Quantum Field Theory on the Lattice

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The Standard Model of particle physics

The constituents are three families of fermions having spin 1/2:

Quarks			
flavor	name	mass $[\mathrm{GeV/c^2}]$	electric charge
uuu	up	0.003	2/3
ddd	down	0.006	-1/3
ccc	charm	1.3	2/3
sss	strange	0.1	-1/3
ttt	top	175	2/3
bbb	bottom	4.3	-1/3

Leptons			
flavor	name	mass $[\mathrm{GeV/c^2}]$	electric charge
ν_e	electron neutrino	$< 10^{-8}$	0
e	electron	0.00511	-1
ν_μ	muon neutrino	< 0.0002	0
μ	muon	0.106	-1
ν_τ	tau neutrino	< 0.02	0
τ	tau	1.777	-1

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- The constituents interact with each other by exchanging gauge bosons, the force carriers, which have spin 1

force	symbol	name	mass [GeV/c^2]	electric charge
strong	g	gluon	0	0
e-m	γ	photon	0	0
weak	W^-	W-boson	80.4	-1
	W^+	W-boson	80.4	+1
	Z^0	Z-boson	91.187	0

- The strong force (or color force) acts only on quarks and gluons, which both carry color charge. It binds, for example, the three quarks that make up a proton and neutron together. The residual strong force also holds the nucleons in a nucleus together.
- The electro-magnetic force acts on all particles that carry electric charge. It binds, for example, the electrons in an atom to the nucleus.
- The weak force causes, for example, beta-decay of radioactive nuclei.
- For two u-quarks, a distance of 3 × 10−17 m apart, the relative strength of the three forces strong, electro-magnetic and weak is. 60:1:10−4 [:10−41].
- For comparison I also included the gravitational force. In particle physics, the gravitational force is certainly negligibly small.

Path integrals (Minkowski space)

- In Quantum Mechanics the probability amplitude for a particle to move from y to x in d dimensions within time t is

$$\langle x | e^{-iHt} | y \rangle$$

- And $H = H_0 + V(x)$ and potential $V(x)$. For a free particle $H_0 = p^2/2m$

$$\langle x | e^{-iH_0 t} | y \rangle = \int dp \langle x | p \rangle \exp\left\{ -i\frac{p^2}{2m}t \right\} \langle p | y \rangle$$

$$= \int \frac{dp}{2\pi} e^{ip(x-y)} \exp\left\{ -i\frac{p^2}{2m}t \right\}$$

$$= \left(\frac{m}{2\pi i t} \right)^{1/2} \exp\left\{ i\frac{m}{2t}(x-y)^2 \right\}$$

- The time evolution operator (transfer matrix) for small ε can be approximated by

$$U_\epsilon = \exp(-iH\epsilon) \quad \approx \quad W_\epsilon = \exp(-iV\frac{\epsilon}{2})\exp(-iH_0\epsilon)\exp(-iV\frac{\epsilon}{2})$$

Path integrals (2)

- Inserting N – 1 complete set of position eigenstates:

$$\langle x|e^{-iHt}|y\rangle = \lim_{N\to\infty}\int dx_1\ldots dx_{N-1}\langle x|W_\epsilon|x_1\rangle\ldots\langle x_{N-1}|W_\epsilon|y\rangle$$

$$= \left(\frac{m}{2\pi i\epsilon}\right)^{1/2}\int dx_1\ldots dx_{N-1}\times \exp(i\frac{m}{2\epsilon}\left[(x-y)^2+\ldots+(x_{N-1}-y)^2\right]$$

$$-i\epsilon\left[\frac{1}{2}V(x)+V(x_1)+\ldots+V(x_{N-1})+\frac{1}{2}V(y)\right])$$

- This last term can be rewritten for small ε

$$S=\int_0^t dt'\left[\frac{m}{2}\dot{x}^2-V(x)\right]$$

- and the amplitude (path integral)

$$\langle x|e^{-iHt}|y\rangle = \int \mathscr{D}x e^{iS}$$

- With the measure

$$\mathscr{D}x = \lim_{N\to\infty}\left(\frac{m}{2\pi i\epsilon}\right)^{1/2} dx_1\ldots dx_{N-1}$$

- Amplitude widely oscillating from “i”. Not well defined but used formally

Path integrals in Euclidean Space

- In “imaginary” time t = −iτ, τ > 0 we have

$$\langle x | e^{-H\tau} | y \rangle = \int \mathcal{D}x e^{S_E}$$

$$S_E = \int_0^\tau d\tau' \left[\frac{m}{2} \dot{x}^2 + V(x) \right]$$

- where $S = iS_E$. Note evolution operator well defined bounded operator. Consider some operator A. Then

$$\mathrm{Tr}\left(e^{-H\tau} A\right) = \sum_{n=0}^{\infty} e^{-E_n \tau} \langle n | A | n \rangle$$

$$Z(\tau) = \mathrm{Tr}\left(e^{-H\tau}\right) = \sum_{n=0}^{\infty} e^{-E_n \tau}$$

- For large τ the n = 0 term dominates, hence the ground state expectation value of A is

$$\langle 0 | A | 0 \rangle = \lim_{\tau \to \infty} \frac{1}{Z(\tau)} \mathrm{Tr}\left(e^{-H\tau} A\right)$$

Path integrals (2)

- With
$$\mathbf{x}(\tau) = e^{H\tau}\mathbf{x}e^{-H\tau}$$
- correlation functions are

$$\langle x(\tau_1)\ldots x(\tau_n)\rangle \equiv \langle 0\,|\,\mathbf{x}(\tau_1)\ldots\mathbf{x}(\tau_n)\,|\,0\rangle$$

$$= \langle 0\,|\,e^{E_0\tau_1}\mathbf{x}e^{-H(\tau_1-\tau_2)}\mathbf{x}\ldots\mathbf{x}e^{-H(\tau_{n-1}-\tau_n)}\,|\,0$$

$$= \lim_{\tau\to\infty}\frac{1}{Z(\tau)}\int dx\langle x\,|\,e^{-H(\tau/2-\tau_1)}\mathbf{x}e^{-H(\tau_1-\tau_2)}\mathbf{x}\ldots e^{-H(\tau_n+\tau/2)}\,|\,x\rangle$$

$$= \lim_{\tau\to\infty}\frac{1}{Z(\tau)}\int \mathscr{D}x\; x(\tau_1)\ldots x(\tau_n)e^{-S_E[x(\tau)]}$$

- Note, Schro¨dinger equation in Euclidean space is
$$\frac{\partial}{\partial\tau}\psi_E(x,\tau) + H\psi_E(x,\tau) = 0$$
- The Euclidean path integral is an average over random paths suitably weighted. It looks like a partition function (functional integral) with a Boltzmann weight S_E
  - **4-D STATISTICAL MECHANICS!!**

Euclidean Quantum Field Theory

- The path integral for a quantum theory follows that of Quantum Mechanics. For example, for a Euclidean scalar field with 4-vector coordinate x

$$\phi(x) = e^{Hx^4}\phi(\mathbf{x},0)e^{-Hx^4}$$

- Treat Euclidean fields as random variables, whose expectation values yield correlation functions. The probability distribution is

$$\langle F[\phi]\rangle = \int d\mu\ F[\phi]$$

- with action $S[\phi]$ and measure

$$d\mu = \frac{1}{Z}e^{-S[\phi]}\prod_x d\phi(x)\,.$$

- For a general action, the n-pt functions are

$$\langle\phi(x_1)\ldots\phi(x_n)\rangle = G(x_1,\ldots,x_n)$$

- By Wick's theorem we have

$$\begin{aligned}\langle\phi(x_1)\phi(x_2)\rangle &= G(x_1,x_2),\\ \langle\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_2)\rangle &= G(x_1,x_2)G(x_3,x_4)+G(x_1,x_3)G(x_2,x_4)+G(x_1,x_4)G(x_2,x_3),\end{aligned}$$

- For a quadratic scalar field action $S = \phi^\dagger(x)D\phi(x)$ and D possibly functions of other fields, we have $D\ G(x,y) = \delta(x-y)$. For example, for a free scalar field, $D = \Box + m^2$

- The $G(x,y)$ are propagators and are the inverse of an operator.

Statistical mechanics

- Problem is a 4D statistical mechanical problem. Want physical masses constant in limit of lattice spacing $a \to 0$.
- Use theory of phase transitions and determine critical exponents, etc.
- Can define (?) a continuum theory where there is a diverging length scale ξ because $\xi \sim 1/ma$ – a second order phase transition.
- Also diverging length scale in chiral limit (of QCD) $mq \to 0$ because of $1/m_\pi a$.
- Have combination of finite volume (lattice size), lattice spacing, and quark-mass extrapolation systematic-errors.

Quantum Electro-Dynamics

- The familiar Maxwell equations for electric and magnetic fields (in units where c = h/2π = 1, c the speed of light, h Planck's constant

$$\vec{\nabla} \cdot \vec{E} = \rho \ , \qquad \vec{\nabla} \times \vec{B} - \frac{\partial \vec{E}}{\partial t} = \vec{j}$$

- can be written in a relativistic covariant form $x_0 = t$, $\partial_\mu = \frac{\partial}{\partial x_\mu}$, $E_i = F_{0i}$,

$$B_i = \frac{1}{2} \sum_{jk=1}^{3} \epsilon_{ijk} F_{jk}, \; j_0 = \rho$$

$$\partial_\mu F_{\mu\nu}(x) = j_\nu(x) \ , \qquad F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)$$

- The covariant form of the Dirac equation is

$$Dslash\psi(x) \equiv \sum_\mu \gamma_\mu \left[\partial_\mu + ieA_\mu(x) \right] \psi(x) = 0$$

- Gauge invariance under a local finite transformation $\Lambda(x)$

$$A_\mu(x) \to \Lambda(x) A_\mu(x) \Lambda^{-1}(x) - \frac{i}{e} \Lambda(x)(\partial_\mu \Lambda^{-1}(x)) \psi(x) \to \Lambda(x)\psi(x)$$
$$\psi(x) \to \Lambda(x)\psi(x)$$

$$F_{\mu\nu}(x) \to \Lambda(x) F_{\mu\nu} \Lambda^{-1}(x), \qquad D\psi(x) \to \Lambda(x) D\psi(x)$$

- These equations can be obtained from extremizing the action

$$S(A, \psi) = \int d^4x \left\{ \frac{1}{4} F_{\mu\nu}^2 + \bar{\psi}(x) D\psi(x) \right\}$$

- with current-charge density $j_\mu(x) = i\bar{\psi}(x)\gamma_\mu\psi(x)$. In Euclidean space, action is real

What is a gauge theory?

- Maxwell's eqns: field strength and vector potentials

$$\vec{B} = \vec{\nabla} \times \vec{A} \qquad \vec{E} = \frac{\partial}{\partial x_0}\vec{A} - \vec{\nabla} A_0$$

$$F_{\mu\nu} = \begin{pmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & B_3 & -B_2 \\ -E_2 & -B_3 & 0 & B_1 \\ -E_3 & B_2 & -B_1 & 0 \end{pmatrix} = \frac{\partial}{\partial x_\mu} A_\nu(x) - \frac{\partial}{\partial x_\nu} A_\mu(x)$$

- Action

$$S = \int d^4x \frac{1}{4} \sum_{\mu,\nu} F_{\mu,\nu} F^{\mu,\nu} = \int d^4x \frac{1}{2} \left(\vec{E}^2 + \vec{B}^2 \right)$$

$$D(A,m) = -\sum_\mu \gamma_\mu D_\mu + m, \qquad D_\mu = \partial_\mu + igA_\mu$$

- Integral - a probability density

$$\langle \mathcal{O} \rangle = \int dA(x)\, \mathcal{O}(\mathcal{A})\, e^{-S(A)}\, \det\left(D(A,m)\right)$$

QED (2)

- For a quantum theory of QED one integrates over fields $A_\mu(x)$, representing the photons, and fields ψ(x), representing the electrons, as

$$\langle \mathcal{O}(A,\psi,\bar{\psi})\rangle = \frac{1}{Z}\left\{\prod_x \int dA(x)d\bar{\psi}(x)d\psi(x)\right\}\mathcal{O}(A,\psi,\bar{\psi})\mathrm{e}^{-\frac{1}{\hbar}S(A,\psi)}$$

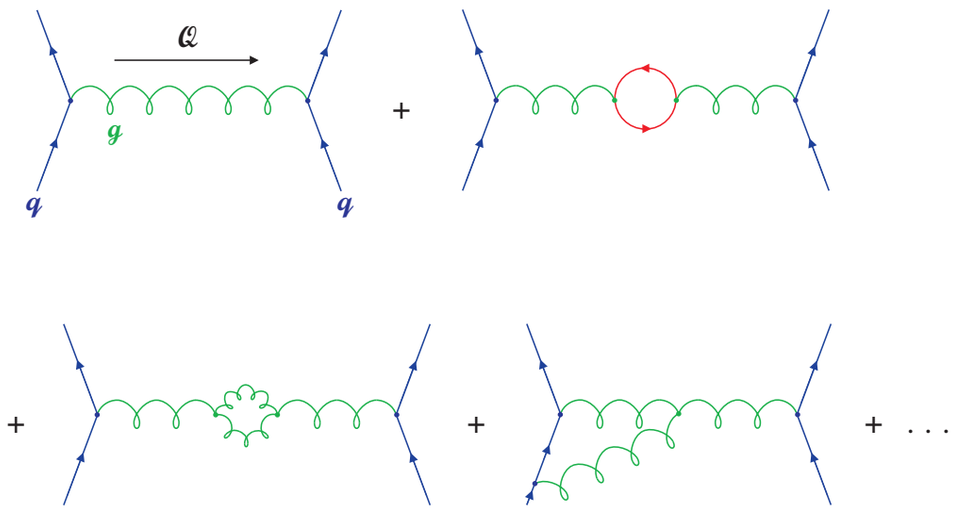
- Z is a normalization factor defined by ⟨1⟩ = 1.
- To do computations in QED, one notices that the electro-magnetic coupling constant, $\alpha = e^2/4\pi$ = 1/137.03 . . . , is small. One can therefore make expansions in powers of α. This is called perturbation theory. Predictions from perturbation theory have been verified, for example for the anomalous magnetic moment of the electron, to 1 part in 10–9!

Quantum Chromo -Dynamics

- The theory of the strong interactions, Quantum Chromo -Dynamics (QCD), is quite similar to QED. The fields ψ(x) now represent quarks, and the fields $A_\mu(x)$ represent gluons. They are now 3 × 3 matrices, $A_\mu(x) = A_\mu^k(x)\lambda_k$ and

$$F_{\mu\nu}(x) = \partial_\mu A_\mu(x) - \partial_\nu A_\mu(x) + g[A_\mu(x), A_\nu(x)]$$

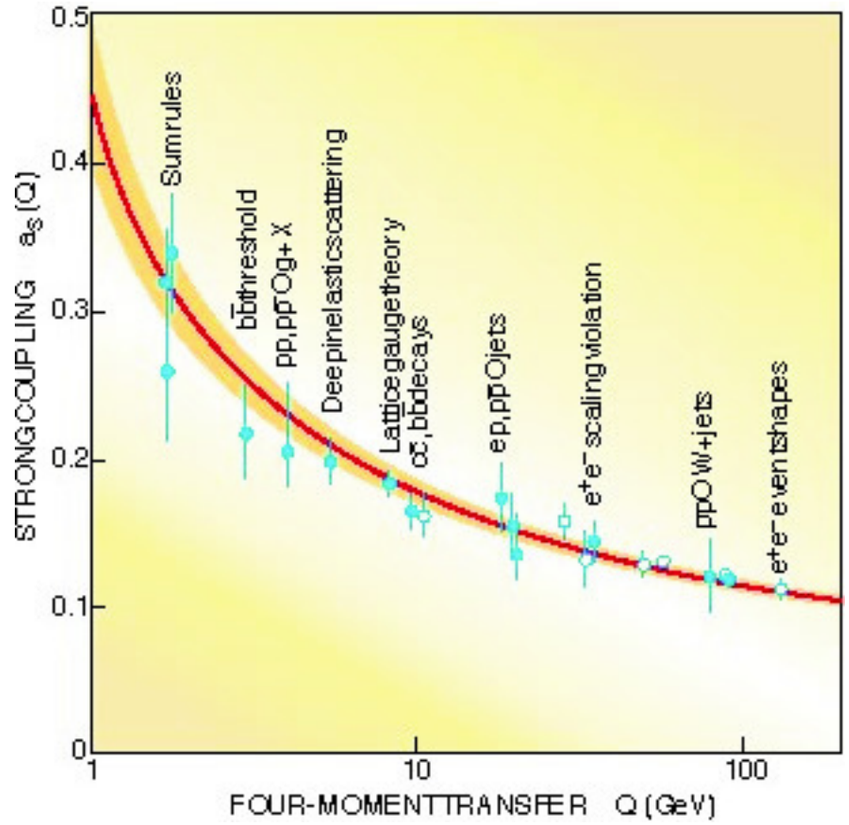
- The last term is new for QCD. As a consequence the gluons interact with each other. This leads to the peculiar property that the coupling constant $\alpha_s(E) = g^2/(4\pi)$ is
  - weak at high energies E: asymptotic freedom
    - ➡ success of perturbation theory for high energy properties



- Last two diagrams show the gluon self-interaction. They don't occur in QED.

QCD (2)

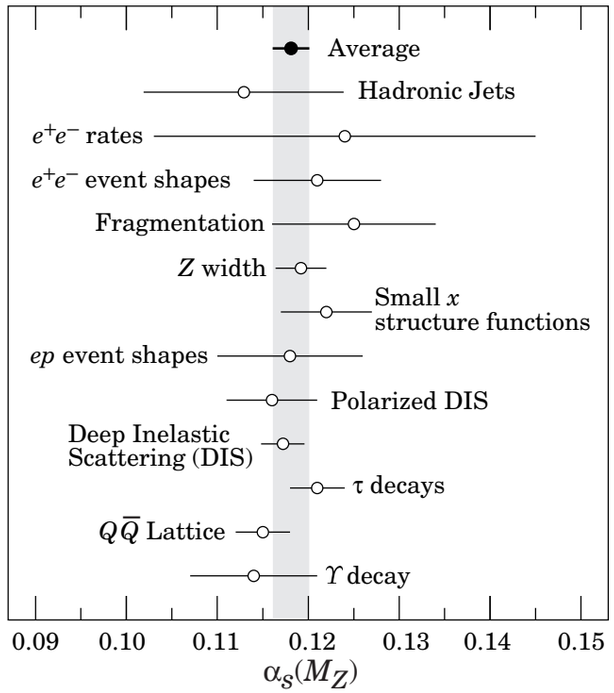
- logarithmic decrease of $\alpha_s(E) = g^2/(4\pi)$ with increasing energy



- strong at low energies (long distances)
  - ➡ confinement: quarks and gluons do not exist as free particles. They are always bound into nucleons, mesons or glueballs.
  - ➡ perturbation theory – expansion in powers of αs not applicable: ⇒ decisive test of low energy properties of QCD from first principles are only emerging
  - ➡ need non-perturbative methods of computation: lattice QCD

Strong coupling constant

- A comparison of lattice calculations of αs with experimental determinations is shown in the following figure from the Particle Data Group, D.E. Groom et al., Euro. Phys. Jour. C15 (2000) 1



- The combined lattice result is: αs (MZ) = 0.115 ± 0.003
- The complete average is: αs (MZ) = 0.118 ± 0.002

Symmetries

There are various important symmetries of the continuum that should be preserved in a lattice discretization:

- Gauge invariance: can change underlying potentials without changing physical fields, like electric and magnetic fields. Was principle used to construct “minimal” coupling theories, like QED and QCD.
- Flavor symmetry: can rotate different types or flavors of fermion fields among each other. This leads to classification of particle families.
- Chiral symmetry: can change fermion fields by an overall phase change

$$\psi(x) \to \exp(i\theta\gamma_5)\psi(x),$$
$$\bar{\psi}(x) \to \bar{\psi}(x)\exp(i\theta\gamma_5)$$

and leaves fermion action invariant

$$\bar{\psi} D \psi \equiv \bar{\psi}\gamma_\mu(\partial_\mu + igA_\mu)\psi$$

Topology of the gauge fields is intimately tied with chiral symmetry – *instantons*

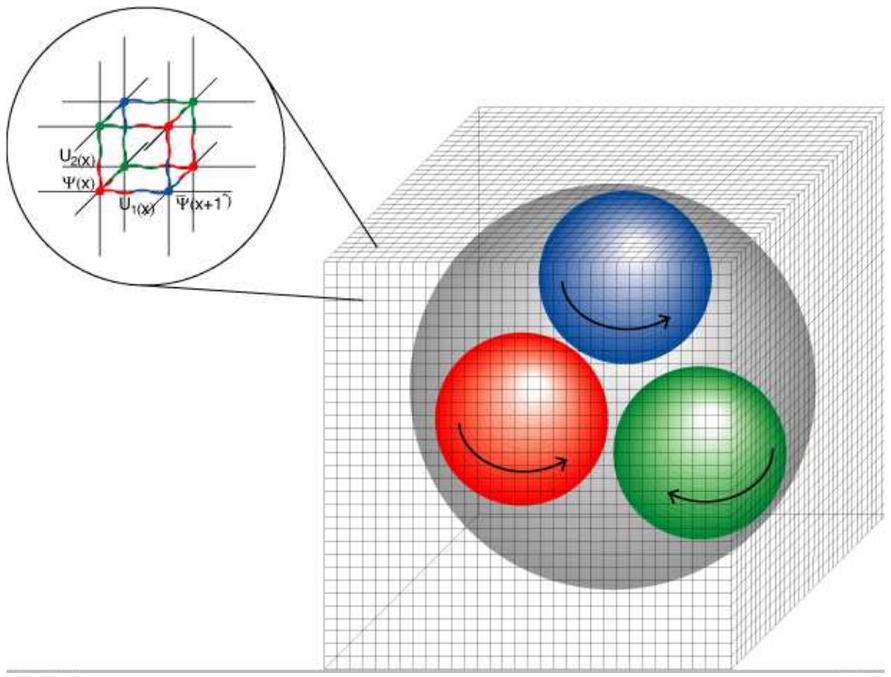
Regularization of QCD on a lattice

- We approximate continuous space-time with a 4-dim lattice, and derivatives by finite differences. Quarks are put on sites, gluons on links. They are represented by 3 × 3 complex unitary matrices $U_{x,\mu} = \exp(igaA_{x,\mu})$, elements of the group SU(3). Then

$$\langle \mathcal{O}(U,\psi,\bar{\psi})\rangle = \frac{1}{Z}\int dU_\mu d\bar{\psi} d\psi \mathcal{O}(U,\psi,\bar{\psi}) \mathrm{e}^{-S_G(U)+\bar{\psi}M(U)\psi}$$

$$= \frac{1}{Z}\int dU_\mu \mathcal{O}(U, M^{-1}(U)) \mathrm{e}^{-S_G(U)} \det M(U)$$

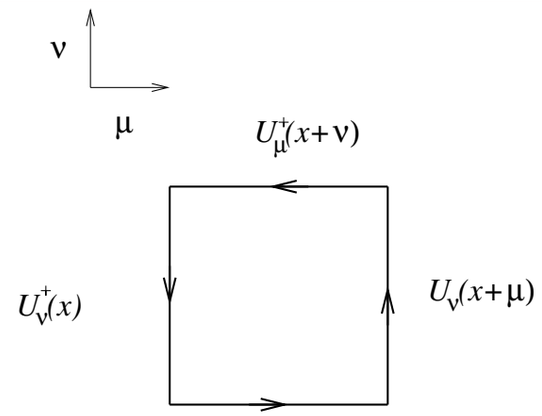
- The Gaussian integration over the anti-commuting fermion fields ψ and ψ was done, resulting in the $\det M(U))$ and $M^{-1}(U)$ factors.



