) = V^\dagger(t)\Gamma_t V(t)$$

$$\tau(t, t') = V^\dagger(t)M^{-1}(t, t')V(t')$$

The "perambulator"

Good news: precision spectroscopy (2)

Isoscalar mesons

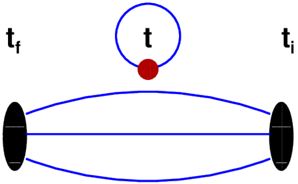


- Correlation functions for $\bar{\psi}\gamma_5\psi$ operator, with different flavour content (s, l).
- 16^3 lattice (about 2 fm). [arXiv:1102.4299]

Limitation

- Distillation does not give direct access to all modes of the Dirac operator, only those low-modes relevant for spectroscopy
- Cannot use the method to calculate eg the strangeness content of the nucleon.

$$\langle N(t_f, \vec{q})| \sum_x e^{-i\vec{q}\cdot\vec{x}} \bar{s}(t', \vec{x}) \Gamma s(t', \vec{x}) |N(0, \vec{0})\rangle$$



- Use standard all to all instead.

Bad news: the bill!

- For constant resolution distillation space scales with N_s
- The cost of a calculation scales with V^2

The problem:

- To maintain constant resolution, need $N_{\mathcal{D}} \propto N_s$
- **Budget:**

Fermion solutions	construct τ	$\mathcal{O}(N_s^2)$
Operator constructions	construct Φ	$\mathcal{O}(N_s^2)$
Meson contractions	$\mathrm{Tr}[\Phi\tau\Phi\tau]$	$\mathcal{O}(N_s^3)$
Baryon contractions	$\bar{B}\tau\tau\tau B$	$\mathcal{O}(N_s^4)$

- Ok for reasonable lattices (eg with $N_s = 16^3$, $N_D = 64$) but scaling this to a 32^3 volume requires $N_D = 512$. Numerically costly.
- Distillation does not preclude stochastic estimation - use both for large V. [See refs for more on stochastic distillation methods and other methods.]

Interpolating Operators

The interpolating operators

- We have spent some time looking at methods for quark propagation
- What about the operators $\mathcal{O} = \bar{\Psi}_{i\alpha}(\vec{x},t)\Gamma_{\alpha\beta}\Psi_{i\beta}(\vec{x},t)$?
- The simplest objects are colour-singlet local fermion bilinears:

$$\mathcal{O}_\pi = \bar{d}\gamma_5 u,\ \mathcal{O}_\rho = \bar{d}\gamma_i u,\ \mathcal{O}_N = \epsilon^{abc}\left(u^a C\gamma_5 d^b\right) u^c,$$

$$\mathcal{O}_\Delta = \epsilon^{abc}\left(u^a C\gamma_n u d^b\right) u^c$$

or more correctly!

$$\mathcal{O}_{A_1} = \bar{d}\gamma_5 u,\ \mathcal{O}_{T_1} = \bar{d}\gamma_i u,\ \mathcal{O}_{G_1} = \epsilon^{abc}\left(u^a C\gamma_5 d^b\right) u^c,$$

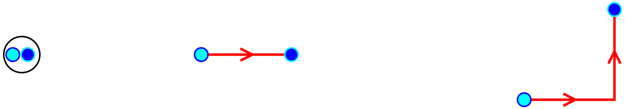
$$\mathcal{O}_H = \epsilon^{abc}\left(u^a C\gamma_n u d^b\right) u^c$$

Access to $J^{PC} = 0^{-+}, 0^{++}, 1^{--}, 1^{++}, 1^{+-}, 1/2, 3/2$

Extended operators

- We would like to access states with $J > 1$
- Would like many more operators that all transform irreducibly under some irrep enabling variational analysis.
- Lattice operators are bilinears with path-ordered products between the quark and anti-quark field; different offsets, connecting paths and spin contractions give different projections into lattice irreps.