Regularization

- The lattice gauge action is constructed from elementary **plaquettes**

$$U_{\Box_{\mu\nu}}(x) = U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)$$



- The gauge action is

$$S_G = \frac{2N_c}{g^2} \sum_x \sum_{\mu>\nu} \left[1 - \frac{1}{N_c} \Re \mathrm{Tr}\, U_{\Box_{\mu\nu}}(x) \right] \equiv -\frac{\beta}{N_c} \sum_x \sum_{\mu>\nu} \Re^x \mathrm{Tr}\, U_{\Box_{\mu\nu}}^{U_u(x)}$$

- where we have ignored the constant term, and introduced

$$\beta = \frac{2N_c}{g^2}$$

- with, for QCD, Nc = 3. ß assumes the rˆole of inverse temperature.
- Exercise: Show that

$$S_G = \frac{1}{4} \int d^4x \, F^a_{\mu\nu} F^a_{\mu\nu} + \mathcal{O}(a^2),$$

- i.e. that the lattice gauge action has O(a2) discretisation errors.
- Gauge invariance: the action is invariant under

$$U_\mu(x) \to V(x) U_\mu(x) V(x+\hat{\mu})^\dagger$$

Static Quark Potential

- Example: relate the static quark potential to Wilson loops. Consider $\Psi^{(n)}$ a complete set of eigenv. of

$$H\Psi^{(n)} = E_n \Psi^{(n)}$$

- The energy E0 of the ground state depend on static quark locations x and y and relative distance R. Thus

$$V(R) \equiv E_0$$

- For an arbitrary state Ψ

$$\langle \Psi | e^{-TH} | \Psi \rangle = \sum_n |\langle \Psi^{(n)} | \Psi \rangle|^2 e^{-TE_n} \quad \overrightarrow{T \to \infty} \quad |\langle \Psi^{(0)} | \Psi \rangle|^2 e^{-TE_0}$$

- For the test-function acting on some vacuum wave function Ω

$$\Psi_{\alpha\beta} = U_{\alpha\beta}(\mathbf{x}, \mathbf{y})\Omega$$

- we obtain

$$\langle \Psi | e^{-TH} | \Psi \rangle = \frac{1}{Z} \int \prod_b dU(b) \mathrm{Tr}\Big(\prod_{b \in loop} U(b) \Big) e^{-S(U)} = W(R,T) \ .$$

- Therefore,

$$V(R,T) = -\lim_{T\to\infty} \frac{1}{T} \log W(R,T)$$

Static quark potential (2)

- Consider strong coupling expansion of the pure gauge action around ß = 0. Compute

$$W(R,T) = \frac{1}{Z}\int \prod dU e^{-S_G(U)} \prod_b U(b),$$
$$S_G = -\frac{\beta}{N_c}\sum_x \sum_{\mu>\nu} \Re \,\mathrm{Tr}\, U_{\square_{\mu\nu}},$$

- Use the identity

$$\int dU \ \mathrm{Tr}(UV_1)\,\mathrm{Tr}(U^{-1}V_2) \ = \ \frac{1}{N}\mathrm{Tr}(V_1V_2), \qquad \int dU \ = \ 1$$

- For the case of a 1 × 2 rectangle

$$W(R,T) = \frac{1}{Z}\int \prod dU\ [1 + \frac{\beta}{N_c}\sum_p \mathrm{Tr}U_p \ + \frac{1}{2}\frac{\beta^2}{N_c^2}\sum_{p_1}\mathrm{Tr}U_{p_1}\sum_{p_2}\mathrm{Tr}U_{p_2} \ + \ldots]\ \mathrm{Tr}U_{1,2}$$
$$= \frac{\beta^2}{4N_c^4}$$

- In general the only non-zero term comes from tiling the loop. So,

$$W(R,T) = \left(\frac{\beta}{2N_c^2}\right)^{RT} = e^{-\alpha_0 RT}, \quad \alpha_0 = -\log\left(\frac{\beta}{2N_c^2}\right)$$

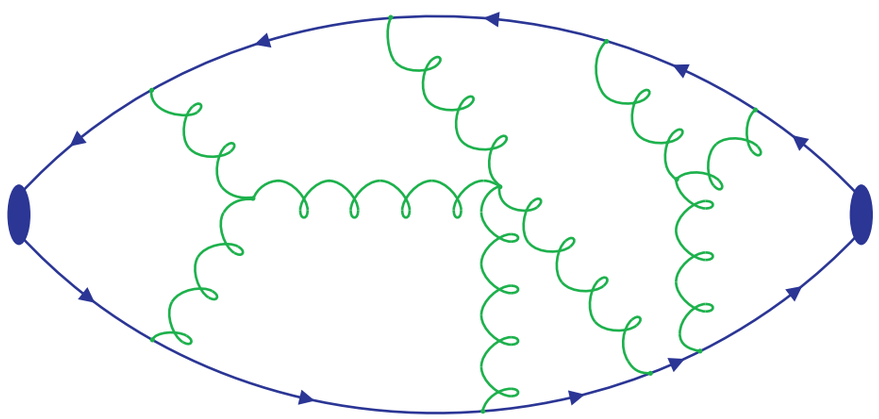
- This is an area law indicating confinement.

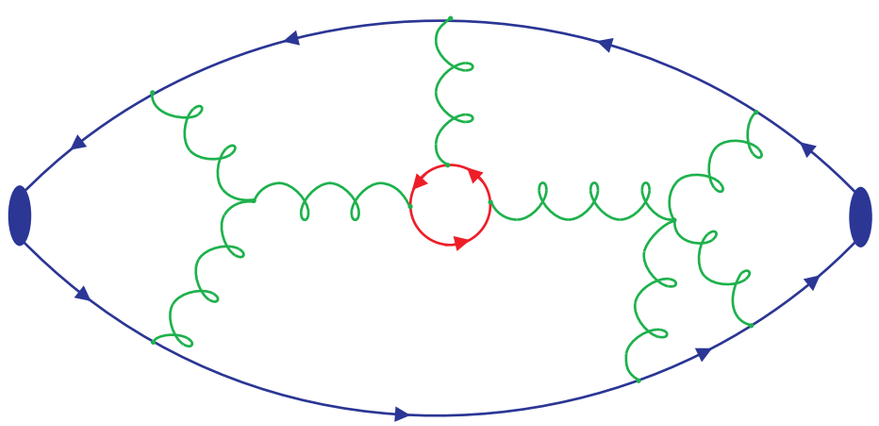
Monte Carlo method

- On a finite lattice we need to compute the integral over a finite, but large, number of U-fields. This can be done numerically, though not by direct integration.
- One uses the stochastic Monte Carlo method instead: generate a series of configurations $U_\mu^{(i)}(x)$ distributed with probability $\mathrm{e}^{-S_G(U)} \det M(U)/Z$ and compute expectation values as averages over those configurations:

$$\langle \mathcal{O}(U,\psi,\bar{\psi}) \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(U^{(i)}, M^{-1}(U^{(i)})$$

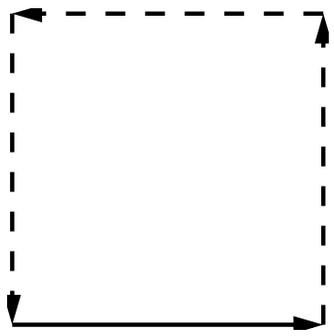
- A sufficient number of configurations is needed to keep the statistical errors of the computation small.
- The detM(U) factor is still a big computational problem, since the matrix M is order V × V , though it is sparse.
- In the quenched approximation, often employed first, one sets det M = 1, i.e. one neglects internal quark loops.





Metropolis algorithm - highly simplified

- Start with some “trial” configuration {U(x)}
- Go through sites of lattice xi,i = 1,...,N in some order, updating each in turn while keeping others fixed
  - Choose new local gauge field U’(xi) with probability PU’←U and Boltzmann density W(U) such that
  - $$\sum_{U'} P_{U'\leftarrow U} = 1; \quad P_{U'\leftarrow U} W(U) = P_{U\leftarrow U'} W(U')$$
  - Calculate change in action ΔS
  - Accept the new configuration with probability
    $$\min\left\{1, \frac{W(U')}{W(U)}\right\} \rightarrow \min\left\{1, e^{-\Delta S}\right\}$$
    - ➡ Ensures correct distribution.
- One complete pass through the lattice is a sweep.
- There are two crucial features that simplify the calculation.
  - The change in the energy can be calculated locally.
  - “Independent” sites can be up- dated in parallel
- These are the features that allow us to make highly effective use of parallel computers.



Statistical and Systematic Uncertainties

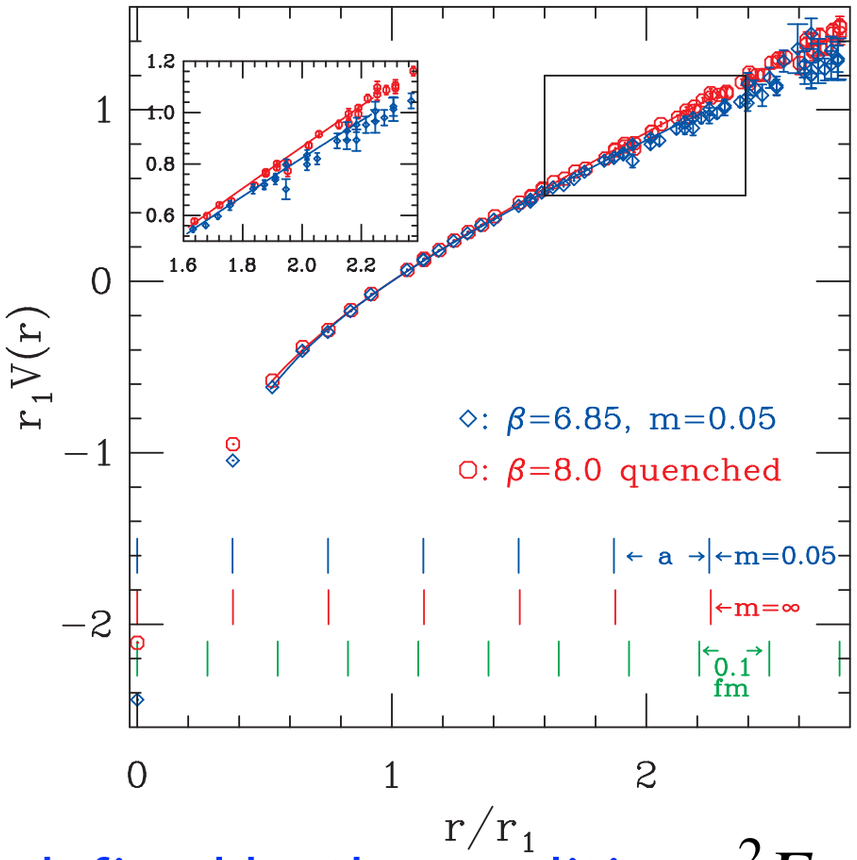
- Statistical uncertainties:
  - gauge configurations generated through Monte Carlo procedure

$$\sigma \simeq \frac{1}{\sqrt{N_{\rm cfg}}}$$

  - where Ncfg is the number of independent gauge configurations; O(100) typical. Lattice data has statistical error bars.
- Systematic Uncertainties
  - Finite volume: we work in a box - it must be big enough to, e.g. contain the hadron. L ~ 2 Fm for hadron masses and properties.
  - Discretisation effects: the lattice spacing a, or inverse coupling ß, must be sufficiently small that these are under control. Standard Wilson gauge action has discretisation errors of O(a2).
- State-of-the-Art: $32^3 \times 64$ lattice, with L ~ 2 Fm, and a ~ 0.07 Fm.

The static quark potential

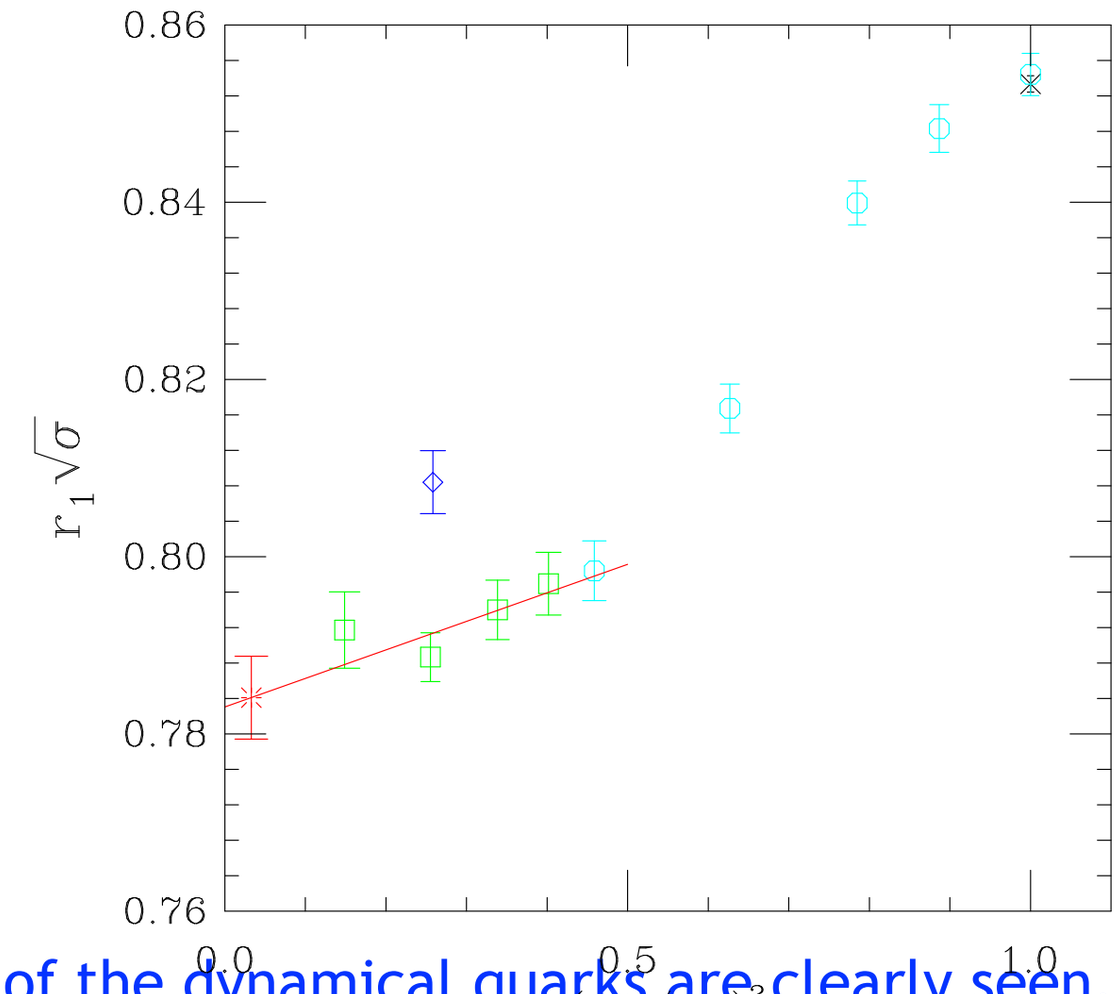
- Confinement was the first property of QCD demonstrated by numerical simulations in (quenched) lattice QCD, by M. Creutz, Phys. Rev. Lett. 43 (1979) 553.
- Confinement is seen as a linear rise of the static potential at large distances. It is by now the best studied property of QCD. Here I shall use it to illustrate the effect of quenching, i.e., of neglecting internal quark loops.



- r_1 is the distance defined by the condition $r_1^2 F_{Q\bar{Q}}(r_1) = 1$. The potentials are matched at r_1.
- The Coulomb well is deeper with dynamical fermions, and the string tension slightly smaller.

Potential (2)

- The difference in the short distance behavior, corresponding to high energies, is due to the different running of the strong coupling constant αs in the presence of dynamical quarks.
- A more detailed comparison of the behavior of a long distance scale √σ and a shorter distance scale r1 ≈ 0.35 fm as function of quark mass, $m_q \propto (m_\pi/m_\rho)^2$, is shown in



- The effects of the dynamical quarks are clearly seen.
  Ref.: C. Bernard et al. (MILC), Phys. Rev. D62 (2000) 034503

Quarks

- The full generating functional for lattice QCD is

$$Z = \int \mathscr{D}U\, \mathscr{D}\psi\, \mathscr{D}\overline{\psi} e^{-S_G(U) + \sum_{x,y} \overline{\psi}(x) M(x,y,U) \psi(y)}$$

- where $M(x, y, U)$ is the fermion matrix which, in its "naive" form, is

$$M(x, y, U) = m\, \delta_{x,y} + \frac{1}{2} \sum_{\mu} \gamma_{\mu} \left(U_{\mu}(x) \delta_{y,x+\hat{\mu}} - U_{\mu}^{\dagger}(x - \hat{\mu}) \delta_{y,x-\hat{\mu}} \right)$$

- Here m is the quark mass. Note that M once again connects only nearest neighbour points

Quarks (2)

- Because the ψ fields are Grassman variables, we can integrate out the fermion degrees of freedom:

$$Z = \int \mathscr{D}U \, \det M(U) \, e^{-S_G(U)} \, .$$

- While M is local, the calculation of det M is a global operation.
  In particular, we have to re-evaluate det M every time we update the gauge fields.
  If you think about this, it is not surprising; quarks are fermions, and therefore have to satisfy Fermi-Dirac statistics, including anti-symmetry under exchange of co-ordinates - a non-local procedure.
- There have been many studies of efficient non-local update algorithms - most noticeably the Hybrid MonteCarlo.
- The cost of including fermions is high - perhaps 1,000 times as expensive as simulations with gluons alone.

Quenched Approximation

- Because of this enormous computational cost, many simulations to date have set

$$\det M = 1$$

- in the path integral - this is the quenched approximation. The best justification for using this approximation is that it applies in the large-Nc limit

Dynamical Fermions

- Recall the partition function for full QCD,

$$Z = \int dU e^{-S_G(U)} \det M(U) .$$

- Computing the determinant is not practical. Consider instead Hamilton's equations. Introduce a fictitious momenta and evolve in fictitious time (computer time, so a 4+1 Hamiltonian).

$$H = \frac{1}{2}\pi^2 + S(\phi) \qquad \frac{d\phi}{dt} = \frac{\delta H}{\delta \pi} = \pi$$

$$\frac{d\pi}{dt} = -\frac{\delta H}{\delta \pi} = -\frac{\delta S}{\delta \phi}$$

- Note, we can rewrite in Z the det(M(U)) using Bosonic fields x

$$Z = \int dU d\chi d\pi \ \exp\left[-\frac{1}{2}\pi^2 - S_G(U) - \sum_{x,y} \chi_x^\dagger M^{-1}(U) \chi_y\right]$$

- In the Hybrid Monte Carlo algorithm, choose some Gaussian distributed π and x, then evolve the U and π according to a discrete version of Hamilton's equations, keeping x fixed. Metropolis accept or reject the proposed U. This is the new U.

- Note, at each step require

$$\frac{\delta H}{\delta U} = \frac{\delta S_G(U)}{\delta U} - \chi^\dagger M^{-1}(U) \frac{\delta M(U)}{\delta U} M^{-1} \chi$$

- So, an inversion at each step – expensive – but tractable

Fermion Doubling and Chiral Symmetry

- The difficulties are not over yet. . . .
- Let us consider the inverse lattice free-fermion propagator in *momentum space*:

$$M_{xy}^{-1} = \int_0^{\frac{\pi}{a}} \frac{d^4p}{(2\pi)^4} \frac{e^{ip\cdot(x-y)}}{m + i\sum_\mu \gamma_\mu \sin ap_\mu}$$

- This has a pole at $p_\mu = 0$ and$p_\mu = \pi/a$; it arises because the Dirac equation is *first order*
- In four dimensions we have a theory with 2^4 non-interacting, equal mass fermions
- This is the "fermion-doubling problem"
  - Kogut-Susskind - preserves chiral symmetry, but with wrong flavor spectrum
  - Wilson fermions - correct spectrum of states, but at the loss of exact chiral symmetry on the lattice.
  - Chiral fermions - an exact lattice symmetry that reduces to chiral symmetry in the continuum and flavor structure.
- For spectroscopy, Wilson fermions are the traditional "flavor of choice"

Wilson fermions

- Solution is to add a second-derivative, or momentum-dependent mass term, to the action

$$S_F^W = \sum_x \left[(m+4r)\bar{\psi}(x)\psi(x) - \frac{1}{2}\sum_\mu \bar{\psi}(x)(r-\gamma_\mu)U_\mu(x)\psi(x+\hat{\mu}) + \bar{\psi}(x+\hat{\mu})(r+\gamma_\mu)U_\mu^\dagger(x)\psi(x) \right]$$

- In the continuum limit

$$S_F^W = \int d^4x\, \bar{\psi}(x)(D + m - \frac{arD^2}{2})\psi(x) + \mathcal{O}(a^2)$$

  - Lifts mass of doublers **but…**
  - Adds $\mathcal{O}(a)$ discretization errors
  - Breaks chiral symmetry *therefore*
  - *Additive mass renormalization*

Symanzik Improvement

- Working at small lattice spacing a is expensive – more lattice sites are needed to keep the (physical) volume fixed. It is worthwhile to improve the approach to the continuum from $\mathcal{O}(a)$ to $\mathcal{O}(a^2)$
- Use the Symanzik improvement program. Near the continuum limit, the lattice action and composite fields can be written as a local effective theory

$$S_{\text{eff}} = S_0 + aS_1 + a^2 S_2 + \ldots$$

$$\phi_{\text{eff}}(x) = \phi_0(x) + a\phi_1(x) + a^2\phi_2(x) + \ldots$$

- where S_0 is the continuum action, $\phi(x)$ are lattice fields (e.g. axial density), and the S_k are combinations of gauge invariant composite fields of dimension $4+k$.
- For the Wilson fermion action, the $\mathcal{O}(a)$ term is a Pauli term of the form

$$c_{SW}(g_0^2)\bar{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi$$

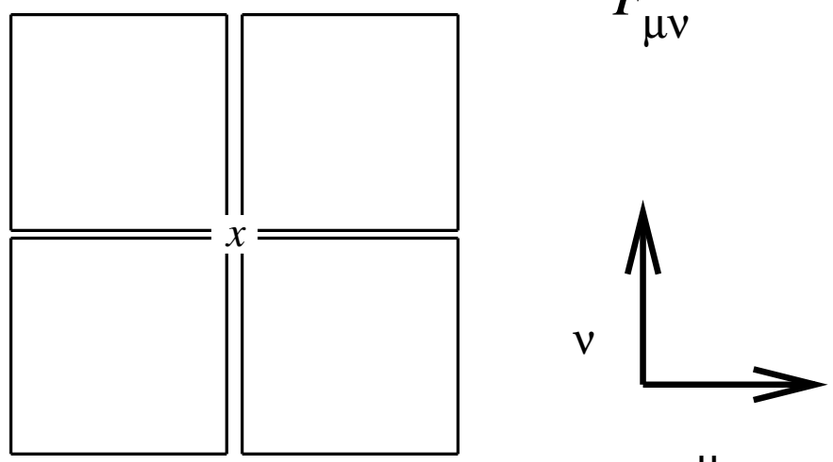
- with some appropriately chosen $c_{SW}(g_0^2)$ which needs to be determined non-perturbatively
- One approach is to simulate a system with Schrodinger Functional, i.e. fixed at initial and final time, boundary conditions that induce a constant chromoelectric field and monitoring the response of the fermions. This program was initiated by the ALPHA collaboration

Improvement

- Because the Wilson term has introduced $\mathcal{O}(a)$ discretisation errors, there has been an emphasis on *removing* those errors - **improvement**
- Sheikholeslami-Wohlert (SW) or "clover" action:

$$S_F = S_F^W - i\frac{c_{\mathrm{SW}}\kappa}{2}\sum_{x,\mu,\nu}\bar{\psi}(x)F_{\mu\nu}\sigma_{\mu\nu}\psi(x)$$

Magnetic moment term looks like four-leaf clover



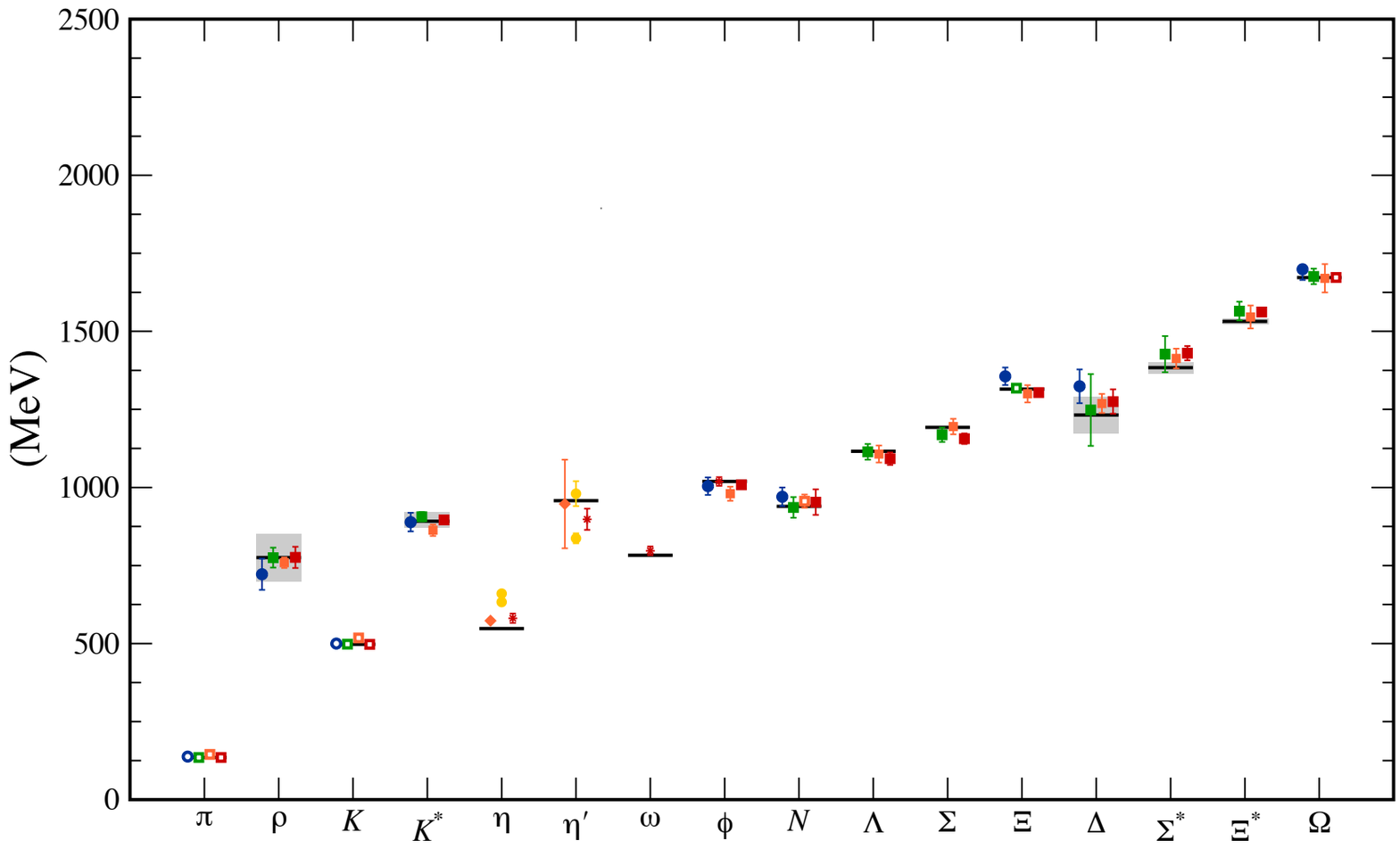
C_{SW} = NP removes all $\mathcal{O}(ma)$ errors from hadron masses.

Hadron spectrum

- The spectrum of hadrons comprising light (u, d, s) quarks is the benchmark test of lattice QCD – also many masses not known!
- In principle, the recipe is to determine the mass of particle P is straightforward:
  - Choose an *interpolating operator* $\mathcal{O}_P$ such that
    $$\langle 0 | \mathcal{O}_P | P \rangle \neq 0$$
  - Construct the time-sliced correlator
    $$C(t) = \sum_{\vec{x}} \langle \mathcal{O}(\vec{x}, t) \mathcal{O}^\dagger(\vec{0}, 0)$$
  - Insert a complete set of states
    $$C(t) = \sum_{\vec{x}} \sum_{P} \int \frac{d^3k}{(2\pi)^3 2E(\vec{k})} \langle 0 | \mathcal{O}(\vec{x}, t) | P(\vec{k}) \rangle \langle P(\vec{k}) | \mathcal{O}^\dagger(\vec{0}, 0) | 0 \rangle$$
    $$= \sum_{\vec{x}} \sum_{P} \int \frac{d^3k}{(2\pi)^3 2E(\vec{k})} \langle 0 | \mathcal{O} | P(\vec{k}) \rangle \langle P(\vec{k}) | \mathcal{O}^\dagger | 0 \rangle e^{ik \cdot x}$$
    $$= \sum_{P} \int \frac{d^3k}{2E(\vec{k})} \delta^3(\vec{k}) \langle 0 | \mathcal{O} | P(\vec{k}) \rangle \langle P(\vec{k}) | \mathcal{O}^\dagger | 0 \rangle e^{iE(\vec{k})t}$$
    $$= \sum_{P} \frac{|\langle 0 | \mathcal{O} | P \rangle|^2}{2m_P} e^{iM_P t}$$
  - Go to *Euclidean space*
    $$C(t) \to \sum_{P} \frac{|\langle 0 | \mathcal{O} | P \rangle|^2}{2m_P} e^{-M_P t}$$

Hadron spectrum from dynamical fermions

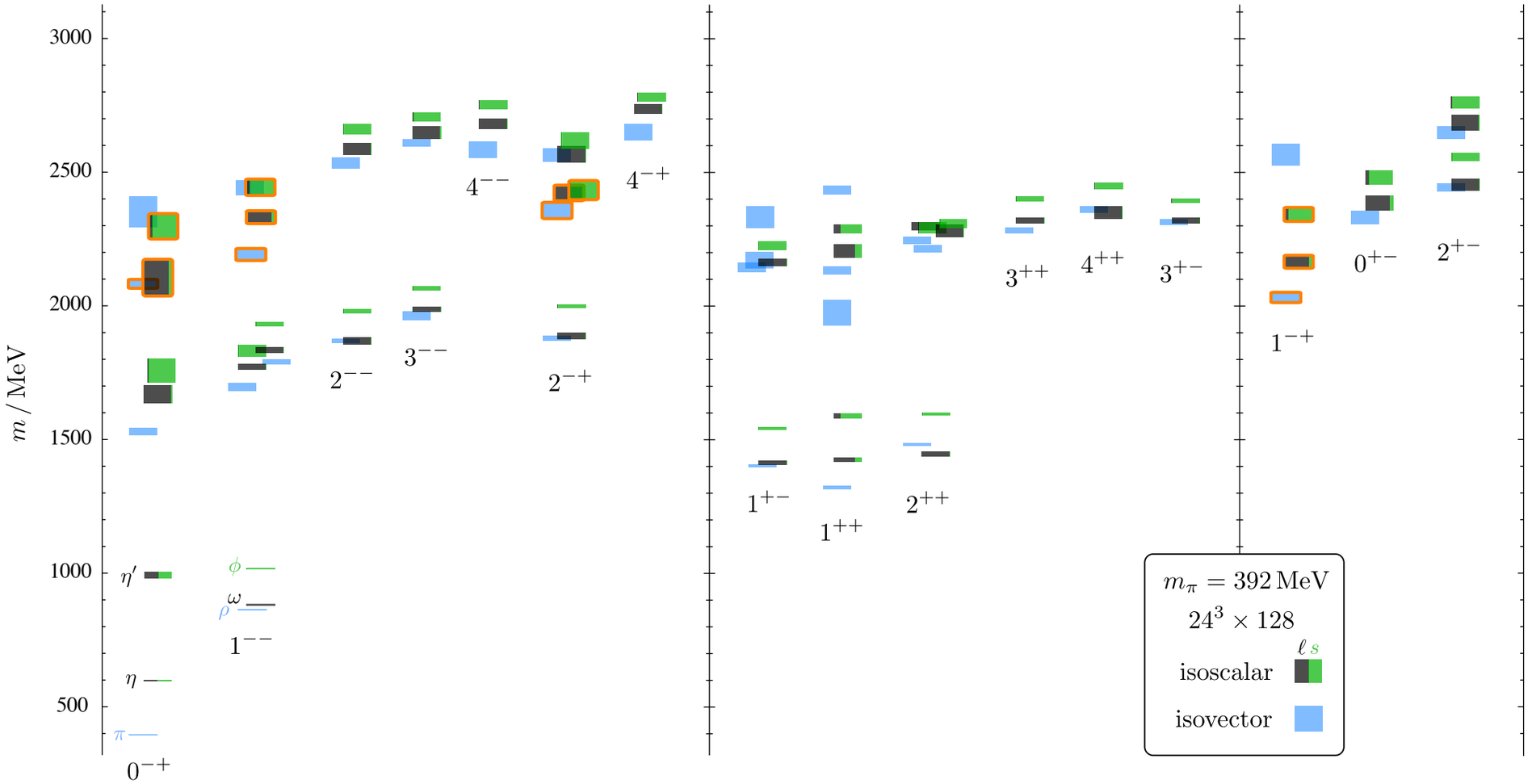
- An amalgamation of dynamical fermion results. Good agreement with expt. Some of these states are unstable under strong interactions (not considered)



Wide-ranging results are from MILC, PACS-CS, BMW, QCDSF. Results for η and η' are from RBC & UKQCD, Hadron Spectrum (also the only ω mass), and UKQCD. Symbol shape denotes the formulation used for sea quarks. Asterisks represent anisotropic lattices. Open symbols denote the masses used to fix parameters. Filled symbols (and asterisks) denote results. Red, orange, yellow, green, and blue stand for increasing numbers of ensembles (i.e., lattice spacing and sea quark mass). Horizontal bars (gray boxes) denote experimentally measured masses (widths). Adapted from Kronfeld (2012).

Hadron spectrum from dynamical fermions

- Excited isoscalar and isovector meson spectrum



Hadron Spectrum (2013): Light-quark meson spectrum resulting from lattice QCD, sorted by the quantum numbers JPC. Note that these results have been obtained with an unphysical pion mass, mπ = 396 MeV

Why supercomputers?

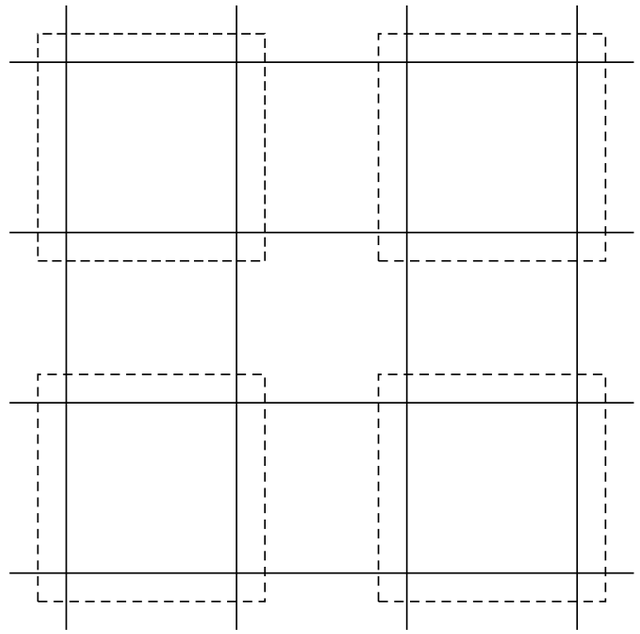
- QCD is a 4 dimensional grid based problem, #sites = L^4
- Want small lattice spacings and large lattice sizes. Typical size is 32^4, corresponding to 33×10^6 degrees of freedom
- In Monte Carlo, integrals are approximated by sums. Each element of the sum is the integration of a differential equation (Hamilton's equations)
- Most time consuming part is repeatedly solving large sparse linear systems of equations. E.g., conjugate gradient
- A cycle estimate is

$$10^3 samples * 10^2 \frac{steps}{sample} * 10^3 \frac{CG}{step} * 10^3 \frac{ops}{CG - site} = 10^{11} \frac{ops}{site}.$$

- For a 1 Gigaflop machine, and a typical medium size of 10^5 sites, then we need 10^7 secs for a complete simulation

QCD on a parallel computing platform

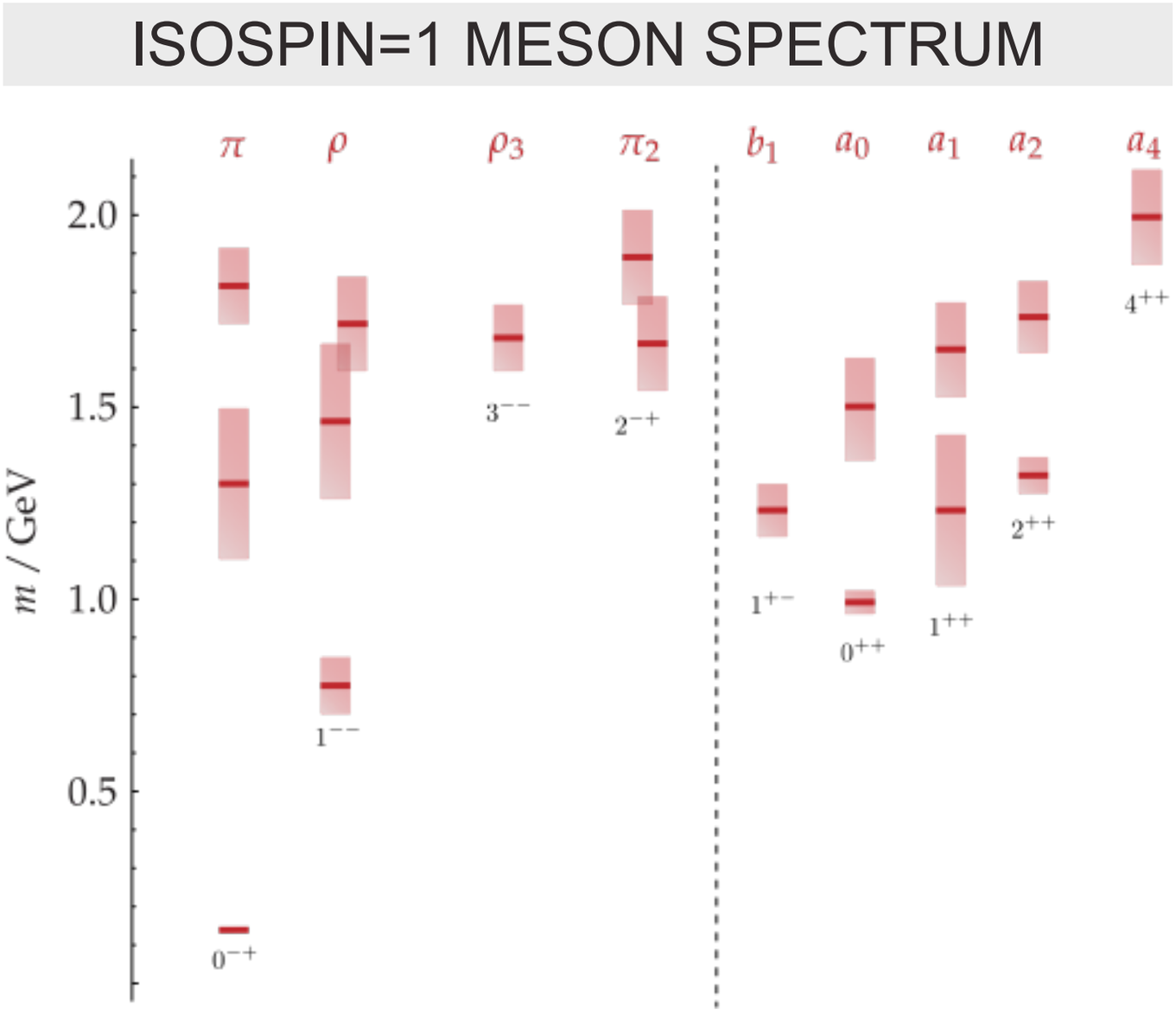
- We want to decrease runtime for a fixed size problem, so we increase # of processors, N
- Consider a 2 dimensional problem. Use a grid mapping
- Amount of data to be communicated between neighboring processors is proportional to the surface area of the subgrid residing on each processor
- Limitation of scalability is communication / computation ratio. Amount of computations is falling faster than the amount of communications when N increases



- Latency is okay - can overlap communication and computations
- Bandwidth okay; however, packet size and overhead too large. For a Teraflop scale computer, we typically need to exchange a few hundred bytes between neighboring processors

Experimental meson spectrum

- Mesons classified by their conserved quantum numbers
  - Spin, isospin, charge-conjugation **J^{PC}**



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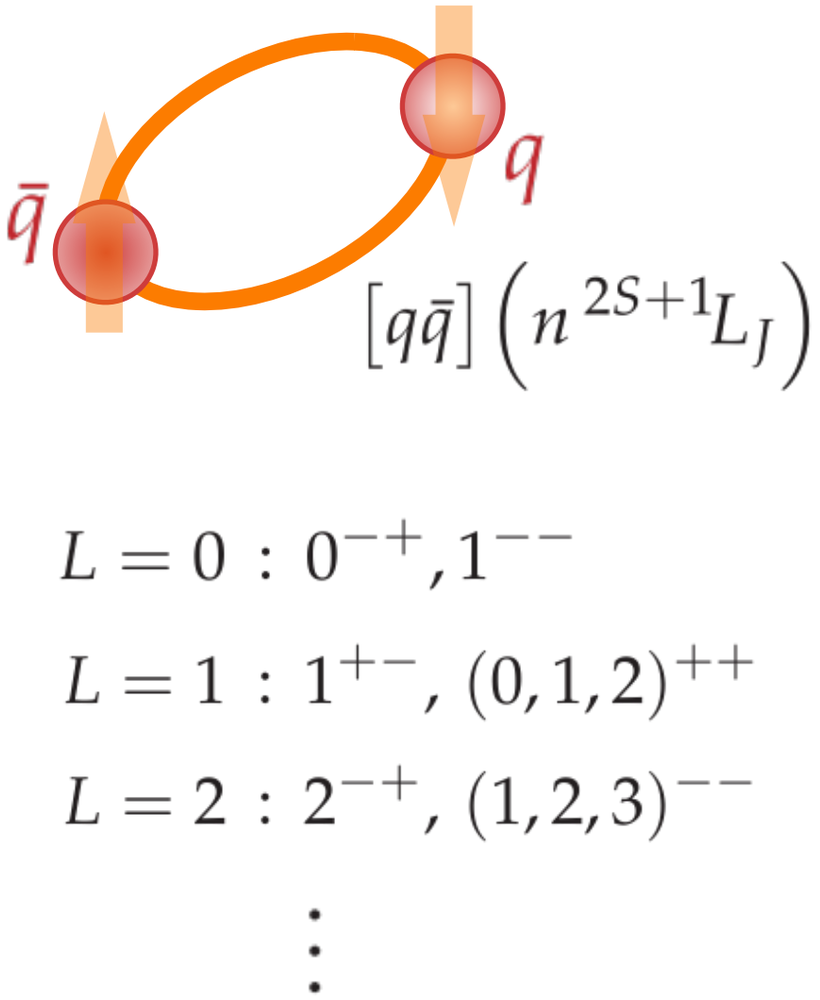
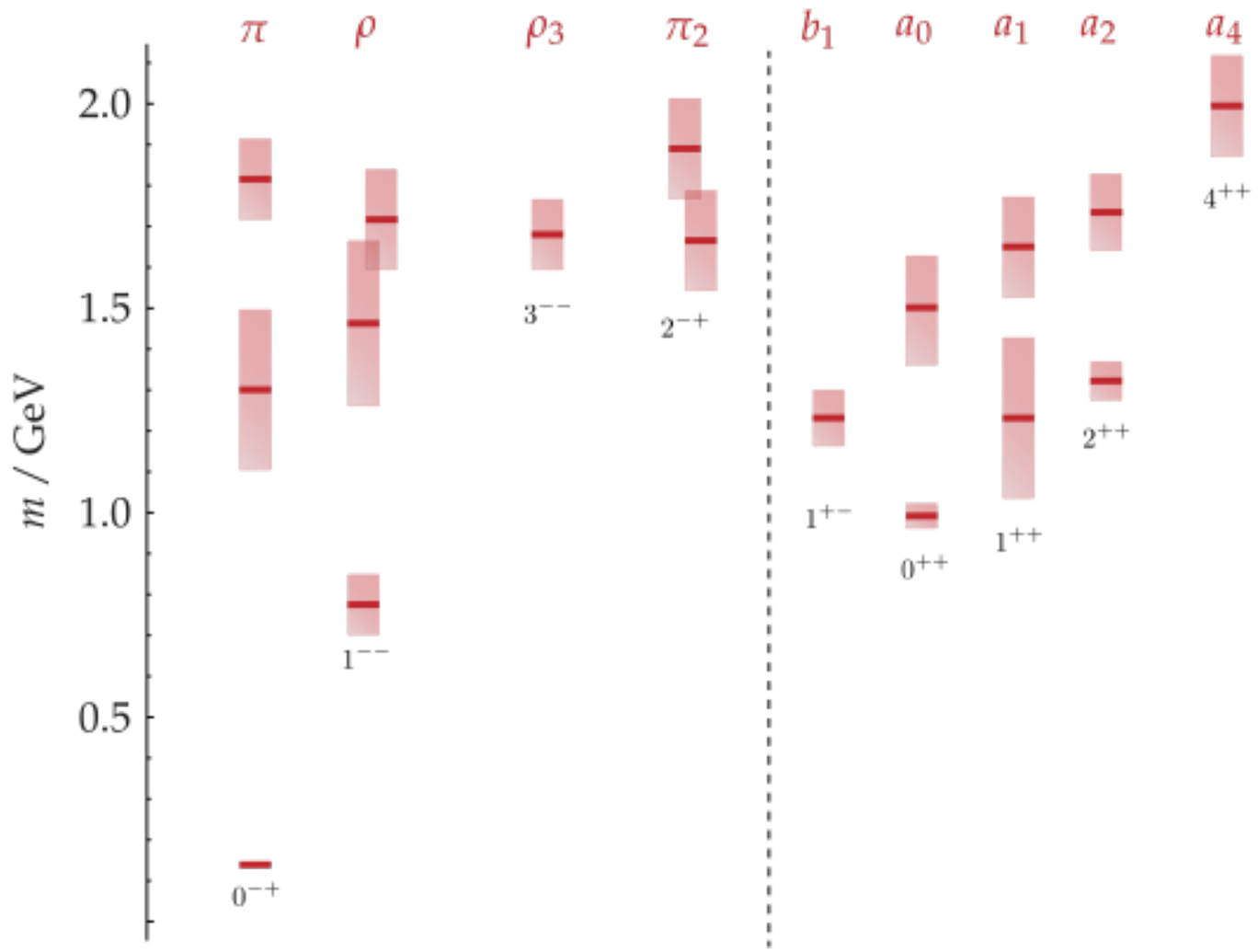


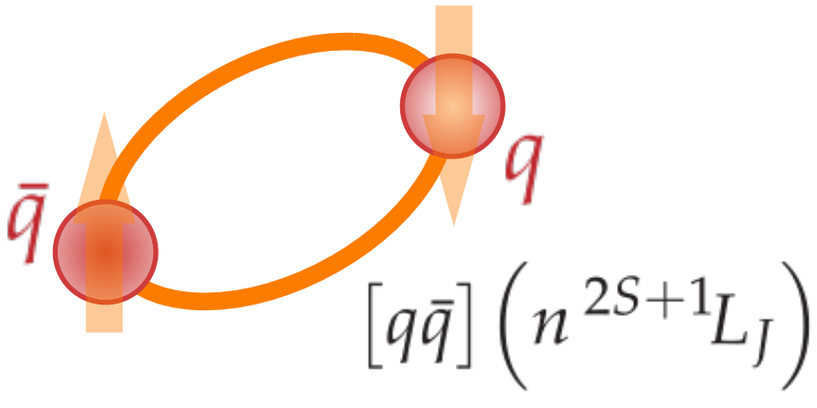
$$L = 0 : 0^{-+}, 1^{--}$$
$$L = 1 : 1^{+-}, (0,1,2)^{++}$$
$$L = 2 : 2^{-+}, (1,2,3)^{--}$$
$$\vdots$$

ISOSPIN=1 MESON SPECTRUM



Experimental meson spectrum

- Mesons classified by their conserved quantum numbers
  - Spin, isospin, charge-conjugation $\mathbf{J^{PC}}$



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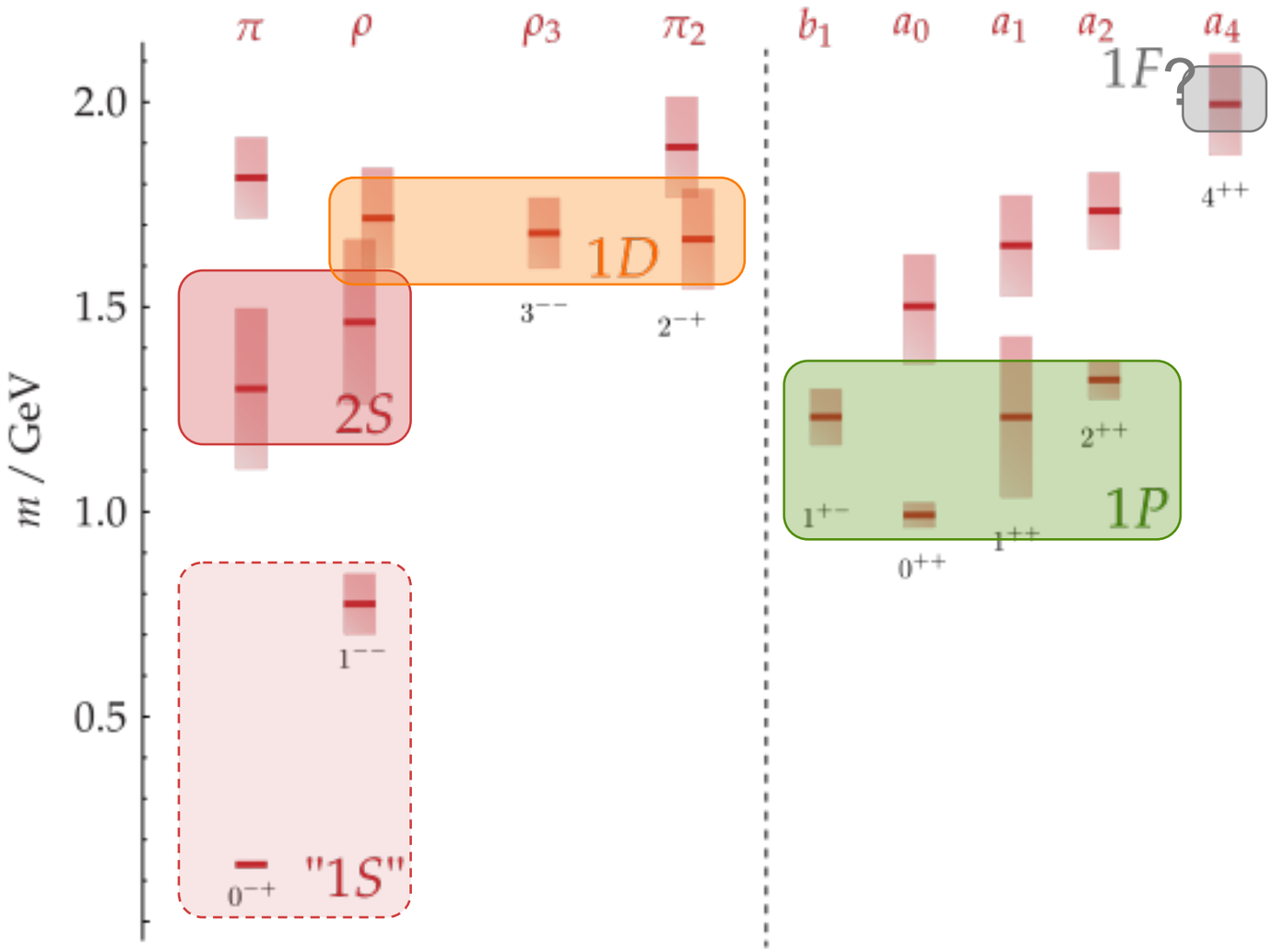
ISOSPIN=1 MESON SPECTRUM