Meson operators examples



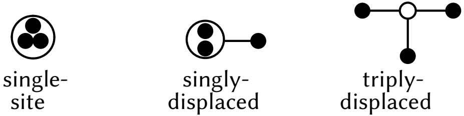
$\mathcal{O}_{\alpha\beta} = \sum_x \bar{\psi}_\alpha(x)\psi_\beta(x)$

$\mathcal{O}^{i}_{\alpha\beta} = \sum_x \bar{\psi}_\alpha(x)U_i(x)\psi_\beta(x+\hat{\imath})$

$\mathcal{O}^{ij}_{\alpha\beta} = \sum_x \bar{\psi}_\alpha(x)U_i(x)U_j(x+\hat{\imath})\psi_\beta(x+\hat{\imath}+\hat{\jmath})$

Extended baryon operators

- The same idea for baryons gives prototype extended operators

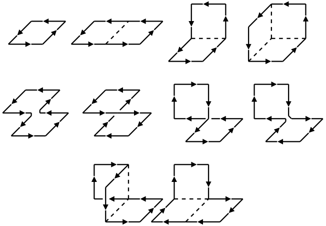


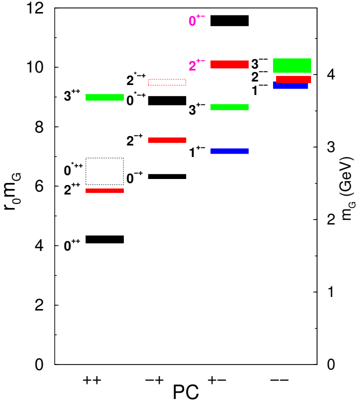
With thanks: 0810.1469

- We can make arbitrarily complicated operators in this way
- An early success was glueball calculations

Glueballs

- QCD nonAbelian ⇒ allows bound states of glue
- Candidates observed experimentally: $f_0(1370)$, $f_0(1500)$, $f_0(2220)$
- Glueballs can be calculated in lattice QCD
- The interpolating fields are purely gluonic, built from Wilson loops





Morningstar and Peardon, 1999. Quenched

Good operators

- What makes a good operator?
- An operator of definite momentum that transforms under a lattice irrep
- An operator that has strong overlap with the (continuum) state you are interested in.
- An operator is not noisy ie that produces an acceptable correlator
- Note that smearing and distillation are rotationally symmetric operations and do not change the quantum numbers.

- But recall from earlier that subduction leads to

Lattice irrep, Λ	Dimension	Continuum irreps, J
A_1	1	0, 4, ...
A_2	1	3, 5, ...
E	2	2, 4, ...
T_1	3	1, 3, ...
T_2	4	2, 3, ...
G_1	3	1/2, 7/2, ...
G_2	3	5/2, 7/2, ...
H	4	3/2, 5/2, ...

- So a correlator $C(t) = \langle 0|\phi(t)\phi^\dagger(0)|0\rangle$ contains in principle information about all (continuum) spin states subduced in Λ^{PC}.

Operator basis — derivative construction

- A closer link to (or “memory” of) the continuum would be good
- There are different approaches to optimise lattice operators. This is one.

Operator basis — derivative construction

- A closer link to (or "memory" of) the continuum would be good
- There are different approaches to optimise lattice operators. This is one.
- Start with continuum operators, built from n derivatives:

$$\Phi = \bar{\psi}\,\Gamma\left(D_{i_1} D_{i_2} D_{i_3} \dots D_{i_n}\right)\psi$$

- Construct irreps of $SO(3)$, then subduce these representations to O_h
- Now replace the derivatives with lattice finite differences:

$$D_j\psi(x) \rightarrow \frac{1}{a}\left(U_j(x)\psi(x+\hat{j}) - U_j^\dagger(x-\hat{j})\psi(x-\hat{j})\right)$$

- On a discrete lattice covariant derivative become finite displacements of quark fields connected by links

arXiV:0707.4162

EXAMPLE: $J^{PC} = 2^{++}$ MESON CREATION OPERATOR

- Trying to gain more information to discriminate spins. Consider continuum operator that creates a 2^{++} meson:

$$\Phi_{ij} = \bar{\psi}\left(\gamma_i D_j + \gamma_j D_i - \frac{2}{3}\delta_{ij}\gamma \cdot D\right)\psi$$