Experimental meson spectrum

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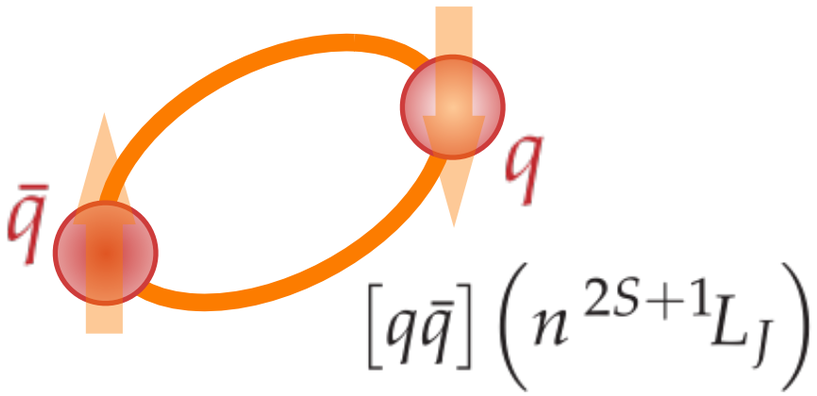
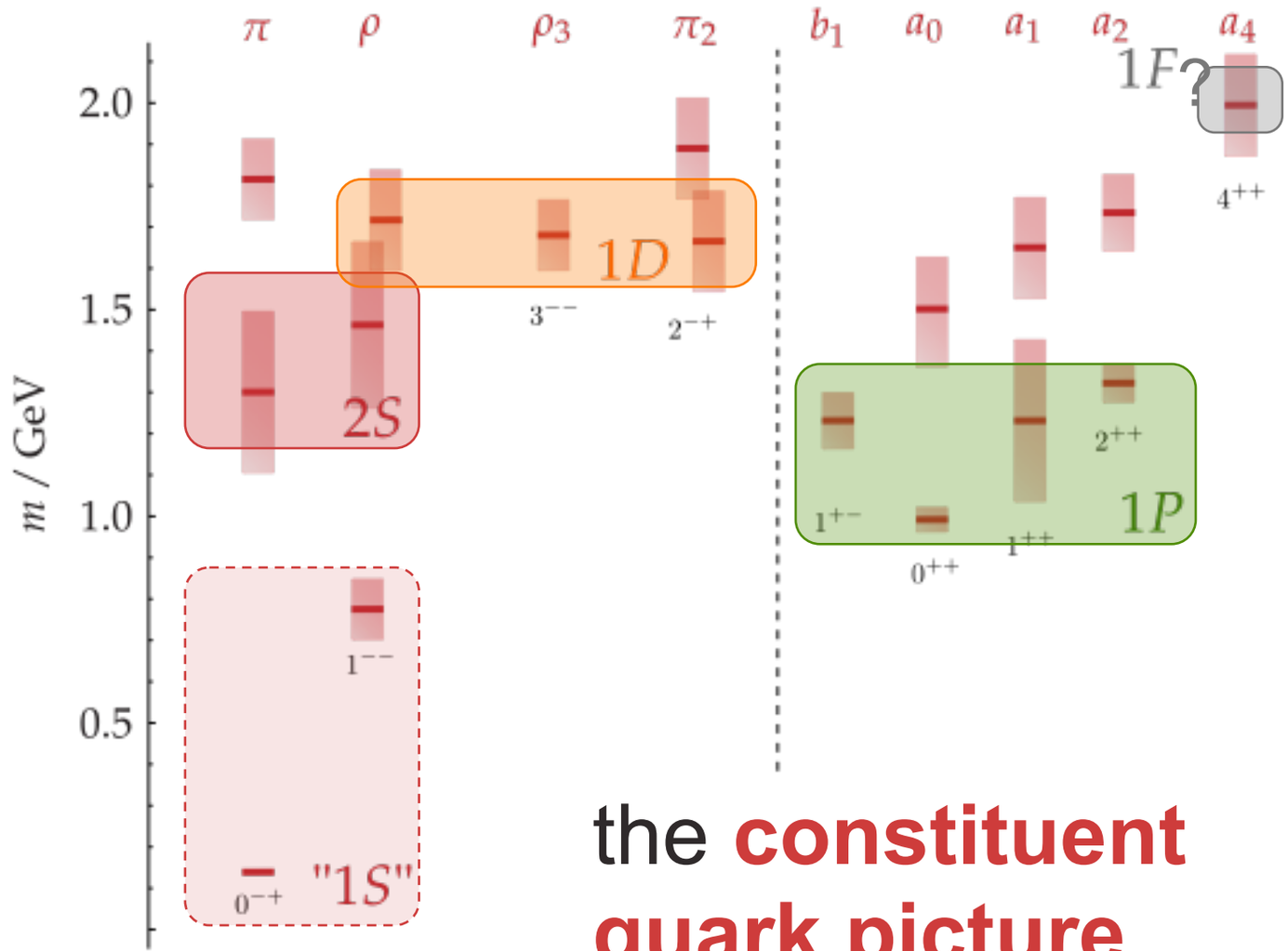


$$[q\bar{q}]\left(n\,^{2S+1}L_J\right)$$

$$L=0:\ 0^{-+},1^{--}$$
$$L=1:\ 1^{+-},(0,1,2)^{++}$$
$$L=2:\ 2^{-+},(1,2,3)^{--}$$
$$\vdots$$

n.b. absent: $0^{--}, 0^{+-}, 1^{-+}, 2^{+-}\ldots$

ISOSPIN=1 MESON SPECTRUM



the **constituent quark picture**

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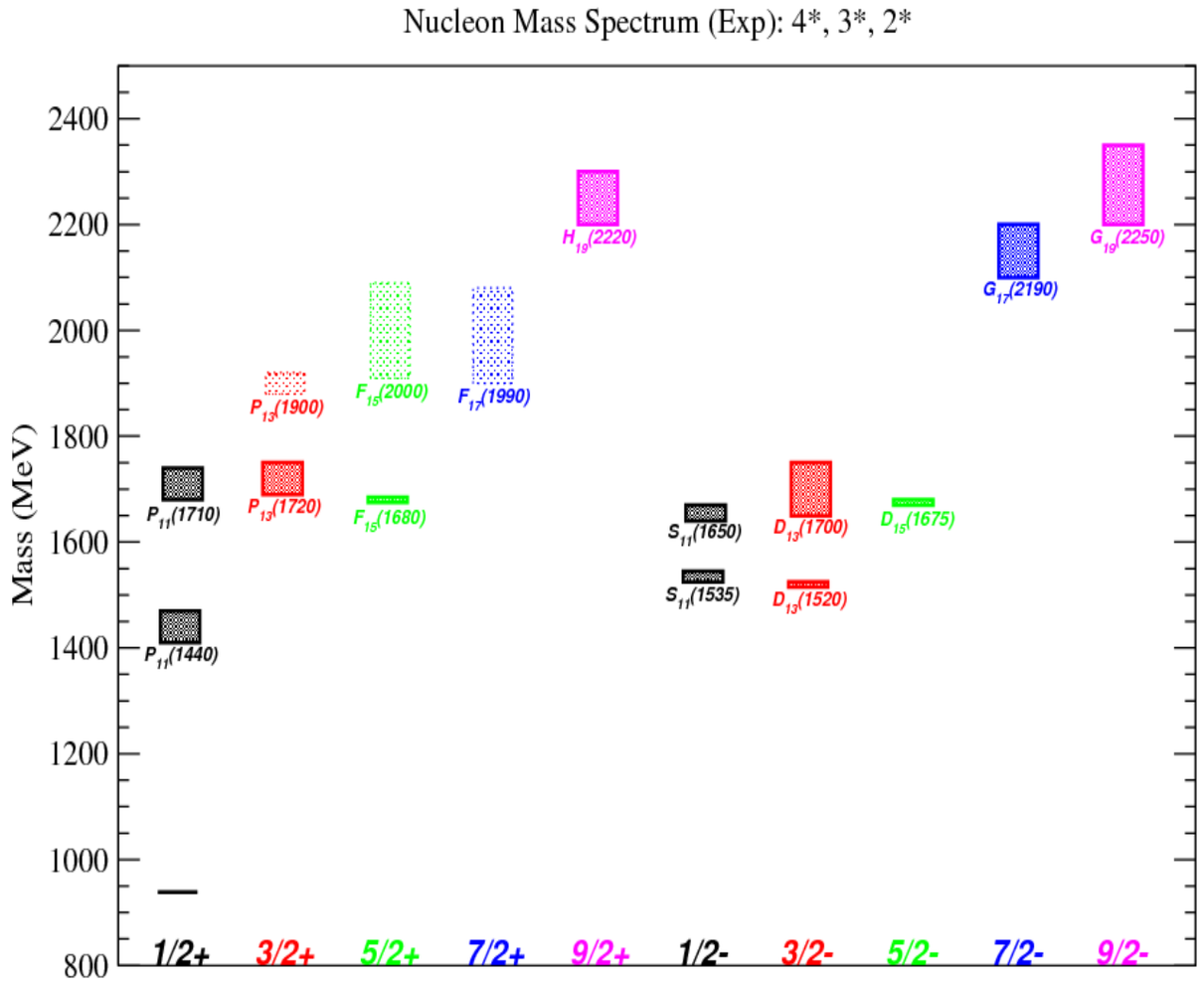
Experimental baryon spectrum

- Baryons classified by their conserved quantum numbers
  - Spin, parity, isospin **J^P**

ISOSPIN=1/2 BARYON SPECTRUM



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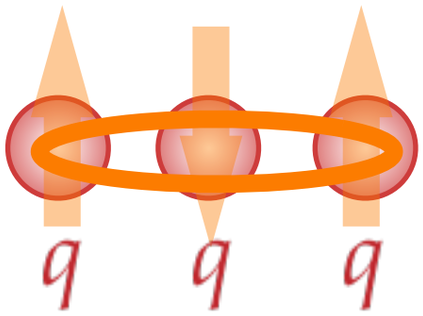


$$[qqq]\left(n^{2S+1}L_{\pi}\right)$$

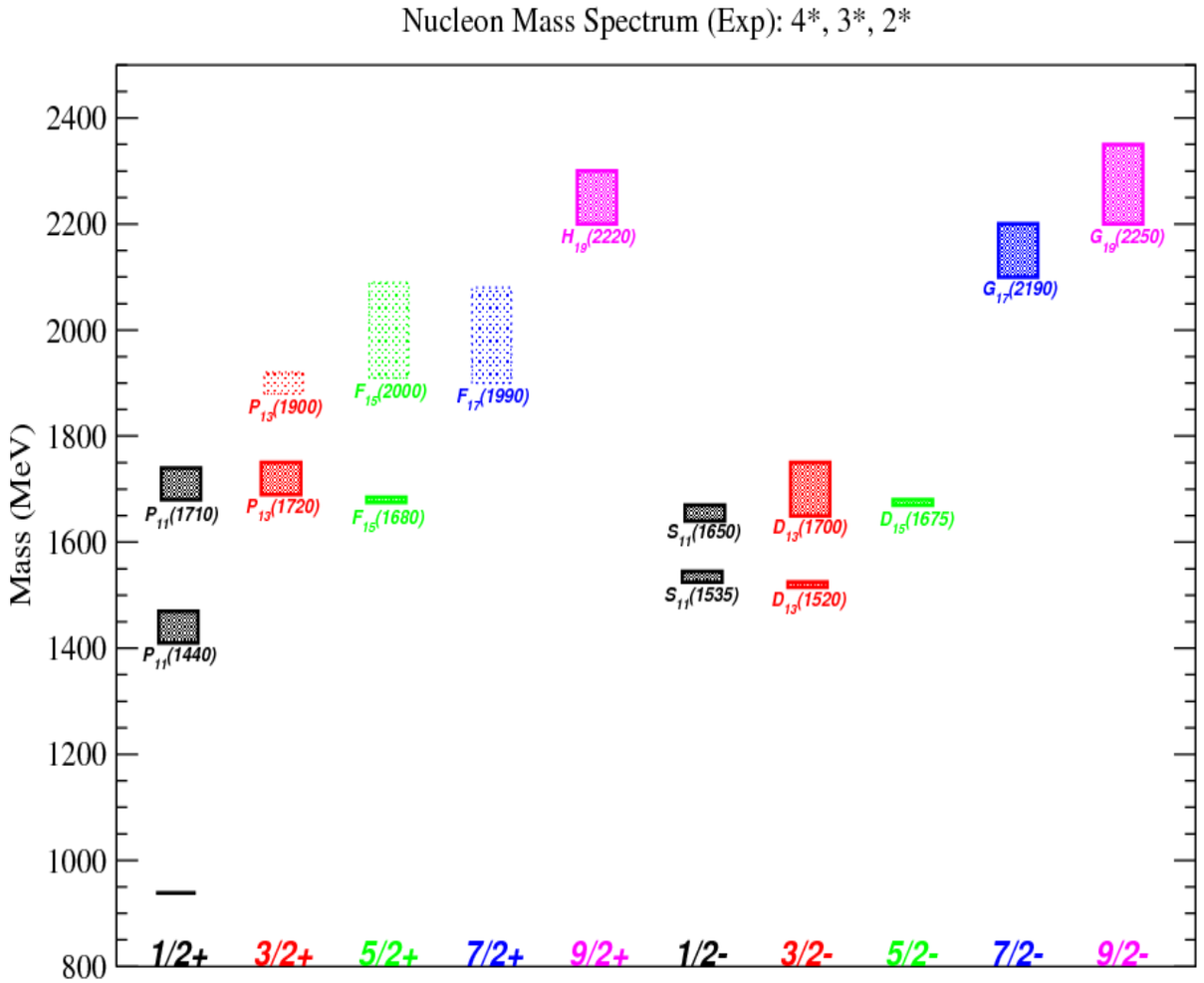
Antisymmetric under interchange

π = permutation of quarks in space

$$\mathrm{L} = \quad 0_S \quad : \quad \frac{1}{2}^+$$

$$\mathrm{L} = \quad 1_M \quad : \quad \left(\frac{1}{2}, \frac{3}{2}\ ,\ \frac{1}{2}, \frac{3}{2}, \frac{5}{2}\right)^-$$

ISOSPIN=1/2 BARYON SPECTRUM



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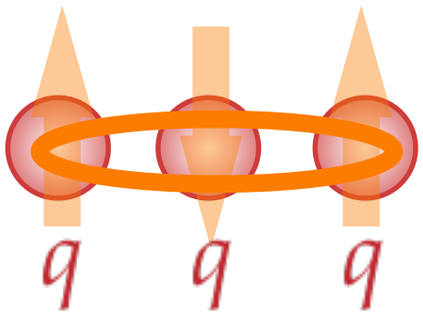

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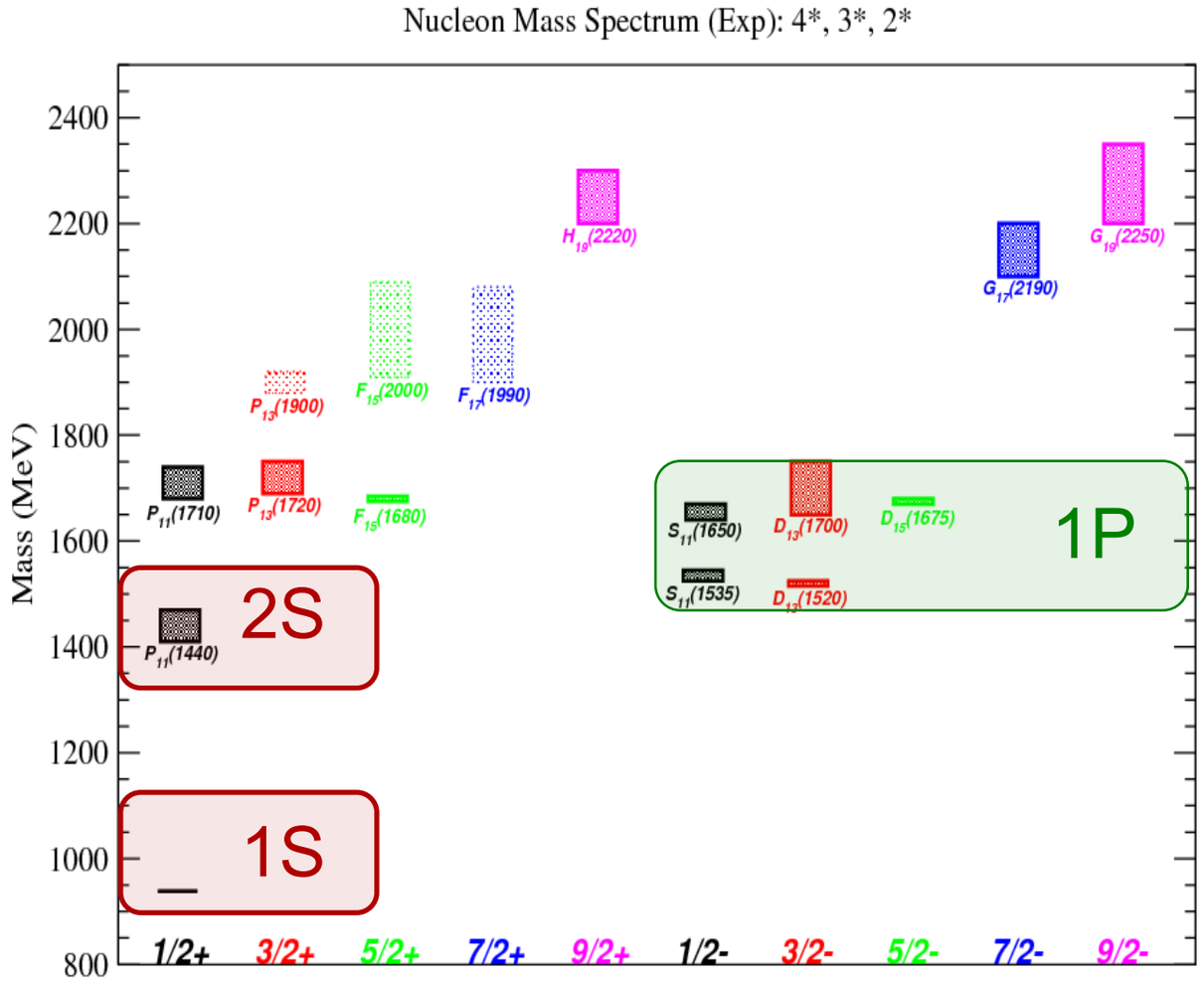
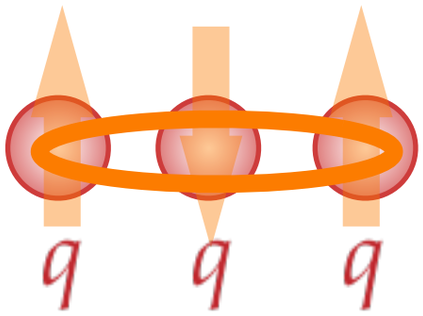
ISOSPIN=1/2 BARYON SPECTRUM



Experimental baryon spectrum

- Some states are “missing” ???



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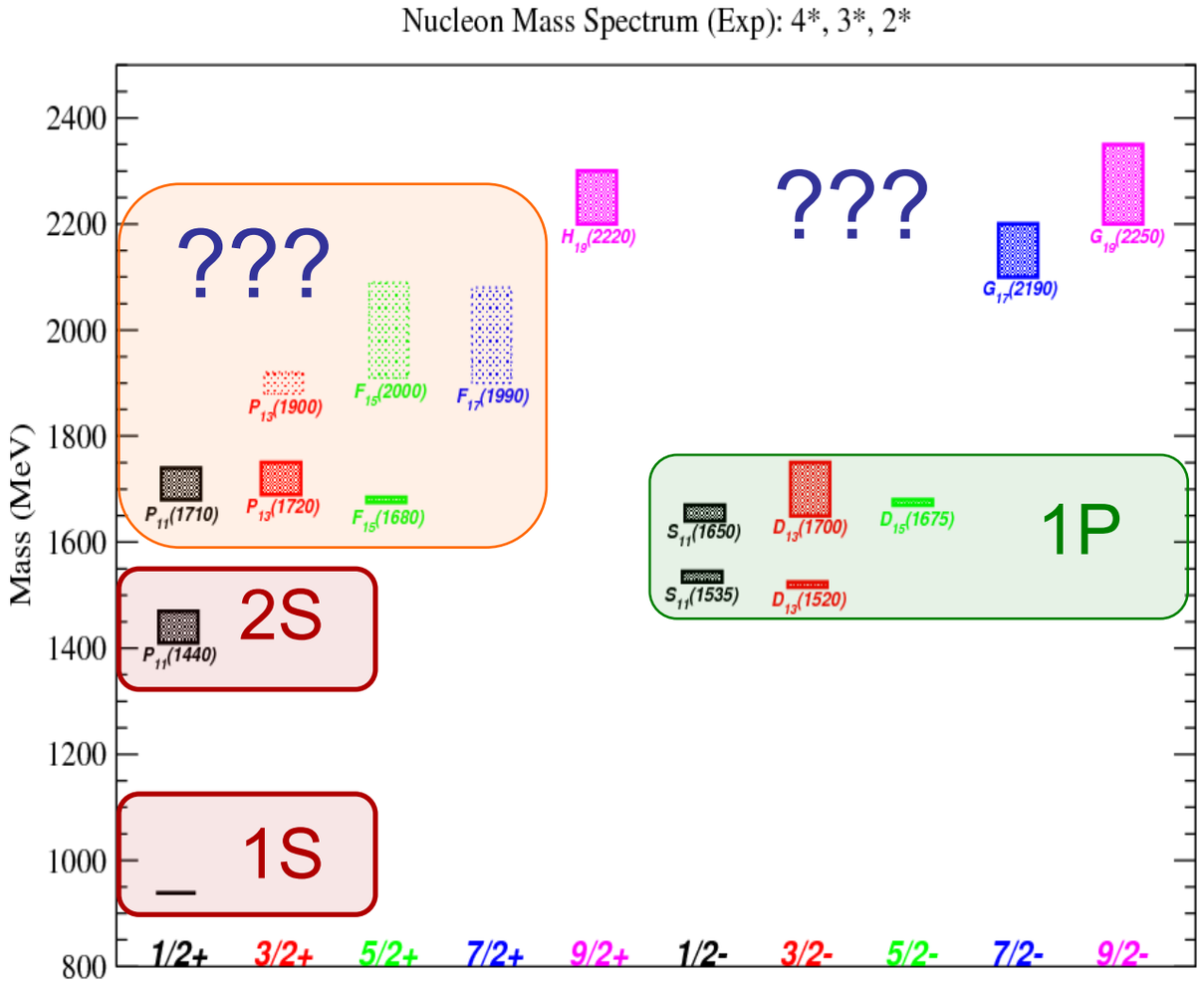
Antisymmetric under interchange

π = permutation of quarks in space

L =	0_S	:	$\frac{1}{2}^+$
L =	1_M	:	$(\frac{1}{2},\frac{3}{2}\ ,\ \frac{1}{2},\frac{3}{2},\frac{5}{2})^-$
L =	2_S	:	$(\frac{3}{2},\frac{5}{2})^+$
L =	2_M	:	$(\frac{3}{2},\frac{5}{2})^+\ ,\ (\frac{1}{2},\frac{3}{2},\frac{5}{2})^+$
L =	1_A	:	$(\frac{1}{2},\frac{3}{2})^+$
L =	0_M	:	$(\frac{1}{2},\frac{3}{2})^+$

ISOSPIN=1/2 BARYON SPECTRUM



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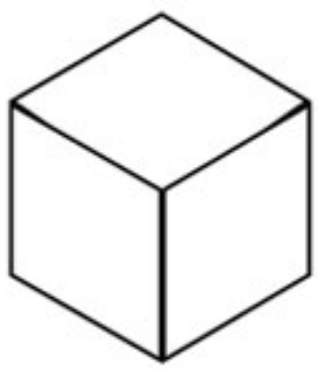
Finite volume QCD & the hadron spectrum

Compute **correlation functions** as an average over field configurations

$$\text{e.g.} \quad \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D} A_\mu \; \bar{\psi}\Gamma\psi(t)\, \bar{\psi}\Gamma\psi(0) \; e^{-\int d^4x\, \mathcal{L}_{\text{QCD}}(\psi,\bar{\psi},A_\mu)}$$

'sum' 'field correlation' 'probability weight'



Field integration within a finite, but continuous, hypercube

Need some kind of ultraviolet regulator….

Spectrum from two-point correlation functions

$$\begin{aligned} C(t) &= \langle 0|\mathcal{O}(t)\, \mathcal{O}^\dagger(0)|0\rangle \\ &= \sum_{\mathfrak{n}} e^{-E(\mathfrak{n})t} \langle 0|\mathcal{O}(0)|\mathfrak{n}\rangle \langle \mathfrak{n}|\mathcal{O}^\dagger(0)|0\rangle \end{aligned}$$

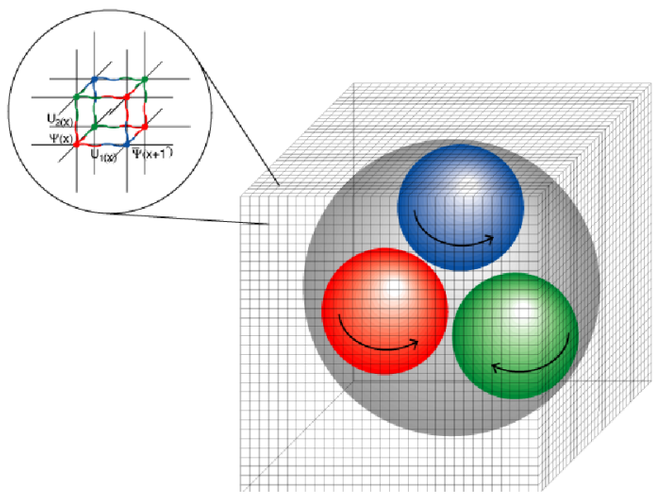
States $|\mathfrak{n}\rangle$ are finite-volume distorted

Lattice QCD & the hadron spectrum

Compute **correlation functions** as a Monte Carlo average over field configurations

$$\text{e.g.} \quad \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A_\mu \; \bar{\psi}\Gamma\psi(t)\, \bar{\psi}\Gamma\psi(0) \; e^{-\int d^4x\, \mathcal{L}_{\text{QCD}}(\psi,\bar{\psi},A_\mu)}$$

'sum' 'field correlation' 'probability weight'



Discretize the action over sites

Serves as an ultraviolet regulator

Spectrum from two-point correlation functions

$$\begin{aligned} C(t) &= \langle 0|\mathcal{O}(t)\, \mathcal{O}^\dagger(0)|0\rangle \\ &= \sum_{\mathfrak{n}} e^{-E(\mathfrak{n})t} \langle 0|\mathcal{O}(0)|\mathfrak{n}\rangle \langle \mathfrak{n}|\mathcal{O}^\dagger(0)|0\rangle \end{aligned}$$

States $|\mathfrak{n}\rangle$ are finite-volume distorted

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Excited states from correlators

- How to get at excited QCD eigenstates ?

  - optimal operator for state $|\mathfrak{n}\rangle$: $\Omega^\dagger_{\mathfrak{n}} \sim \sum_i v_i^{(\mathfrak{n})} \mathcal{O}_i^\dagger$

    for a basis of meson operators $\{\mathcal{O}_i\}$

  - can be obtained (in a variational sense) from the matrix of correlators

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

  - by solving a generalized eigenvalue problem

'diagonalize the correlation matrix'

$$C(t) v^{(\mathfrak{n})} = C(t_0) v^{(\mathfrak{n})}\, \lambda_{\mathfrak{n}}(t)$$

eigenvalues $\lambda_{\mathfrak{n}}(t) \sim e^{-E_{\mathfrak{n}}(t-t_0)}$

  - a large basis can be constructed using covariant derivatives :

$$\mathcal{O} \sim \bar{\psi} \Gamma \overleftrightarrow{D} \ldots \overleftrightarrow{D} \psi$$

Operators - quark bilinears

- Scalar/Vector Dirac structures & covariant derivatives

$$\bar{\psi}\gamma_5\psi \qquad \rightarrow J = 0$$
$$\bar{\psi}\gamma_i\psi \qquad \rightarrow J = 0$$
$$\bar{\psi}\overleftrightarrow{D_i}\psi \qquad \rightarrow J = 1$$

  - ➡ Combine gamma & derivatives

$$\bar{\psi}\Gamma\overleftrightarrow{D}\overleftrightarrow{D}\psi$$

in terms of

$$\langle 1m_1\ 1m_2|Jm\rangle\bar{\psi}\overleftrightarrow{D}_{m_1}\overleftrightarrow{D}_{m_2}\psi \qquad \rightarrow J = 0,1,2$$
$$\langle 1s\ Ll|Jm\rangle\langle 1l_1\ 1l_2|Ll\rangle\bar{\psi}\Gamma_s\overleftrightarrow{D}_{l_1}\overleftrightarrow{D}_{l_2}\psi \qquad \rightarrow J = 0,1,2,3$$

- Subduction of continuum to cubic reps.

$$\mathcal{O}^{[J]}_{\Lambda\lambda} = \sum_M \mathcal{S}^{JM}_{\Lambda\mu}\mathcal{O}^{JM}$$

arxiv:1004.4930, 1104.5152, 1201.2349

Operators - three quarks

- Baryons operators are projectors acting on flavor, Dirac spin, and spatial indices

$$(\mathrm{Flavor}_{\pi_F} \otimes \mathrm{Spin}_{\pi S} \otimes \mathrm{Space}_{\pi D})\{\psi_1\psi_2\psi_3\}$$

- Symmetric under quark permutations π & color is antisymmetric

- Now CG-s in permutations π and coupling spin and derivatives/space

e.g., two derivatives

$$\mathcal{O}_i \sim (\mathrm{CGCs})_{i,j,k}\ \{\overrightarrow{D}\overrightarrow{D}\}_j\ \{\psi\psi\psi\}_k \qquad 1\times 1\times \mathcal{S} \rightarrow\ J=\tfrac{1}{2},\tfrac{3}{2},\tfrac{5}{2},\tfrac{7}{2}$$

arxiv:1004.4930, 1104.5152, 1201.2349

Distillation

- Define a low rank (spatial) smearing operator

  e.g., quark bilinear

$$C_{ij}(t) \;=\; \langle \bar{\psi}\Box\Gamma^i_t\Box\psi \;\cdot\; \bar{\psi}\Box\Gamma^j_0\Box\psi\rangle \qquad \Box_{xy} = V_x V_y^\dagger$$

- Factorize propagators and operator constructions

$$C_{ij}(t) \;=\; \mathrm{Tr}\left[\Phi^i(t)\; P(t,0)\; \Phi^j(0) P(0,t)\right]$$

$$\Phi^i_{\alpha\beta}(t) \;=\; V(t)^\dagger \Gamma^i_{\alpha\beta}(t) V(t)$$ **matrix rep. of operator**

$$P_{\alpha\beta}(t,0) \;=\; V(t)^\dagger \mathcal{M}^{-1}_{\alpha\beta}(t,0) V(0)$$ ***perambulator***

Multigrid & GPUs have been key to construction quark line

`and a powerful ally it is'

arxiv:0905.2160

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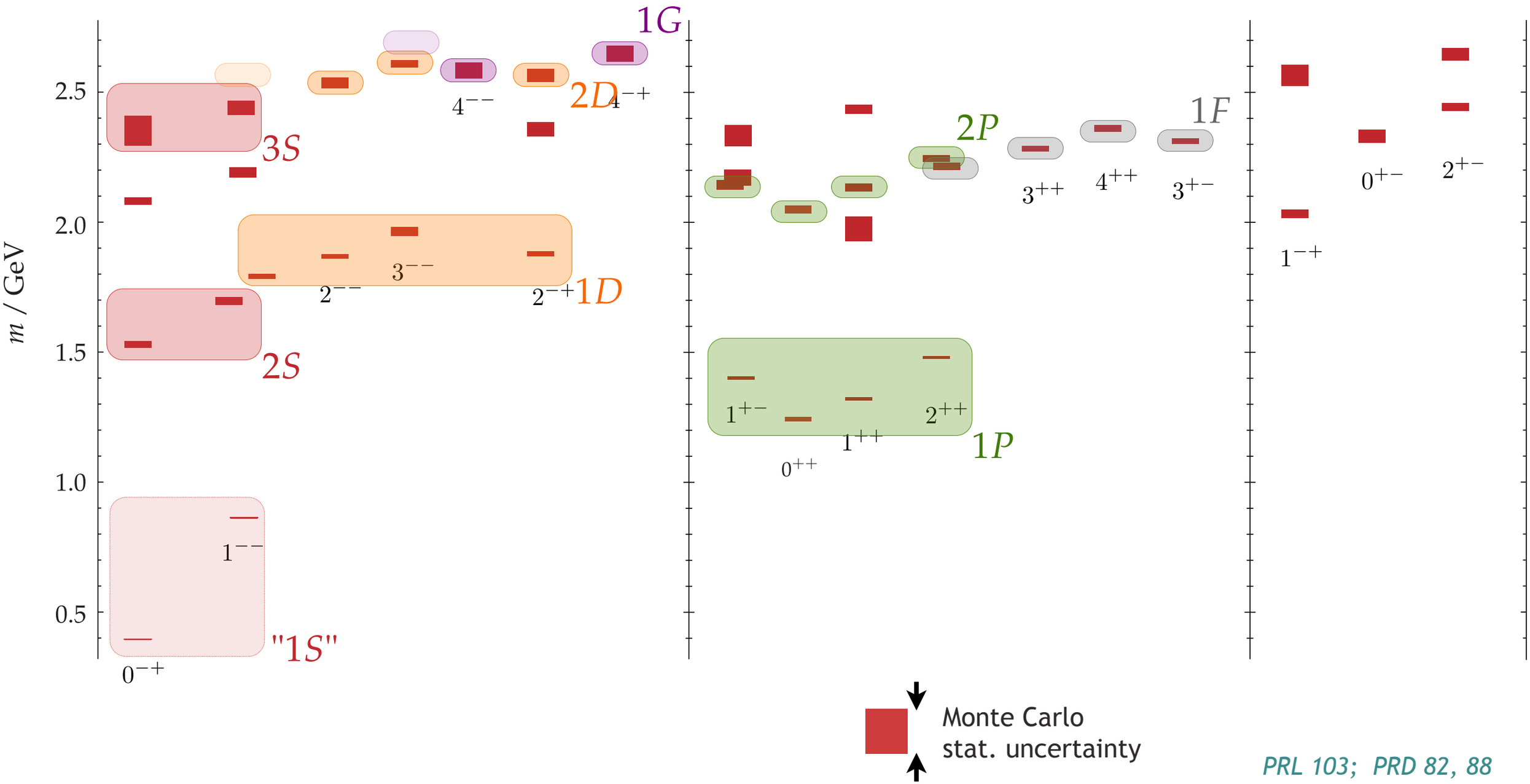
Glimpse of meson spectrum from lattice QCD

- Appears to be some $q\bar{q}$-like near-degeneracy patterns - isovectors

$m_\pi \sim 391\,\mathrm{MeV}$



PRL 103; PRD 82, 88

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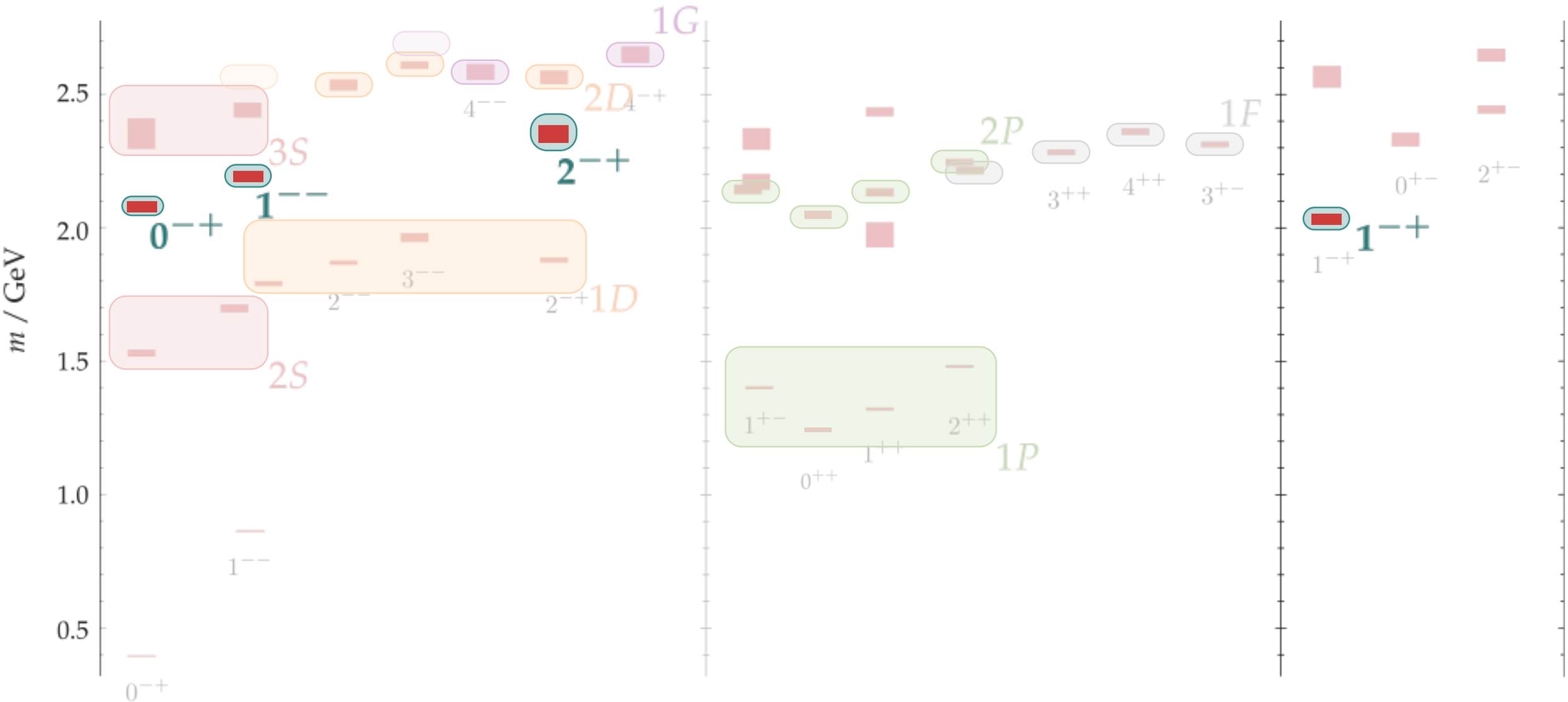
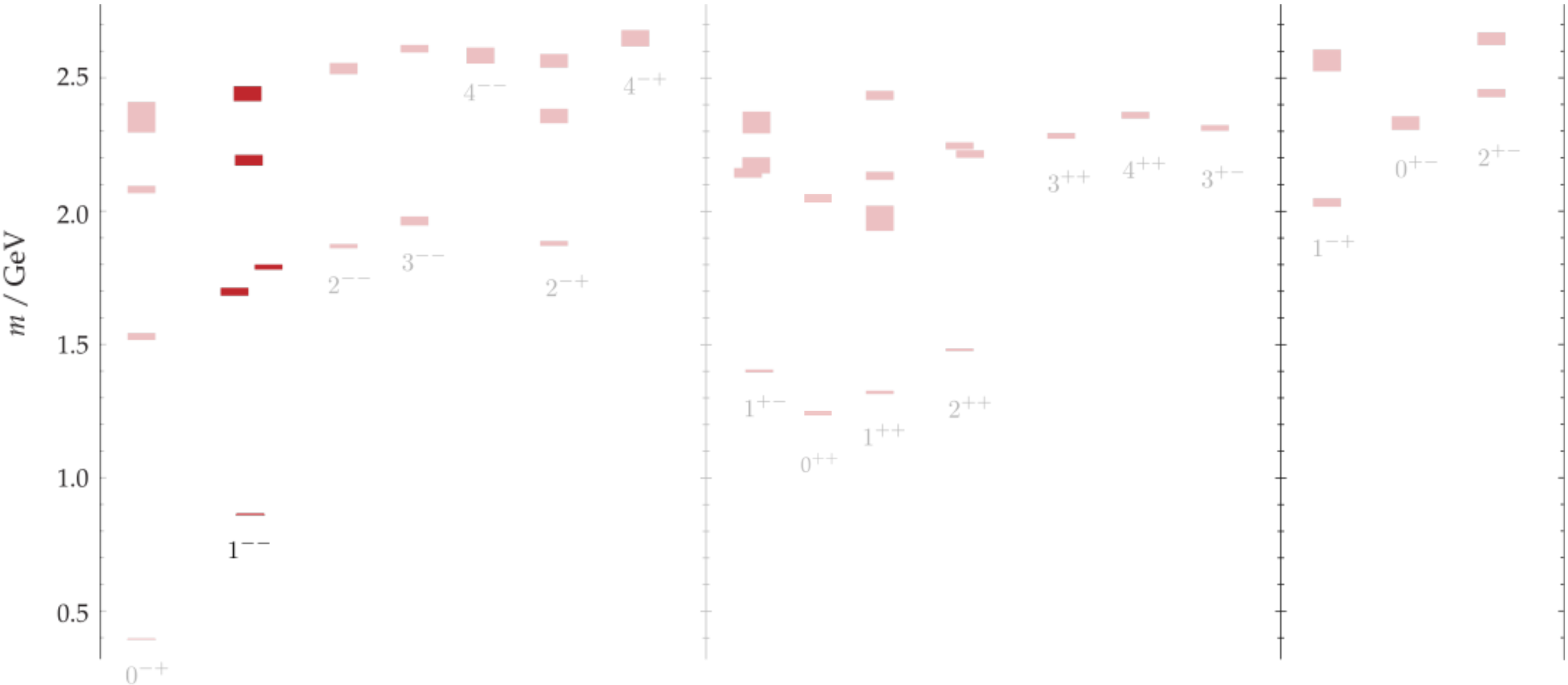
qq interpretation?

- "Extra" non-exotic states at same energy scale as lightest exotic?



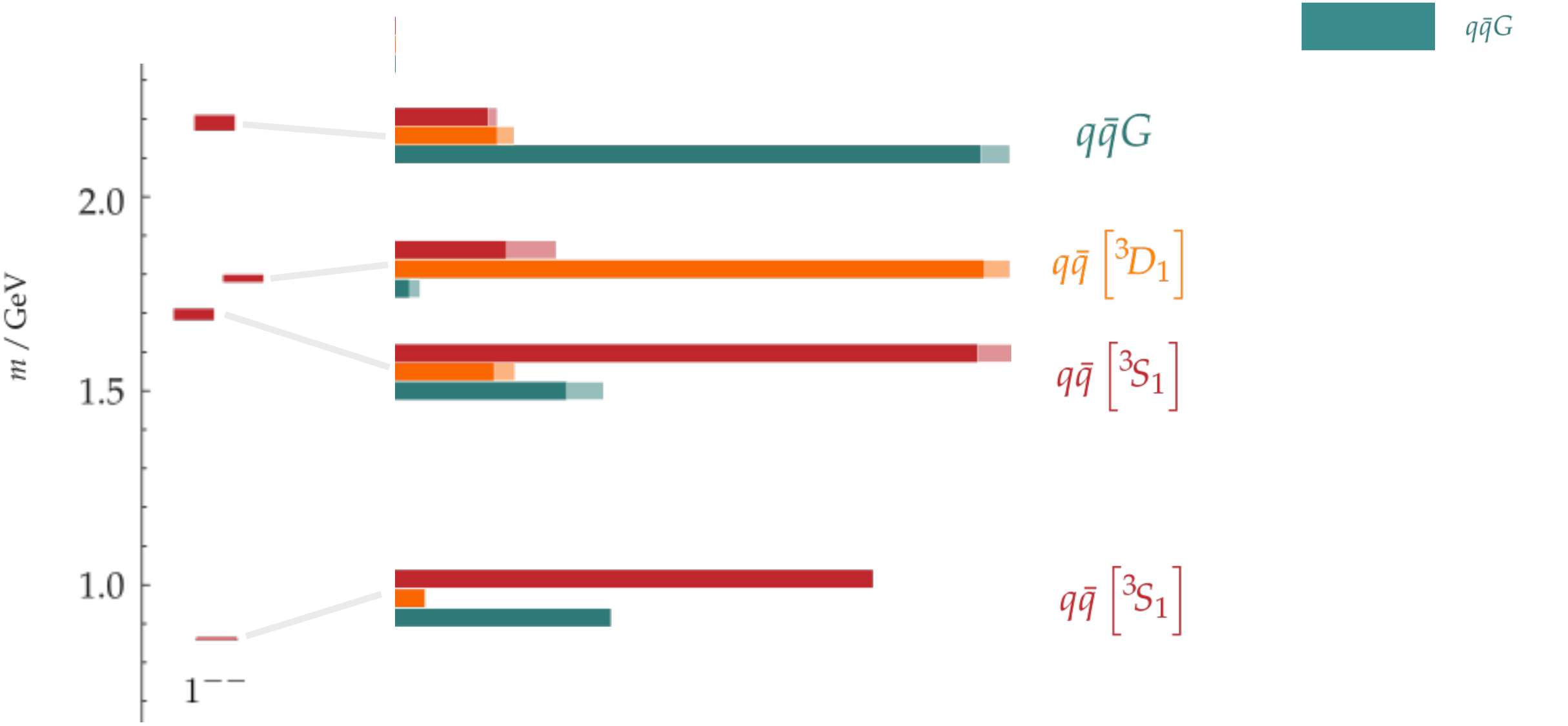
qq interpretation?

- Consider the relative size of operator overlaps $\langle n | \mathcal{O}_i^\dagger | \varnothing \rangle$



1^{--} operator overlaps

- Consider the relative size of operator overlaps $\langle \mathfrak{n} | \mathcal{O}_i^\dagger | \varnothing \rangle$



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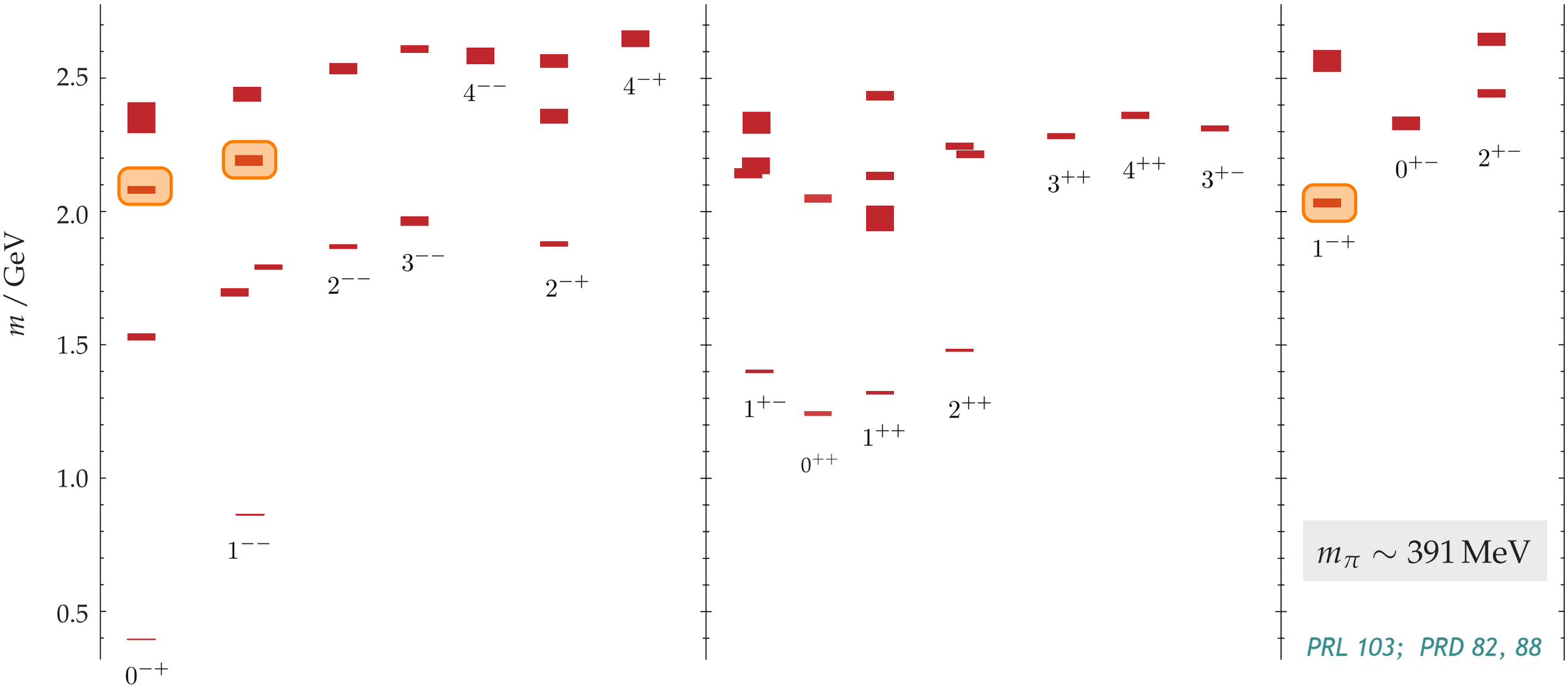
Glimpse of meson spectrum from lattice QCD

- ‘super’-multiplet of **hybrid mesons** roughly 1.2 GeV above the ρ

$(0,\mathbf{1},2)^{-+},\,1^{--}$



PRL 103; PRD 82, 88

- these states have a dominant overlap onto $\bar{\psi}\Gamma[D,D]\psi \;\sim\; [q\bar{q}]_{\mathbf{8}_c} \otimes B_{\mathbf{8}_c}$

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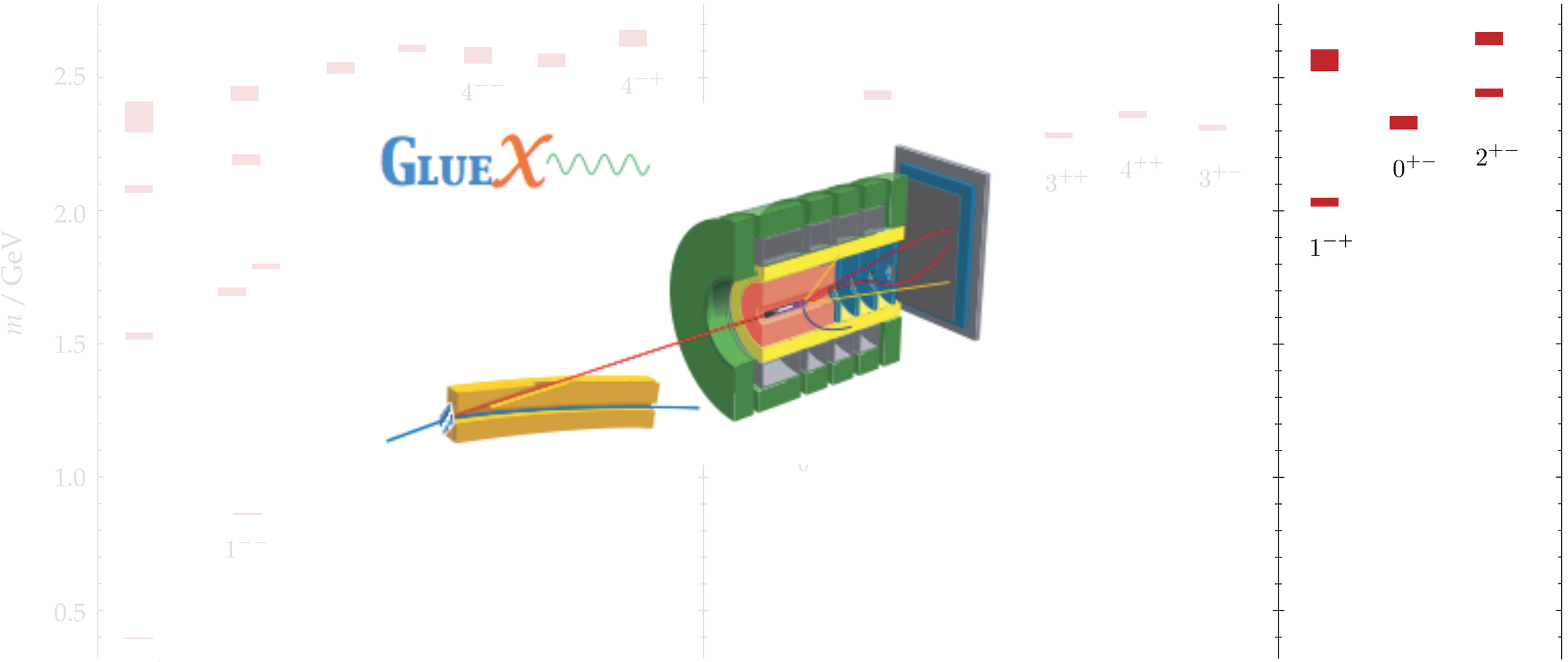
Glimpse of meson spectrum from lattice QCD