- Lattice: Substitute gauge-covariant lattice finite-difference D_{latt} for D
- A reducible representation:

$$\Phi^{T_2} = \{\Phi_{12}, \Phi_{23}, \Phi_{31}\}$$

$$\Phi^{E} = \left\{\frac{1}{\sqrt{2}}(\Phi_{11} - \Phi_{22}), \frac{1}{\sqrt{6}}(\Phi_{11} + \Phi_{22} - 2\Phi_{33})\right\}$$

- Look for signature of continuum symmetry:

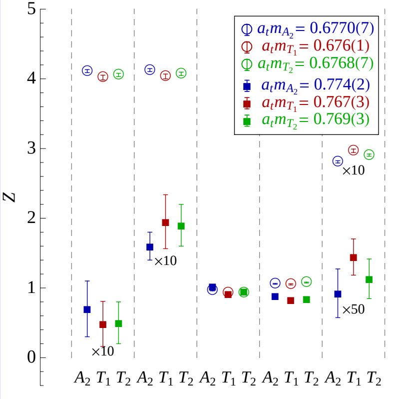
$$\mathcal{Z} = \langle 0|\Phi^{(T_2)}|2^{++(T_2)}\rangle = \langle 0|\Phi^{(E)}|2^{++(E)}\rangle$$

up to rotation-breaking effects

This idea appears to work well

E.g. in charmonium - arXiv:1204.5425

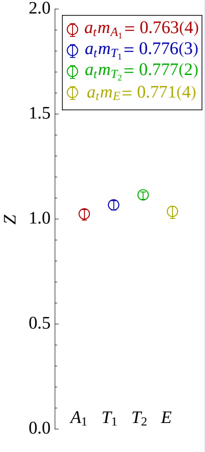
Spin-3 identification



$J = 3$ in A_2, T_1, T_2

$J = 4$ in A_1, T_1, T_2, E

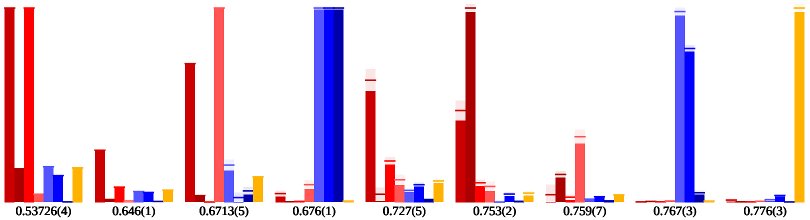
Spin-4 identification



- operators of definite J^{PC} constructed in step 1 are subduced into the relevant irrep
- a subduced irrep carries a "memory" of continuum spin J from which it was subddduced - it **overlaps** predominantly with states of this J.

J	0	1	2	3	4
A_1	1	0	0	0	1
A_2	0	0	0	1	0
E	0	0	1	0	1
T_1	0	1	0	1	1
T_2	0	0	1	1	1

- Using $Z = \langle 0|\Phi|k\rangle$, helps to identify continuum spins
- For high spins, can look for agreement between irreps
- Data below for T_1^{--} irrep, colour-coding is **Spin 1**, **Spin 3** and **Spin 4**.



Spectroscopy - selected results

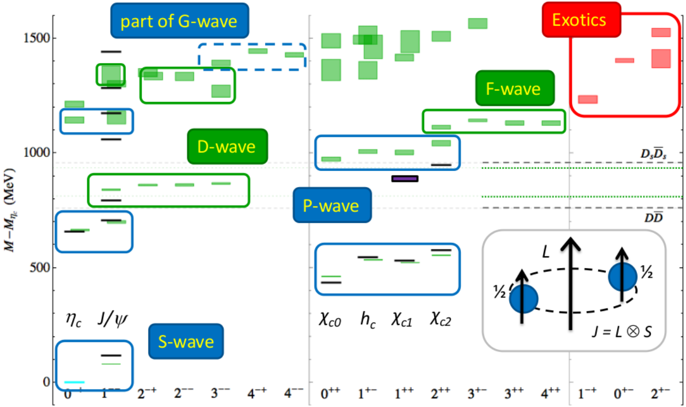
Single hadron states: Charmonium exotics