Multiple exotic mesons within range of GlueX

EXOTIC MESONS

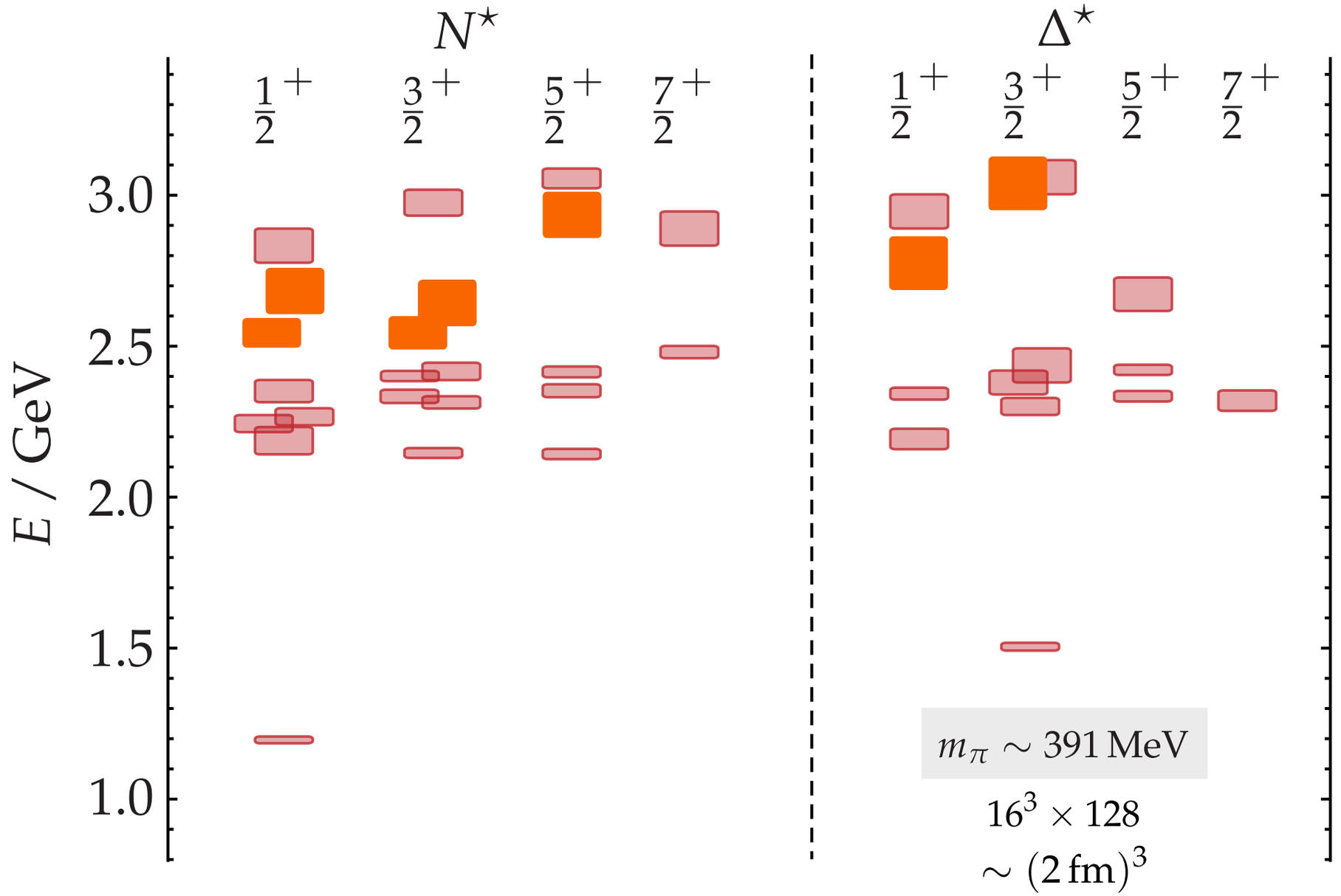


PRL 103; PRD 82, 88

Excited light quark baryons

- A ‘super’-multiplet of **hybrid baryons**

Searches in CLAS12



spectrum from large basis of baryon operators

PRD84 074508 (2011)
PRD85 054016 (2012)

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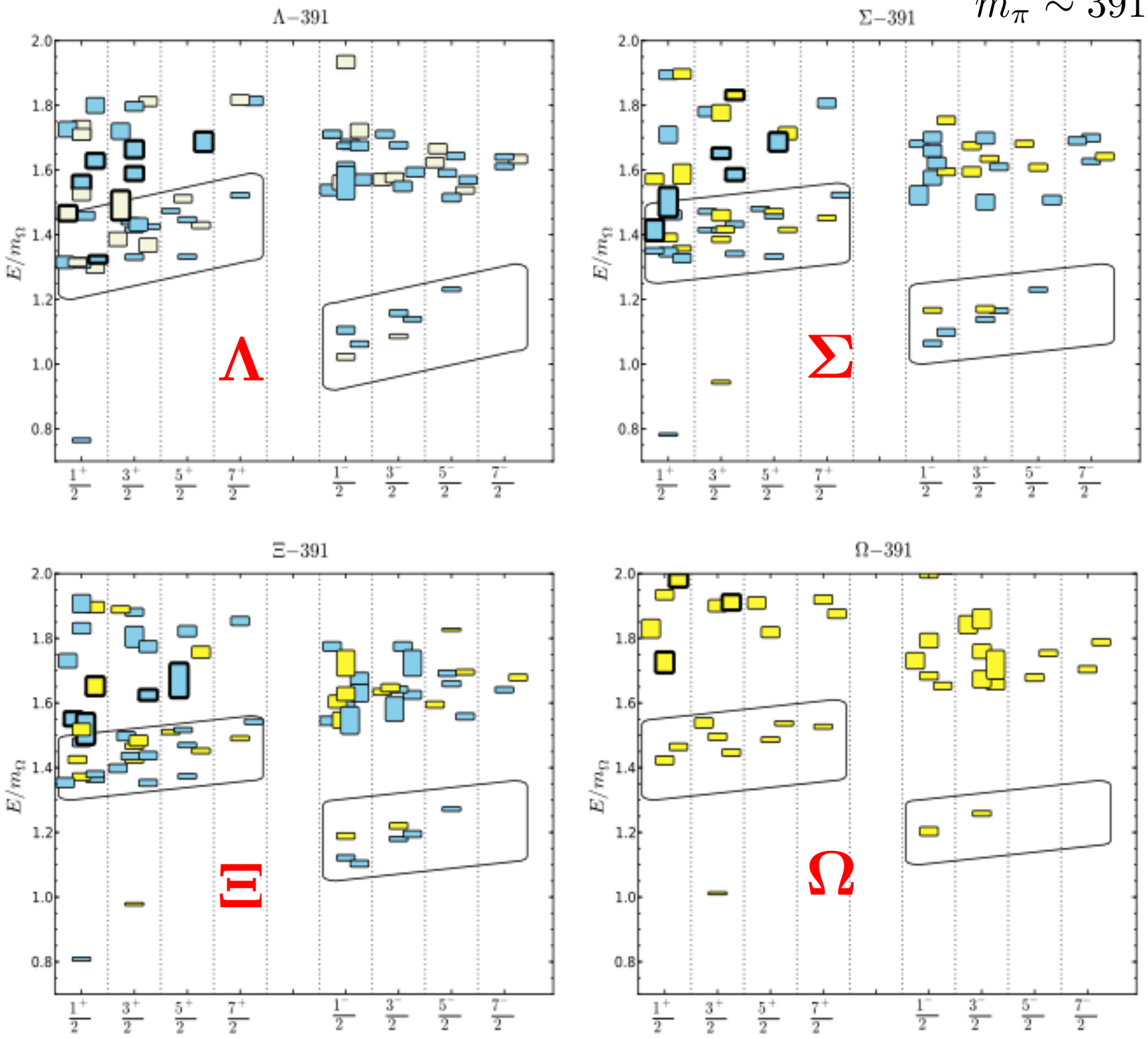
Excited strange (and charm) quark baryons

$m_\pi \sim 391$ MeV

Light quarks – SU(3) flavor broken

Full non-relativistic quark model counting

Some mixing of SU(3) flavor irreps



PRD87 054506 (2013)
PRD90 074504 (2014)
PRD91 054502 (2015)

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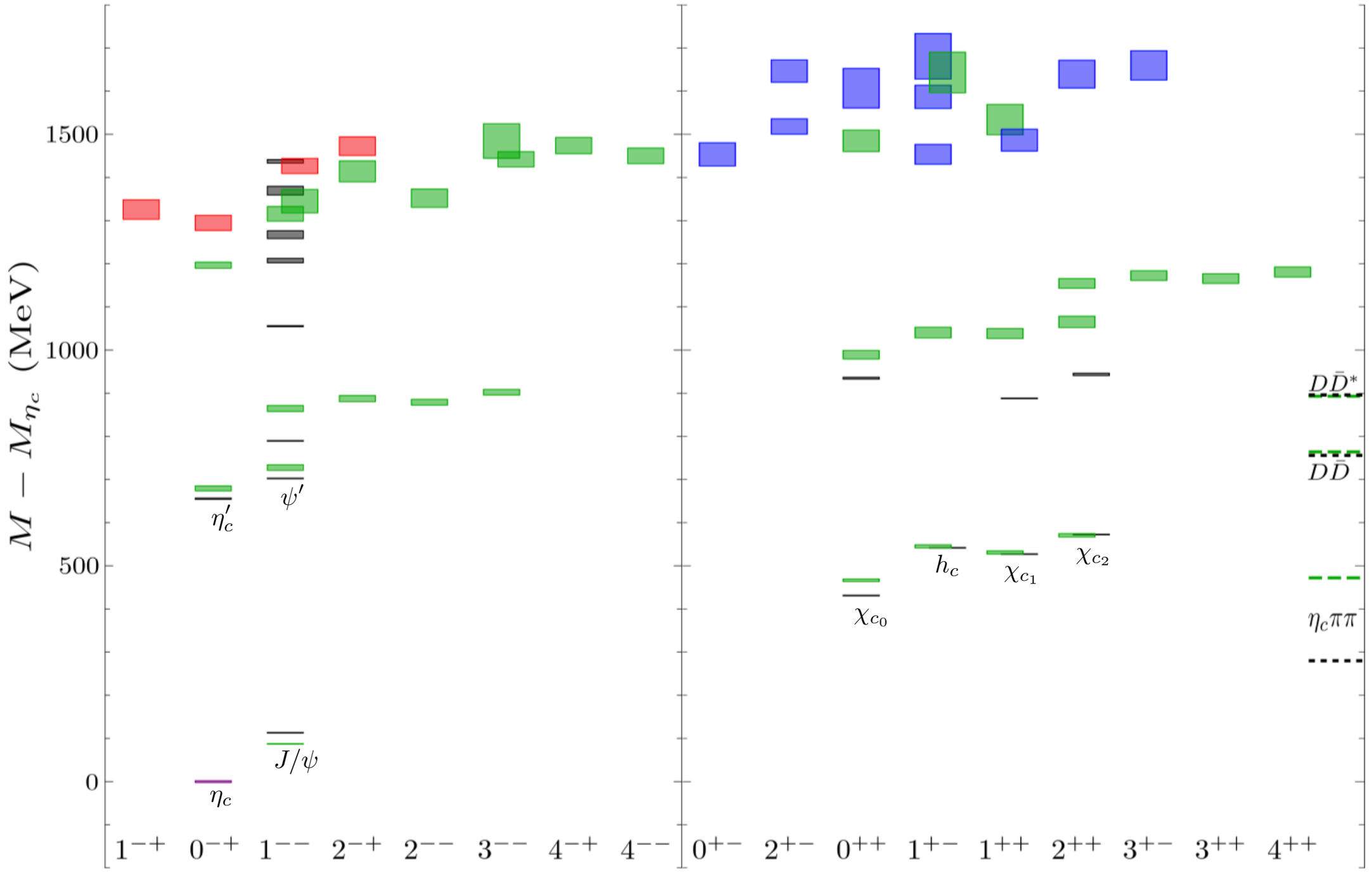
Charmonium spectrum

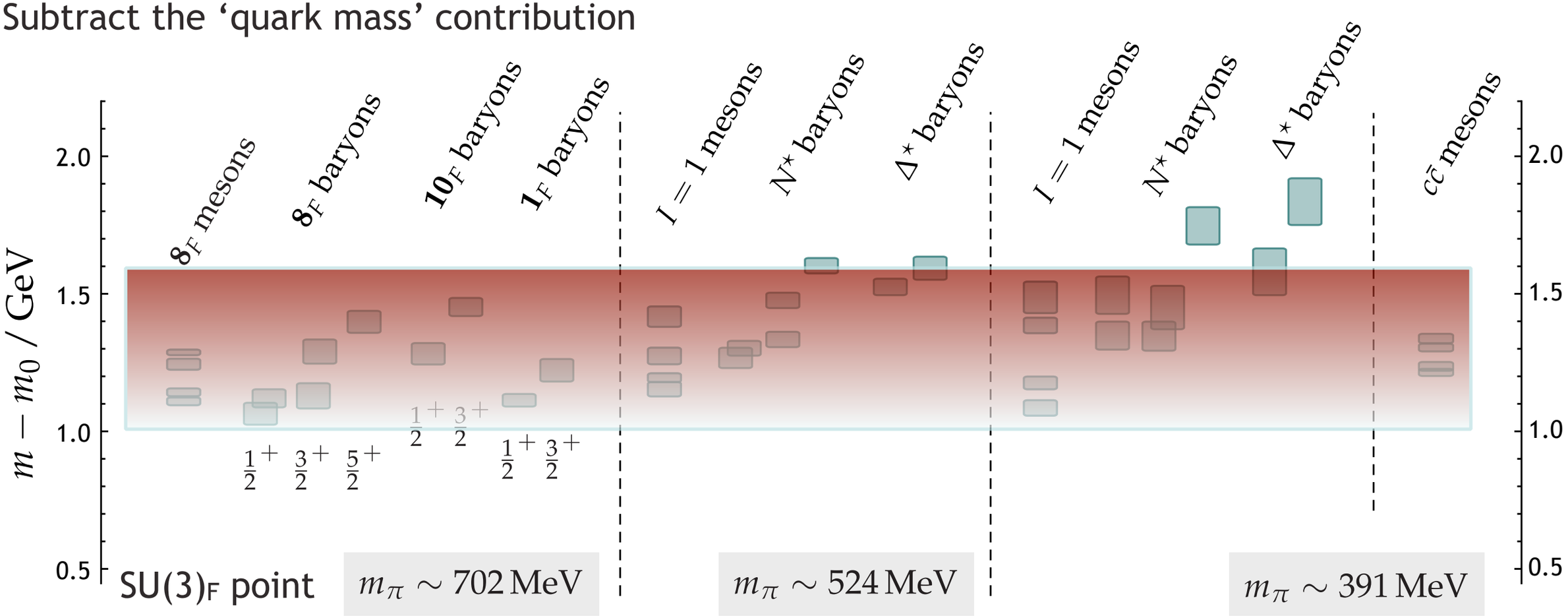
- A ‘super’-multiplet of **hybrid mesons**

Cheung, O’Hara, Tims, Moir, Peardon, Ryan, Thomas (2016)

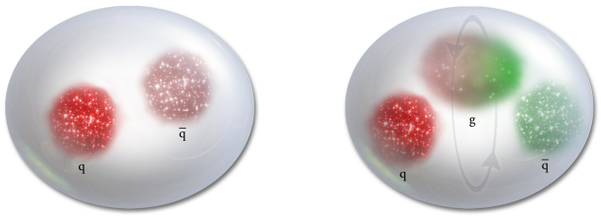


Chromo-magnetic excitation

- Subtract the ‘quark mass’ contribution



Pattern of states suggest gluonic excitations



Conventional Meson Hybrid Meson

- Common energy scale of gluonic excitation $\sim 1.3\,\mathrm{GeV}$

➡ Need to know decay modes and rates to compare to expt.

HADRON SPECTRUM: PRD83 (2011); PRD88 (2013)

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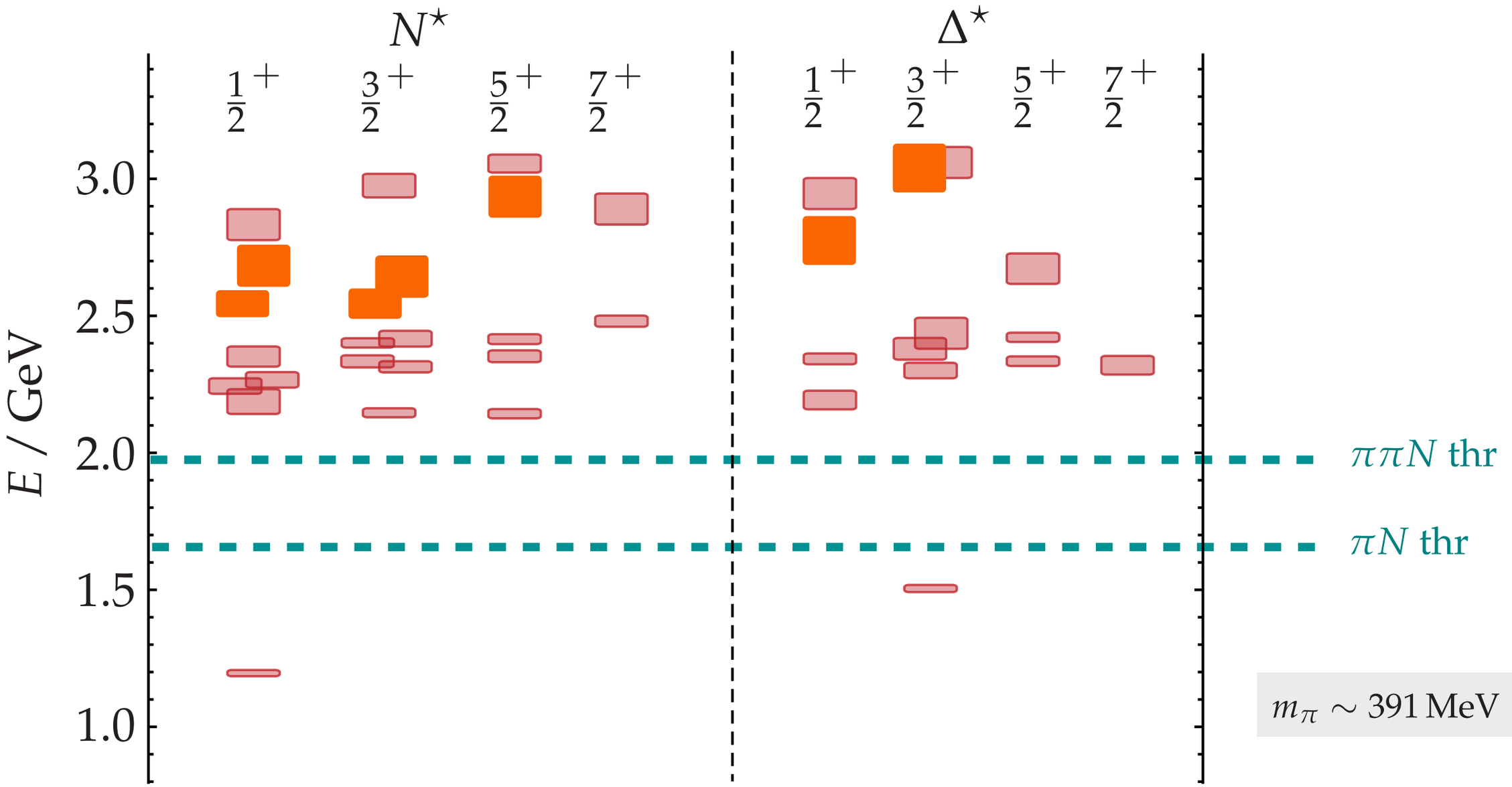
Excited states are resonances

- Initial determination of spectrum with only qqq style operators
  → missing scattering states

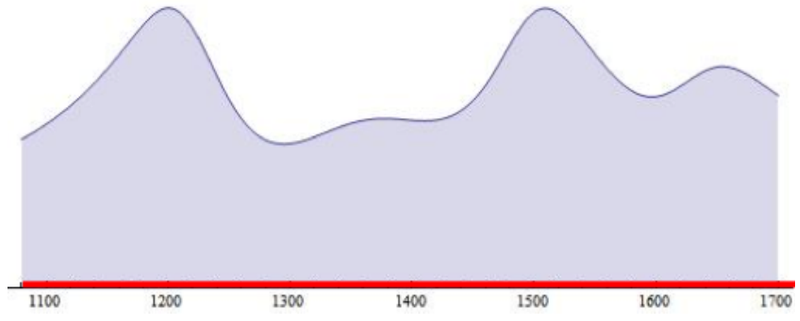


- Some initial results in S11 & P33 have appeared (Graz group)

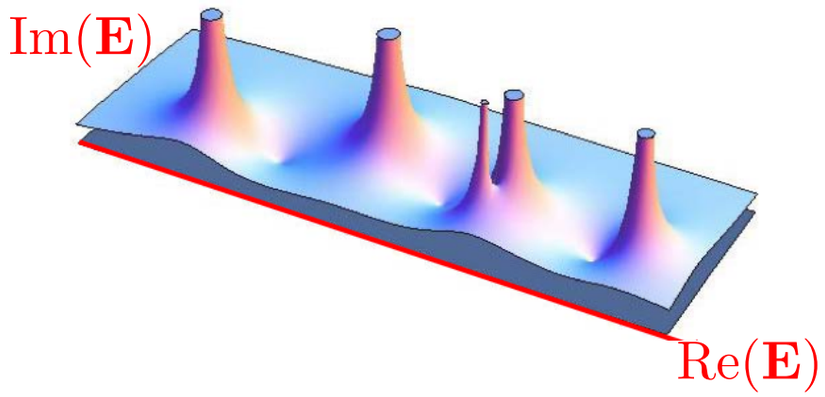
Resonances

Manifest as behavior of real scattering amplitudes

- E.g., πN πN

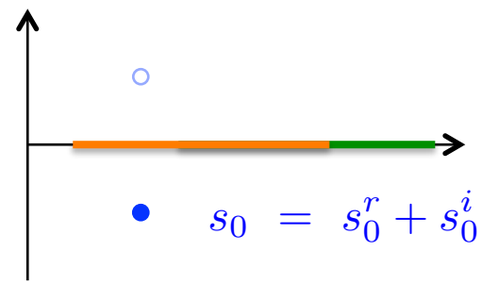


$\mathbf{E}$ (MeV)



Formally defined as a pole in a partial-wave scattering amplitude

$$t_l(s) \sim \frac{R}{s_0 - s} + \ldots$$



Different channels should have same pole location

Pole structure (location and residue) gives decay information

QFT in a periodic cube

Lüscher (1986) : application to 3+1dim quantum field theories

subsequent extensions for moving frames, coupled-channel systems - will come back to this

quantization condition:

solutions, E_n, of

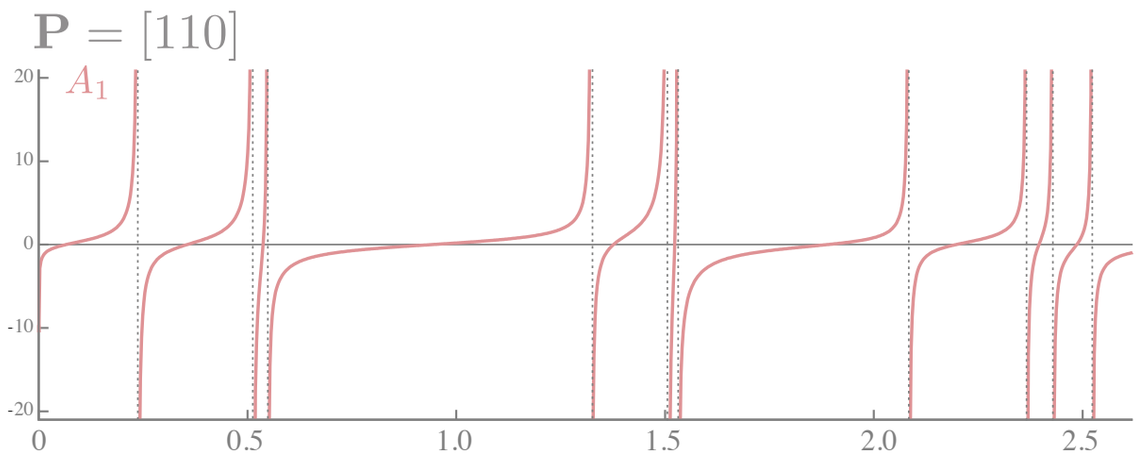
$$\det\left[\mathbf{1} + i\boldsymbol{\rho}\cdot\mathbf{t}\cdot(\mathbf{1}+i\boldsymbol{\mathcal{M}})\right] = 0$$

$\boldsymbol{\rho}(E)$ phase-space

$\mathbf{t}(E)$ scattering matrix $\quad\left(\mathbf{S} = \mathbf{1} + 2i\sqrt{\boldsymbol{\rho}}\cdot\mathbf{t}\cdot\sqrt{\boldsymbol{\rho}}\right)$

$\boldsymbol{\mathcal{M}}(E,L)$ finite-volume function

technicalities: partial-wave basis not ‘diagonal’ in a cube



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solutions, E_n, of

$$\det\left[\mathbf{1} + i\boldsymbol{\rho}\cdot\mathbf{t}\cdot(\mathbf{1}+i\boldsymbol{\mathcal{M}})\right] = 0$$

simplest case — elastic scattering of a single partial wave:

$$t^{(\ell)} = \frac{1}{\rho} e^{i\delta_\ell}\sin\delta_\ell \quad \Rightarrow \quad \cot\delta(E) = \mathcal{M}(E,L)$$

E_n value maps to $\delta(E_n)$

need to compute the spectrum …

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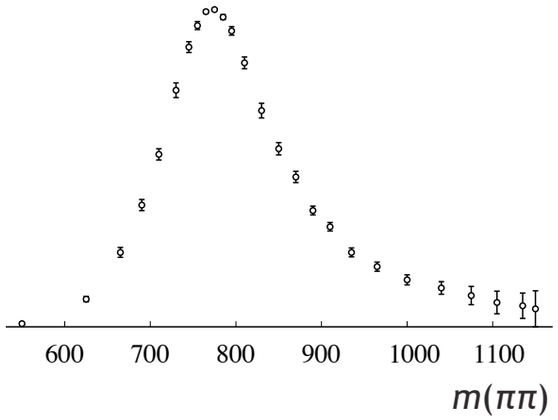
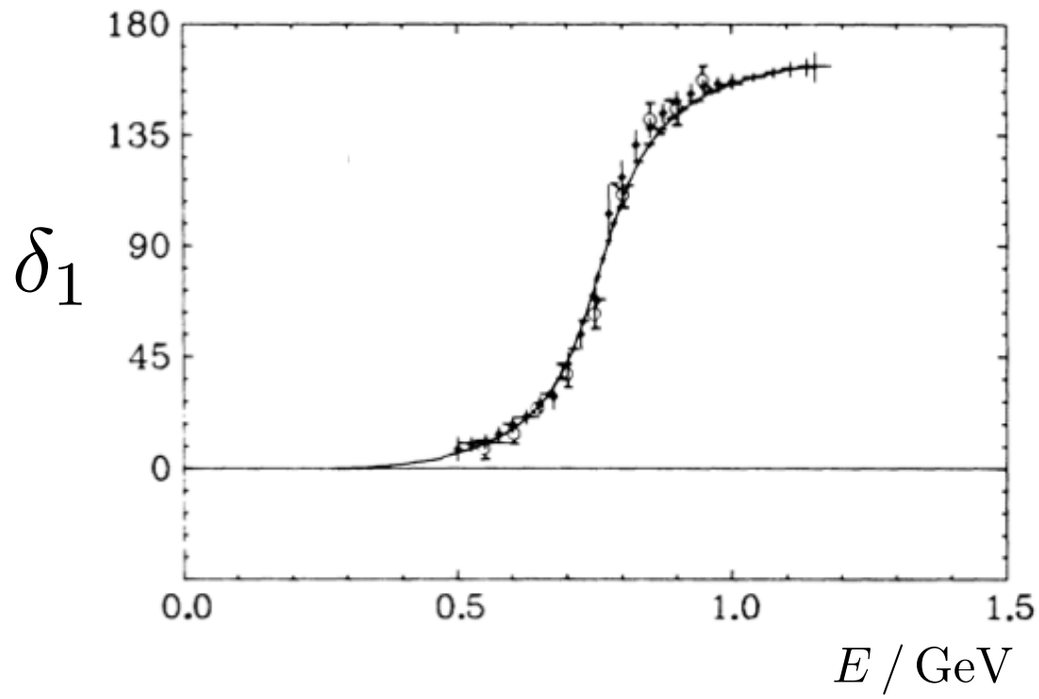
An elastic resonance — the ρ in $\pi\pi$



canonical resonance ‘bump’
described by a rapidly rising phase-shift

scattering phase-shift



PHYSICAL REVIEW D VOLUME 7, NUMBER 5 1 MARCH 1973

$\pi\pi$ Partial-Wave Analysis from Reactions $\pi^+p \to \pi^+\pi^-\Delta^{++}$ and $\pi^+p \to K^+K^-\Delta^{++}$ at 7.1 GeV/c†