Precision calculation of high spin ($J \geq 2$) and exotic states is relatively new

Caveat Emptor

- Only single-hadron operators
- Physics of multi-hadron states appears to need relevant operators
- No continuum extrapolation
- $m_\pi \sim 400$MeV ← already changing

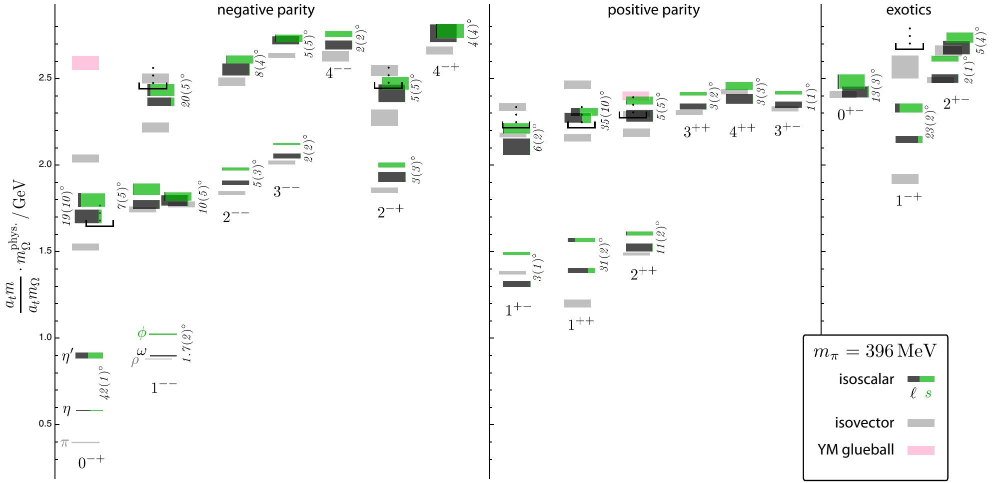
Charmonium



from HSC 2012

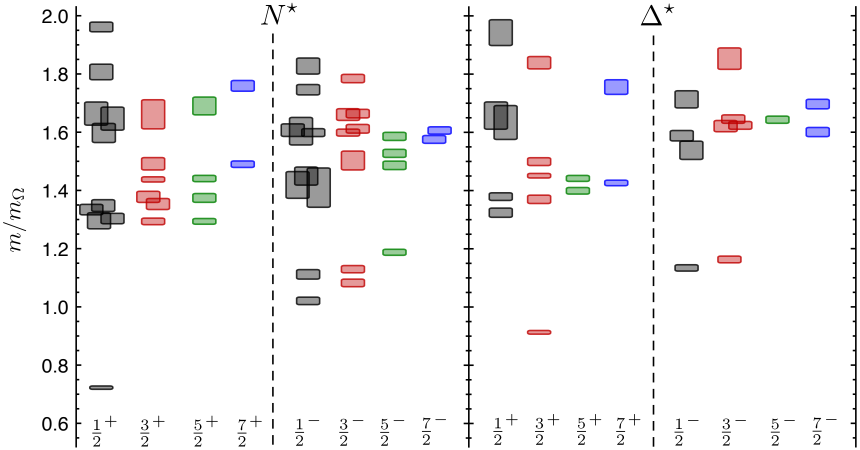
→ Expect improvements now methods established

Single-hadron states: light exotics

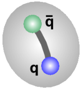
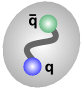


from HSC 2010

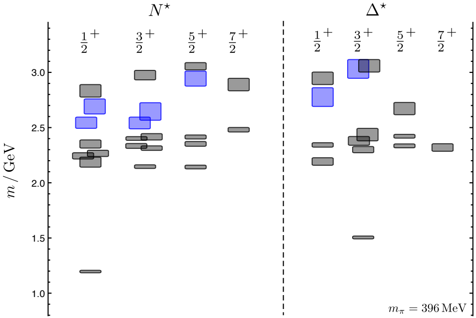
Single-hadron states: baryons @ 396MeV



from HSC 2011

Hybrids  

Expect a large overlap with operators $\mathcal{O} \sim F_{\mu\nu}$



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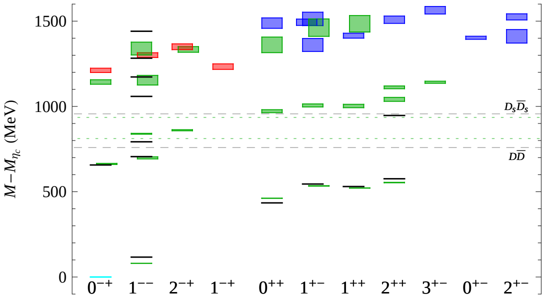
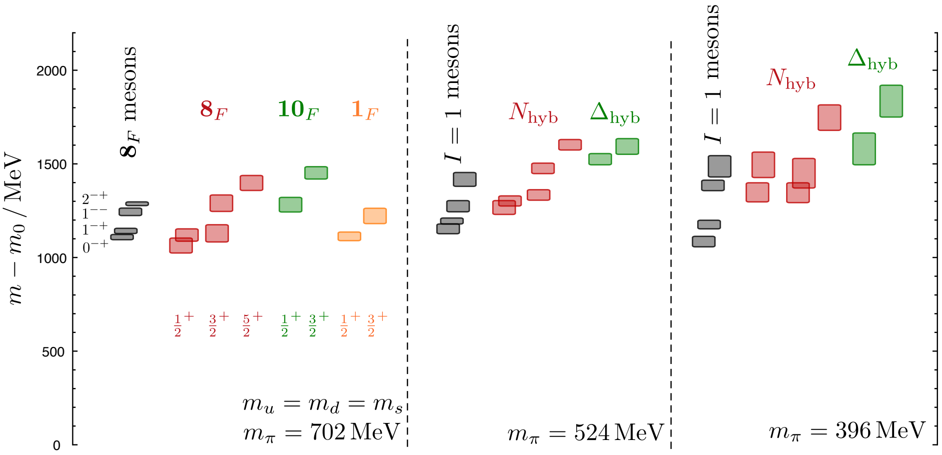


$c\bar{c}$ *from HSC*

Lightest hybrid supermultiplet and excited hybrid supermultiplet same pattern and scale in meson and baryon, heavy and light[*HadSpec*:1106.5515] sectors.

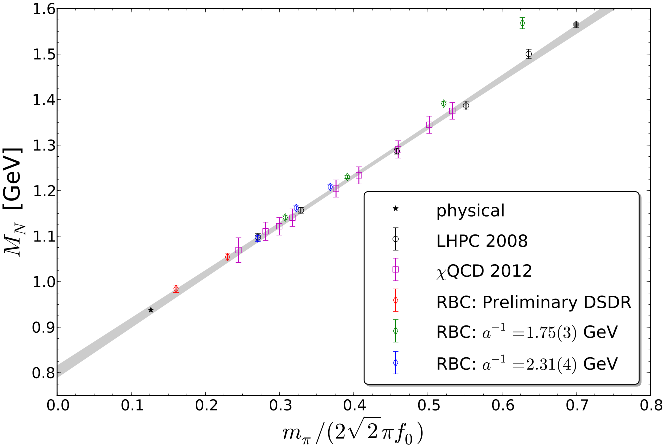
Energy scale for hybrids



$m_0 = m_\rho$ for mesons and $m_0 = m_N$ for baryons.

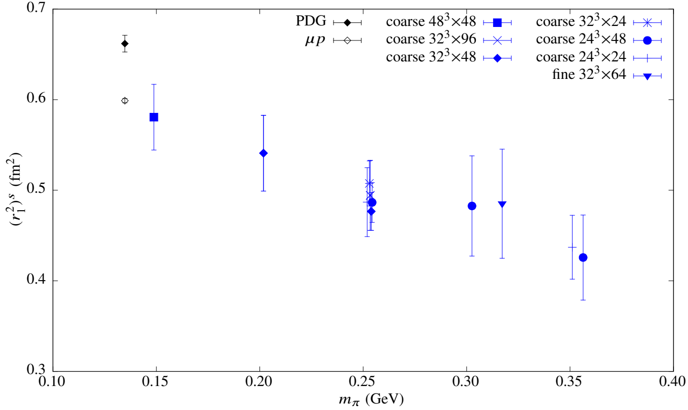
The nucleon mass - unexpected behaviour!