S. D. Protopopescu,* M. Alston-Garnjost, A. Barbaro-Galtieri, S. M. Flatté,‡
J. H. Friedman,§ T. A. Lasinski, G. R. Lynch, M. S. Rabin,‖ and F. T. Solmitz
Lawrence Berkeley Laboratory, University of California, Berkeley, California 94720
(Received 25 September 1972)

Lattice QCD spectrum

Variational analysis of a matrix of correlation functions $C_{ij}(t) = \left\langle 0 \middle| \mathcal{O}_i(t) \mathcal{O}_j(0) \middle| 0 \right\rangle$

$$= \sum_{\mathfrak{n}} e^{-E_{\mathfrak{n}} t} \left\langle 0 \middle| \mathcal{O}_i \middle| \mathfrak{n} \right\rangle \left\langle \mathfrak{n} \middle| \mathcal{O}_j \middle| 0 \right\rangle$$

operator basis: ‘single-meson’ + ‘meson-meson’

$$\overline{\psi} \mathbf{\Gamma} \psi \qquad \sum_{\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2} C(\mathbf{p}_1, \mathbf{p}_2; \mathbf{p})\, M_1(\mathbf{p}_1)\, M_2(\mathbf{p}_2)$$

(& tetraquark & …)

$$\mathbf{p} = \tfrac{2\pi}{L} [n_x, n_y, n_z]$$

maximum momentum guided by non-interacting energies

$$\sqrt{m_1^2 + \mathbf{p}_1^2} + \sqrt{m_2^2 + \mathbf{p}_2^2}$$

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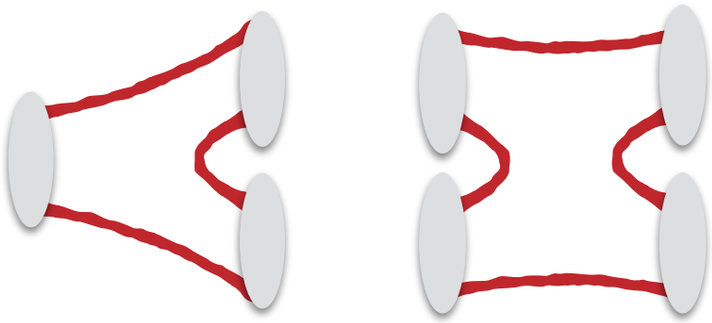
now need to evaluate diagrams like



Distillation handles quark annihilation lines

Linear ops from KNLs+GPUs

`Don’t underestimate the power…’

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Lattice QCD spectrum

Variational analysis of a matrix of correlation functions $C_{ij}(t) = \langle 0 | \mathcal{O}_i(t) \mathcal{O}_j(0) | 0 \rangle$

$$= \sum_{\mathfrak{n}} e^{-E_{\mathfrak{n}} t} \langle 0 | \mathcal{O}_i | \mathfrak{n} \rangle \langle \mathfrak{n} | \mathcal{O}_j | 0 \rangle$$

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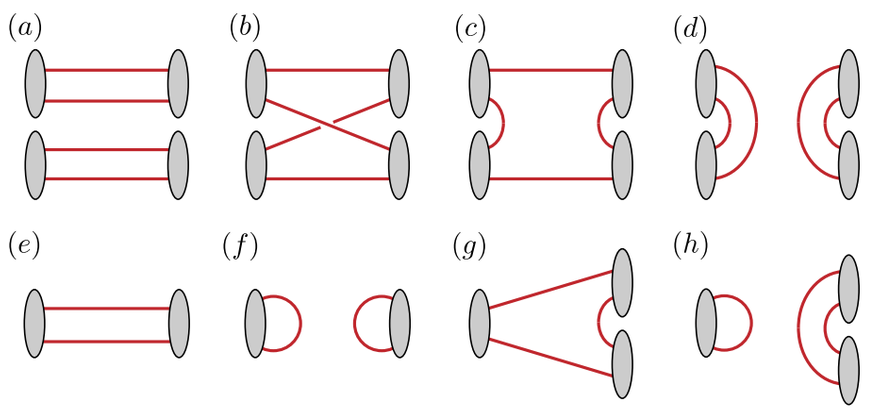
maximum momentum guided by non-interacting energies

$$\sqrt{m_1^2 + \mathbf{p}_1^2} + \sqrt{m_2^2 + \mathbf{p}_2^2}$$

Can be lots of Wick contractions, and momentum projections

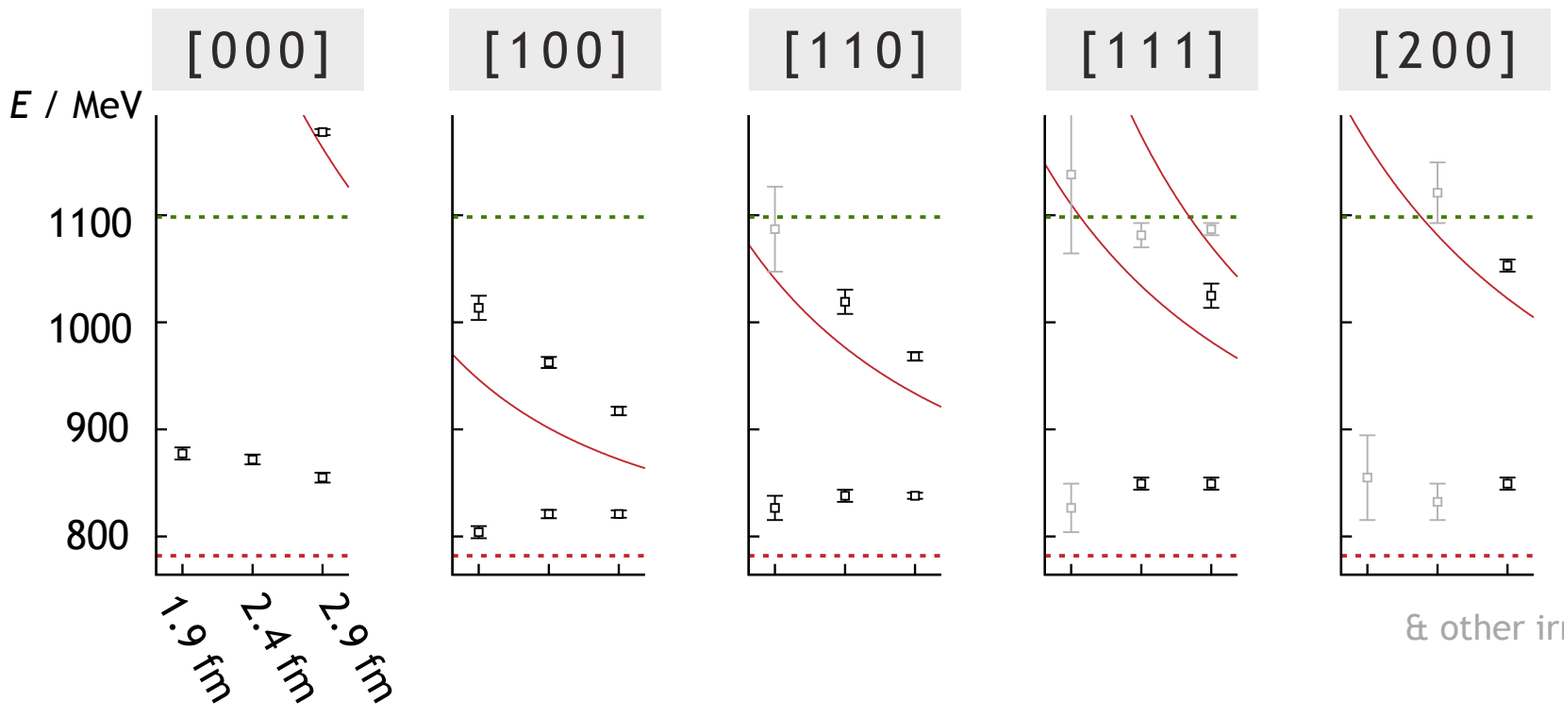
Worst case: rest-frame —> p=100 -> 6x, p=110 -> 12x, p=111 -> 8x



An elastic resonance — the ρ in $\pi\pi$ — lattice QCD

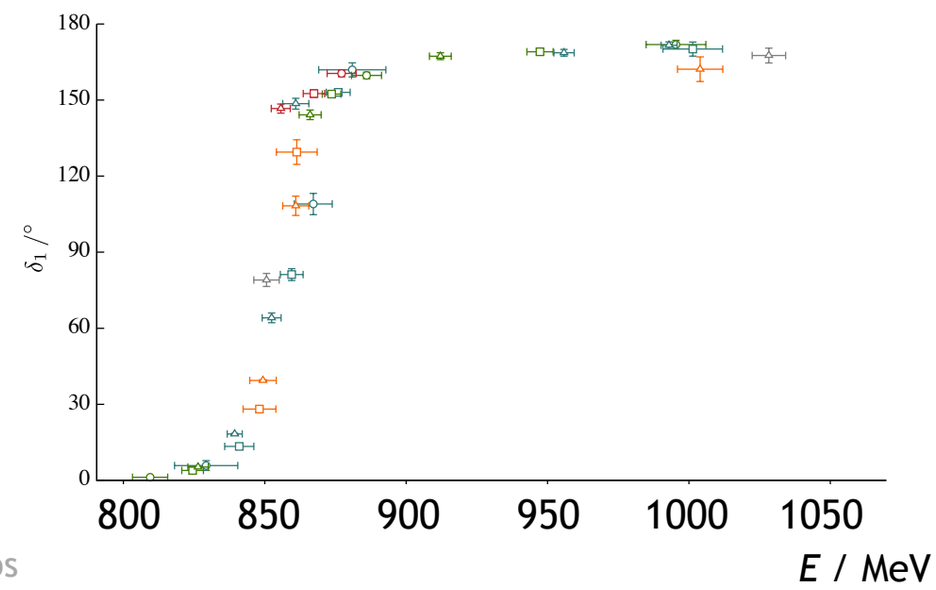
PRD87 034505 (2013)

m_π ~ 391 MeV



& other irreps

scattering phase-shift



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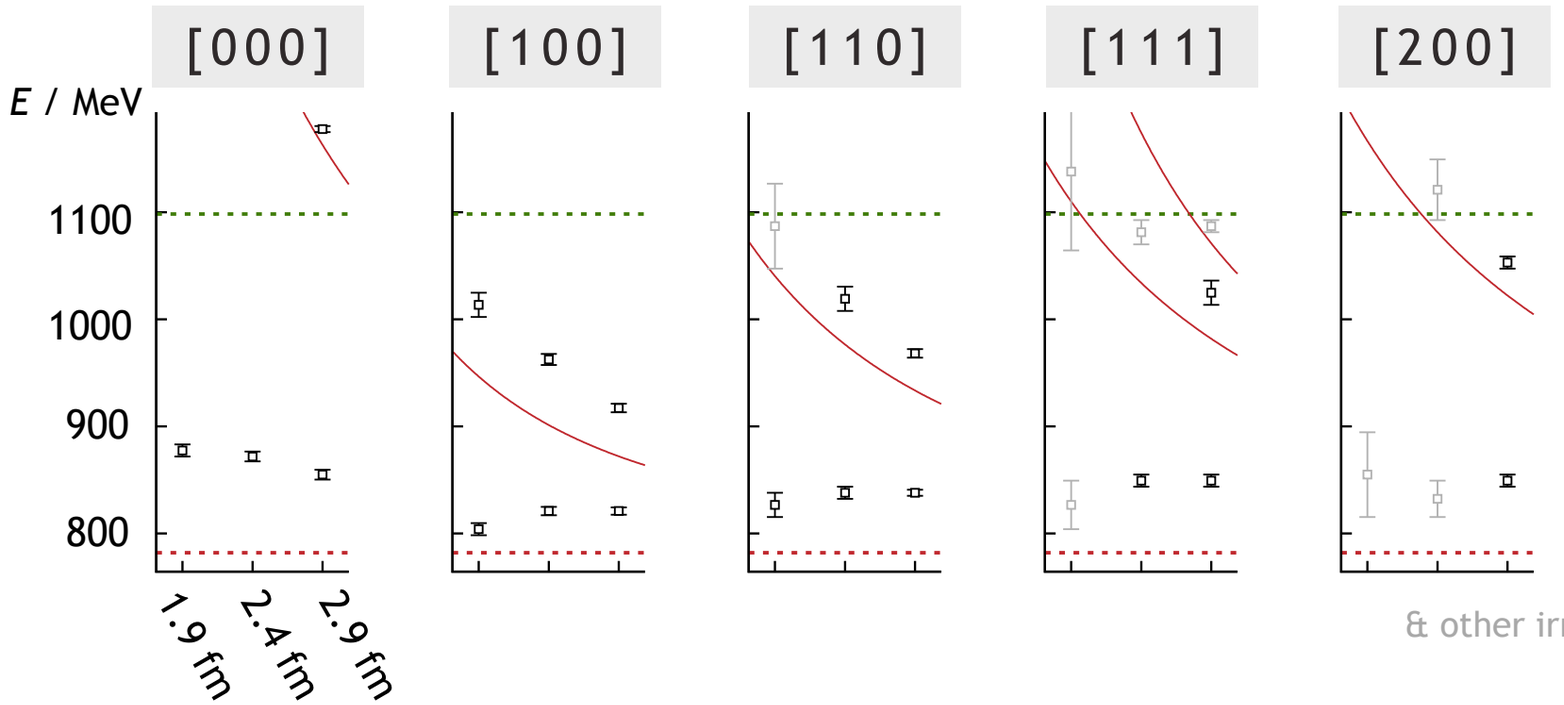
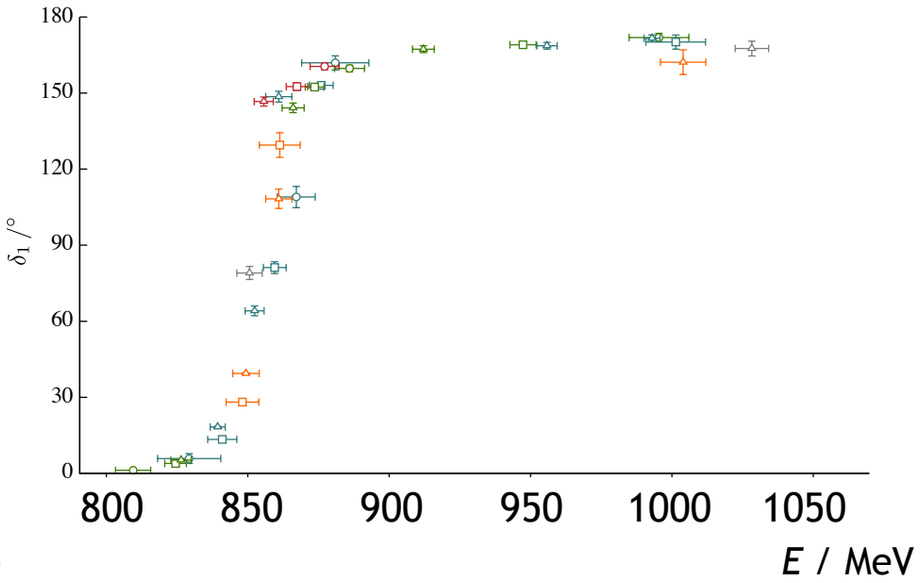


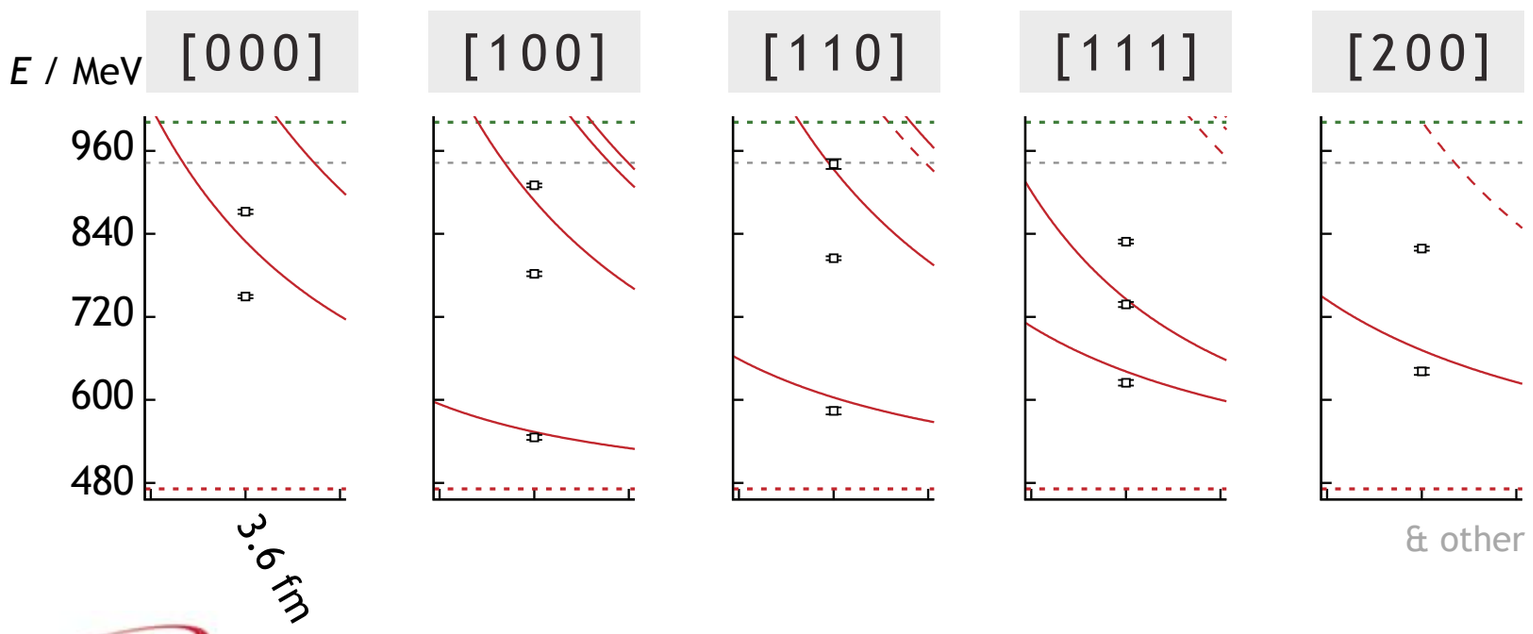
& other irreps

scattering phase-shift



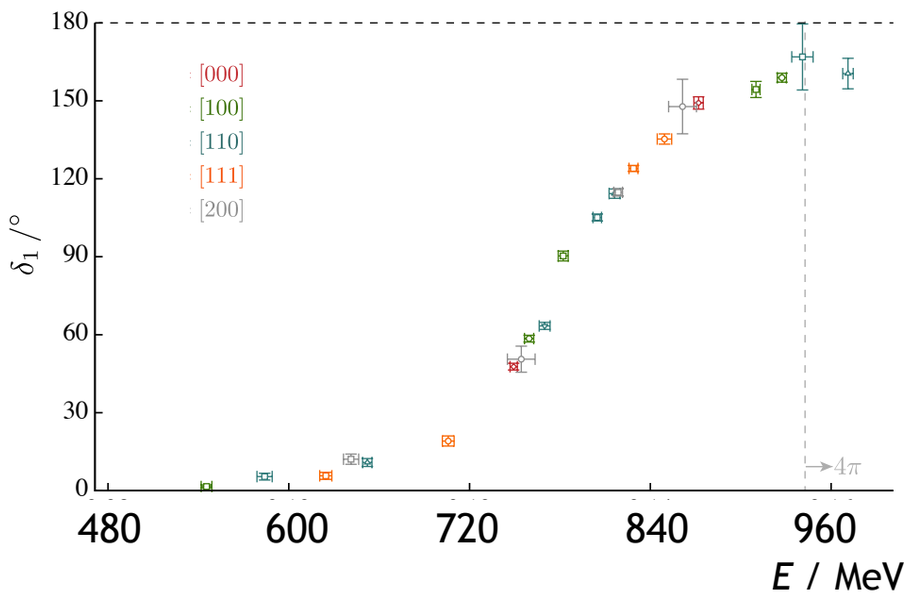
PRD92 094502 (2015)

m_π ~ 236 MeV



& other irreps

scattering phase-shift



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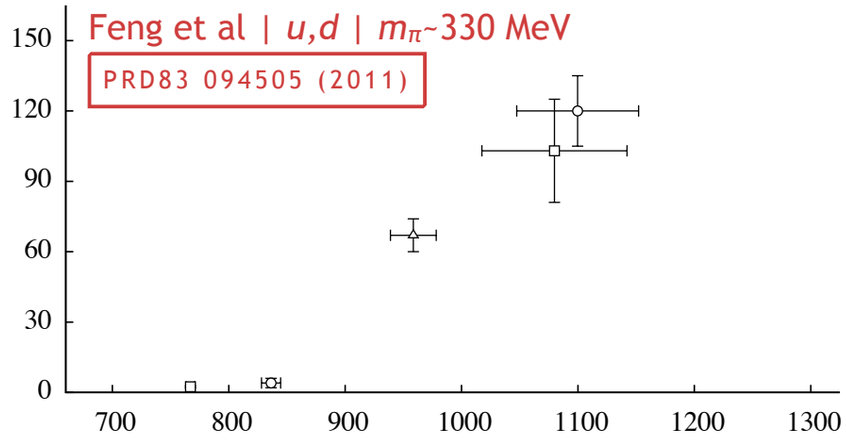
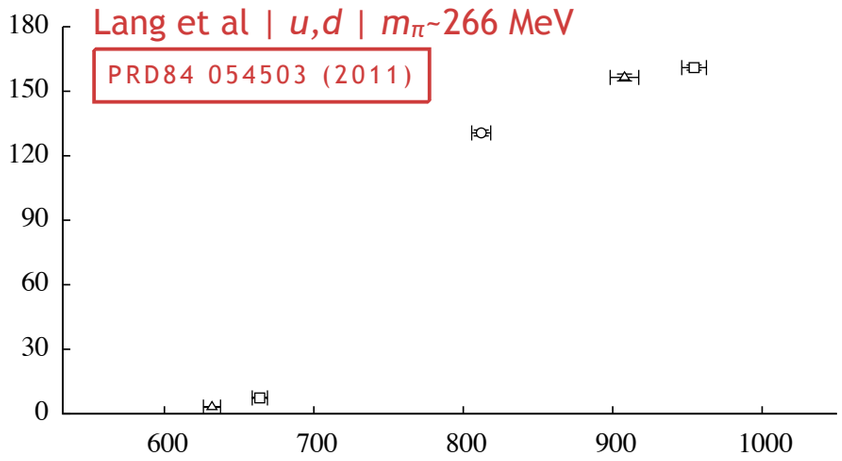
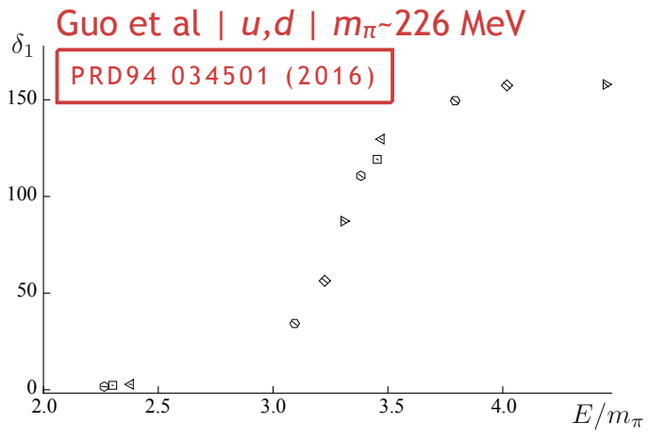
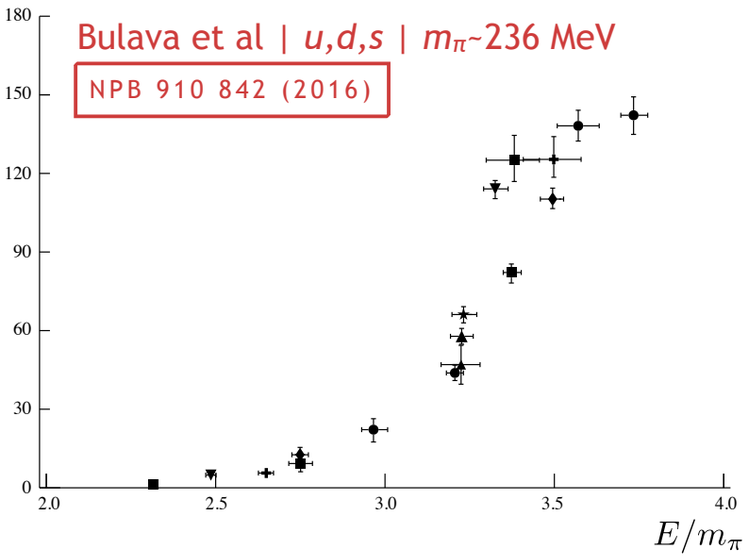
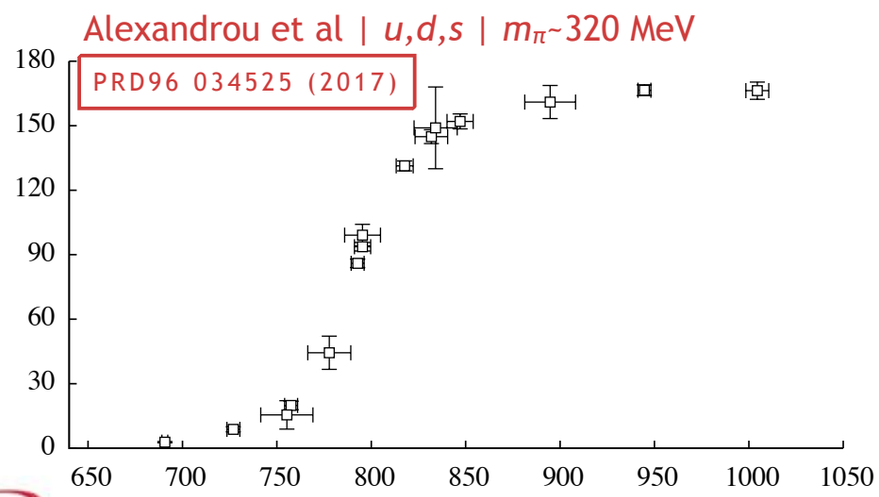
An elastic resonance — the ρ in $\pi\pi$ — lattice QCD