A. Walker-Loud @Lat2014



- A **ruler plot** ie linear in quark mass
- Taking this seriously then $M_N(MeV) = \alpha_0^N + \alpha_1^N m_\pi = 800 + m_\pi$ parameterises the numerial results in the available range and agrees with the physical point!
- But it predicts the wrong quark mass dependence at/near the chiral limit.

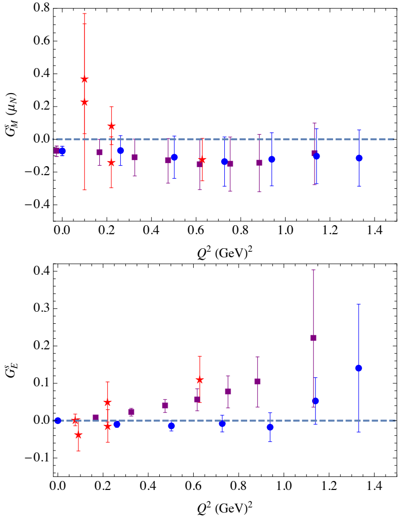
Nucleon size with physical quark masses

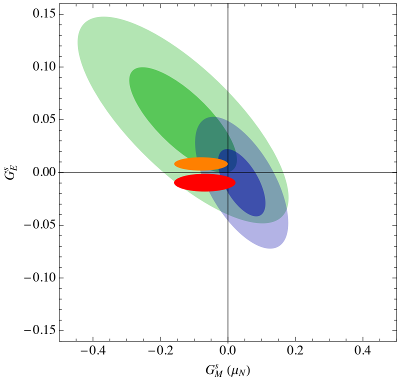


- LHPC 2014 at multiple lattice spacings & volumes and physical pion masses.

Nucleon strangeness - snapshot of activity

- needs disconnected diagrams - distillation not suitable so other all-to-all methods needed.

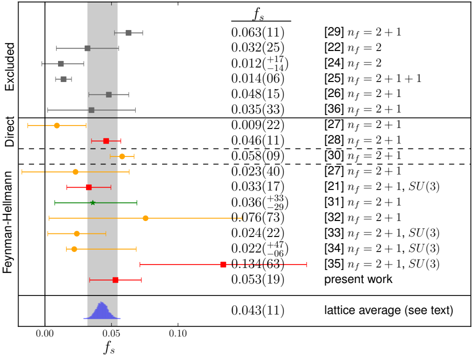




Shanahan et al 1403.6537: deducing disconnected effects from experiment and lattice data. Direct calculations underway.

A COMPLILATION - NUCLEON STRANGENESS

From Junnakar & Walker-Loud (PRD.87 (2013))



Their average: $m_s\langle N|\bar{s}s|N\rangle = 48 \pm 10 \pm 15 MeV$ and $f_s = 0.051 \pm 0.011 \pm 0.016$.

Summary

- New ideas are enabling rapid progress.
- Lots of precision and pioneering calculations of hadronic and nuclear quantities.
- Next - multi-hadron, many-body systems. A rapidly moving field!

References

- APE smearing APE collaboration, M. Albanese et al., *Glueball masses and string tension in lattice QCD*, Phys. Lett. B192 (1987) 163.
- Hyper-cubic (HYP) smearing A. Hasenfratz and F. Knechtli, *Flavor symmetry and the static potential with hypercubic blocking*, Phys. Rev. D64 (2001) 034504.
- Stout-link smearing C. Morningstar and M.J. Peardon, *Analytic smearing of SU(3) link variables in lattice QCD*, Phys. Rev. D69 (2004) 054501.
- All-to-all propagators Foley et al, hep-lat/0505023 and references 1-13 therein.
- Distillation Peardon et al, arXiV:0905.2160
- Stochastic distillation: LaPH, Morningstar et al, arXiv:1104.3870
- All mode averaging (AMA), Shintani et al, arXiv:1402.0244