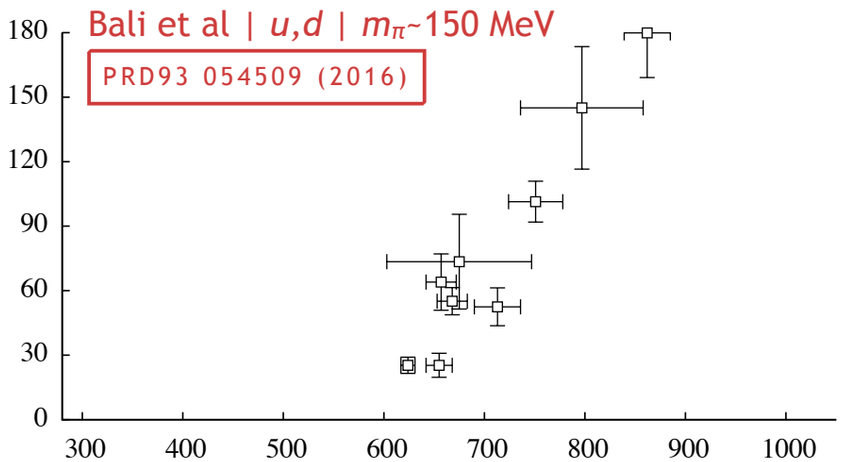












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Coupled-channel resonances

Most resonances decay into more than one final state

e.g. two-channel scattering described by a ***t***-matrix $\mathbf{t}(E) = \begin{pmatrix} t_{11}(E) & t_{12}(E) \\ t_{21}(E) & t_{22}(E) \end{pmatrix}$

Finite-volume spectrum as a function of scattering becomes more complicated

coupled-channel spectrum

solutions $E_n(L)$ of

$$\det\left[\mathbf{1} + i\boldsymbol{\rho}(E)\cdot\boldsymbol{t}(E)\cdot(\mathbf{1} + i\boldsymbol{\mathcal{M}}(E,L))\right] = 0$$

No longer a one-to-one mapping from energy to scattering …

Coupled-channels

solutions, E_n, of

$$\det\left[\mathbf{1} + i\boldsymbol{\rho}\cdot\mathbf{t}\cdot(\mathbf{1}+i\boldsymbol{\mathcal{M}})\right] = 0$$

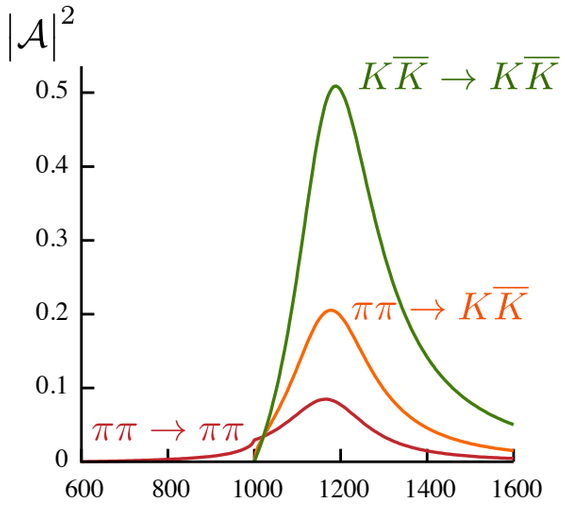
$$\mathbf{t} = \begin{pmatrix} \pi\pi\to\pi\pi & \pi\pi\to K\bar{K} \\ K\bar{K}\to\pi\pi & K\bar{K}\to K\bar{K} \end{pmatrix}$$

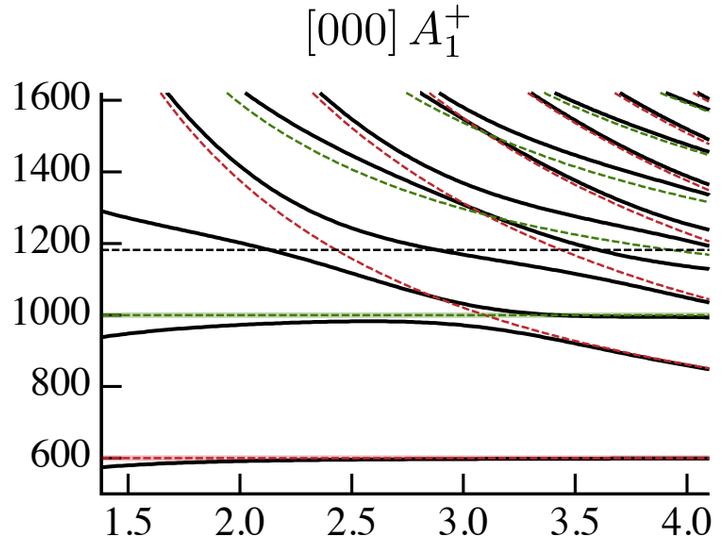
$\boldsymbol{\rho}(E)$ phase-space

$\mathbf{t}(E)$ scattering matrix

$\boldsymbol{\mathcal{M}}(E,L)$ finite-volume function

for a known $\boldsymbol{t}$(E) → can predict E_n





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Coupled-channels

solutions, E_n, of

$$\det\left[\mathbf{1} + i\boldsymbol{\rho}\cdot\mathbf{t}\cdot(\mathbf{1}+i\boldsymbol{\mathcal{M}})\right] = 0$$

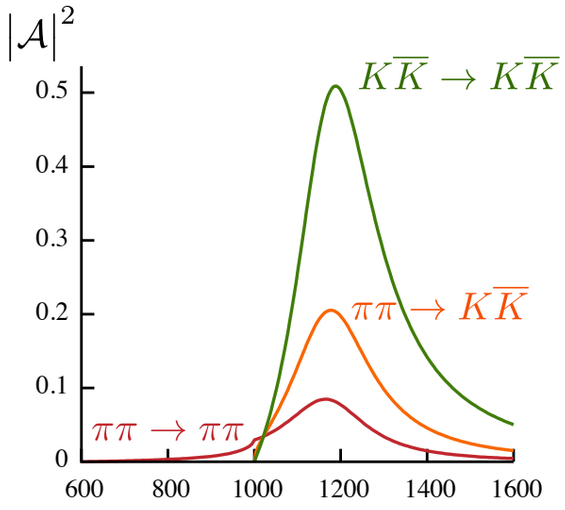
$$\mathbf{t} = \begin{pmatrix} \pi\pi\to\pi\pi & \pi\pi\to K\bar{K} \\ K\bar{K}\to\pi\pi & K\bar{K}\to K\bar{K} \end{pmatrix}$$

$\boldsymbol{\rho}(E)$ phase-space

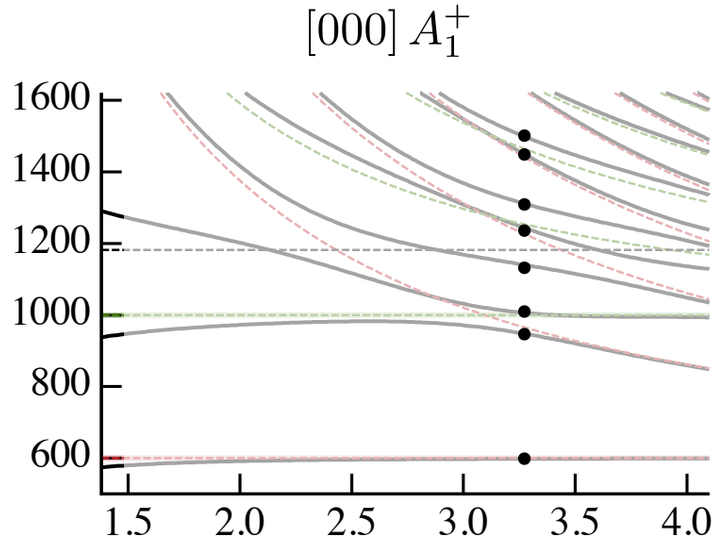
$\mathbf{t}(E)$ scattering matrix

$\boldsymbol{\mathcal{M}}(E,L)$ finite-volume function

for a known $\boldsymbol{t}$(E) → can predict E_n



?



but how do we perform the inverse mapping ?

Coupled-channels

solutions, E_n, of

$$\det\Big[\mathbf{1} + i\boldsymbol{\rho}\cdot\mathbf{t}\cdot(\mathbf{1}+i\boldsymbol{\mathcal{M}})\Big] = 0$$

$\boldsymbol{\rho}(E)$ phase-space

$\mathbf{t}(E)$ scattering matrix

$\boldsymbol{\mathcal{M}}(E,L)$ finite-volume function

parameterize the energy dependence of the ***t*-**matrix

***K*-**matrix is a convenient approach (manifest unitarity)

$$\mathrm{Im}\, t_{ij}(s) = -\delta_{ij}\,\rho_i(s)\,\Theta\big(s - s^{(i)}_{\mathrm{thr.}}\big)$$

$\mathbf{t}^{-1}(E) = \mathbf{K}^{-1}(E) - i\boldsymbol{\rho}(E)$ where ***K*-**matrix is “any” real matrix

Coupled-channels

solutions, E_n, of

$$\det\Big[\mathbf{1} + i\boldsymbol{\rho}\cdot\mathbf{t}\cdot(\mathbf{1}+i\boldsymbol{\mathcal{M}})\Big] = 0$$

$\boldsymbol{\rho}(E)$ phase-space

$\mathbf{t}(E)$ scattering matrix

$\boldsymbol{\mathcal{M}}(E,L)$ finite-volume function

parameterize the energy dependence of the ***t*-matrix**

***K*-matrix is a convenient approach** (manifest unitarity)

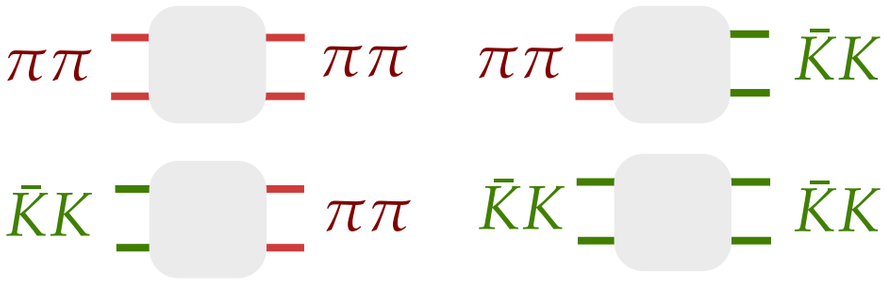
$$\mathrm{Im}\, t_{ij}(s) = -\delta_{ij}\,\rho_i(s)\,\Theta\big(s - s^{(i)}_{\mathrm{thr.}}\big)$$

$\mathbf{t}^{-1}(E) = \mathbf{K}^{-1}(E) - i\boldsymbol{\rho}(E)$ where ***K*-matrix is "any" real matrix**

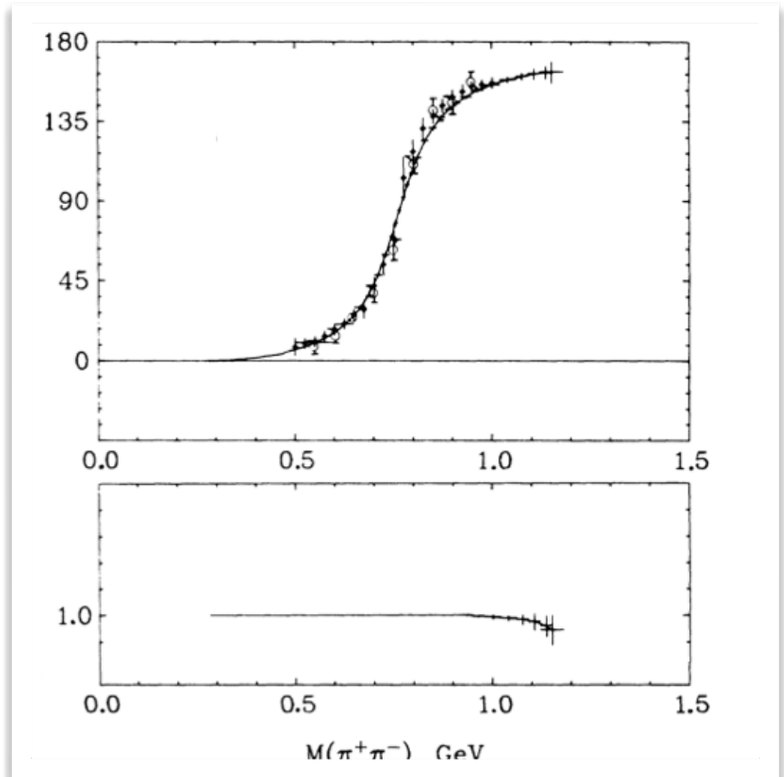
Want pole mass and residues/couplings of t-matrix

In recent years, progress towards establishing this approach

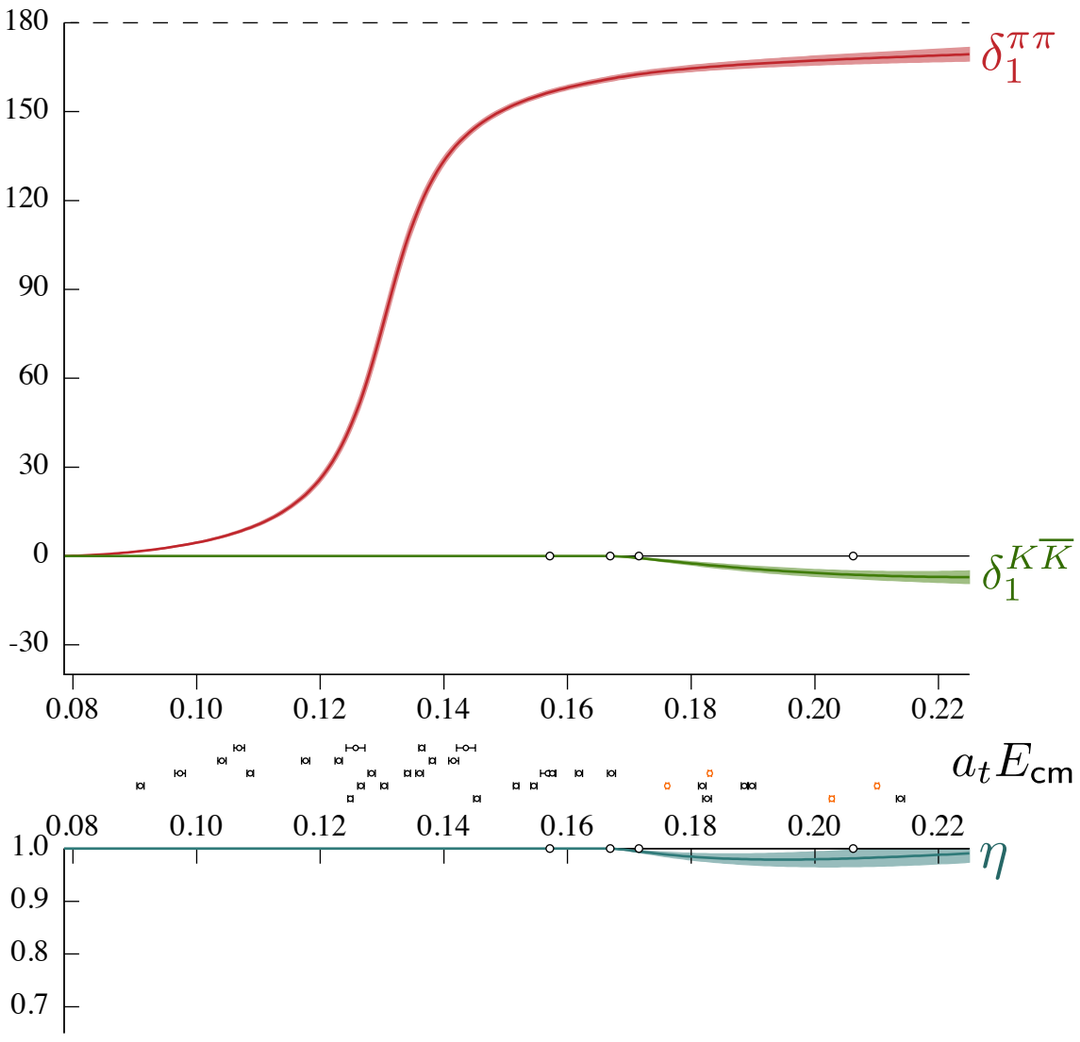
ρ resonance as a coupled channel system



PRD87 034505 (2013)

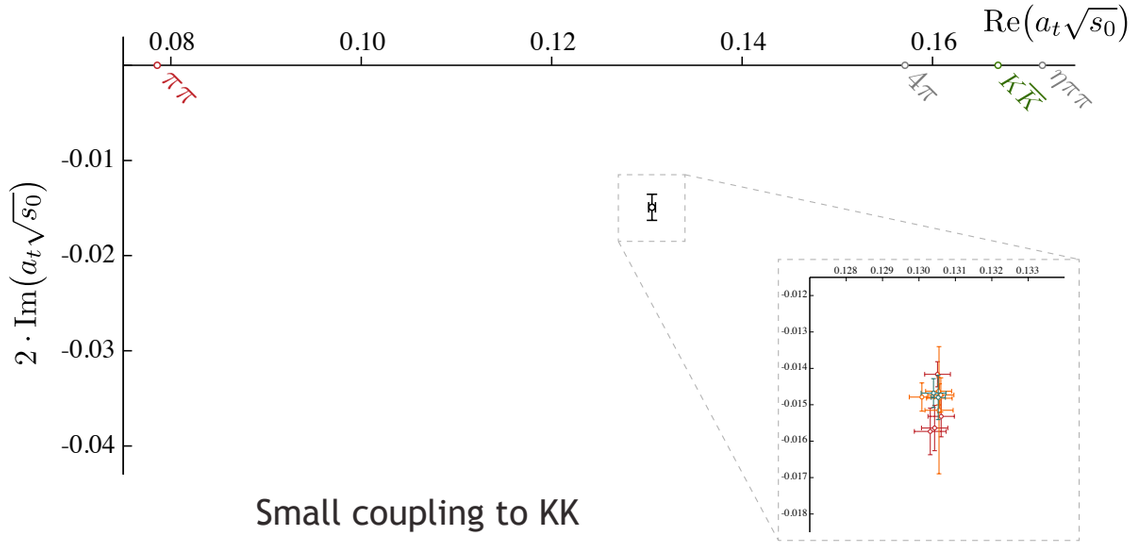


Phase shifts & inelasticity



$m_\pi \sim 236$ MeV

t-matrix pole location



Small coupling to KK

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Side comment: four-particle effects

PRD95 074510 (2017)

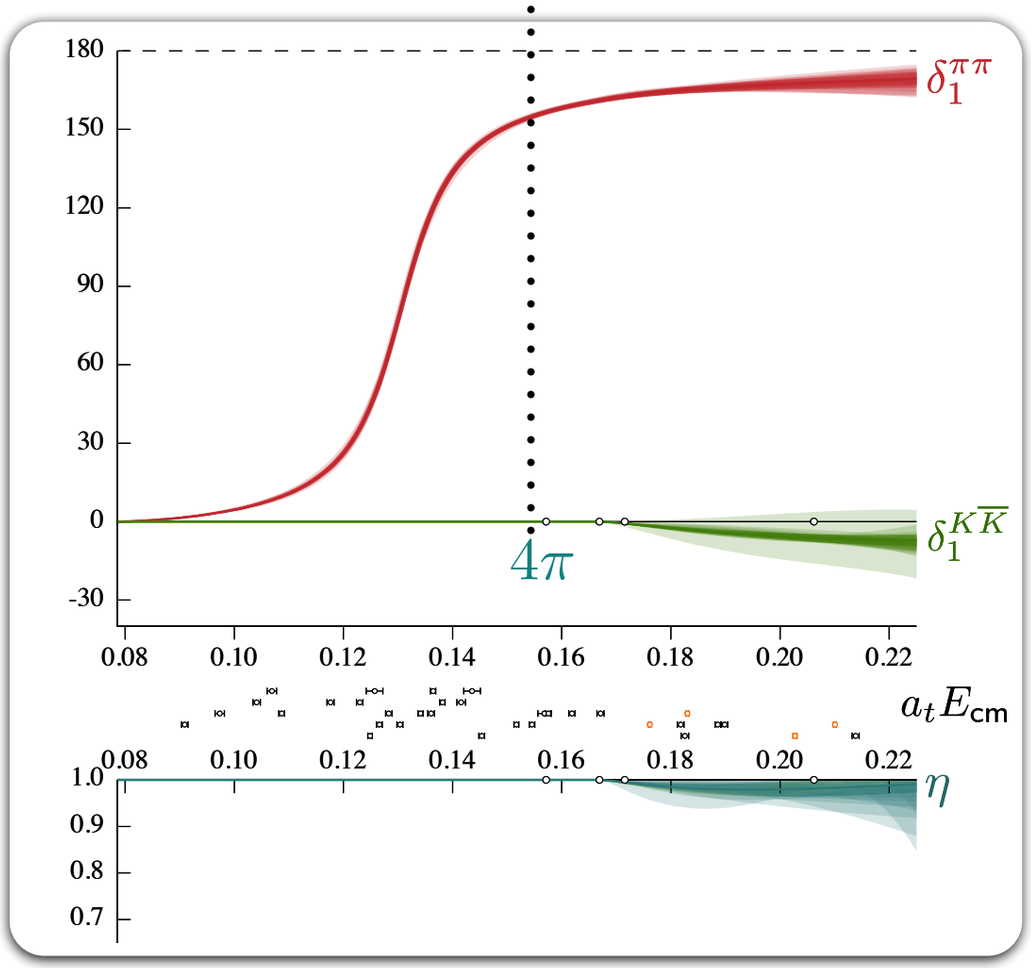
Don't know the equation that describes 2π - 4π, but must have the form:

$$\det\left[\begin{pmatrix}\mathcal{M}_{2\pi} & \\ & \mathcal{M}_{4\pi}\end{pmatrix}^{-1} + \begin{pmatrix}\tilde{K}_{2\pi,2\pi} & \tilde{K}_{2\pi,4\pi} \\ \tilde{K}_{4\pi,2\pi} & \tilde{K}_{4\pi,4\pi}\end{pmatrix}\right] = 0$$

If $\tilde{K}_{2\pi,4\pi} \sim \mathcal{O}(\epsilon)$, then factorizes

$$\det\left[\mathcal{M}_{2\pi}^{-1} + \tilde{K}_{2\pi,2\pi}\right] \times \det\left[\mathcal{M}_{4\pi}^{-1} + \tilde{K}_{4\pi,4\pi}\right] + \mathcal{O}(\epsilon) = 0$$

See no clear evidence of 4π



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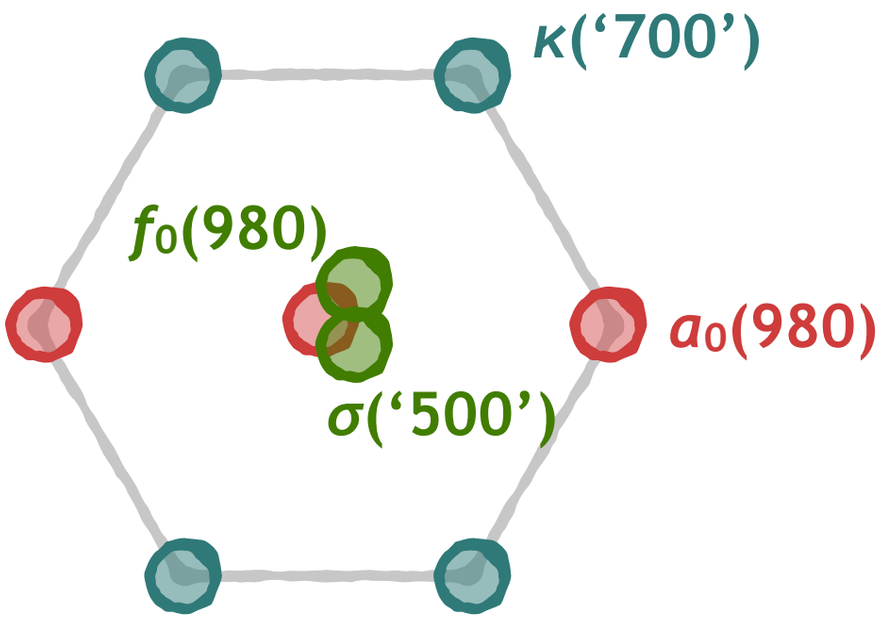
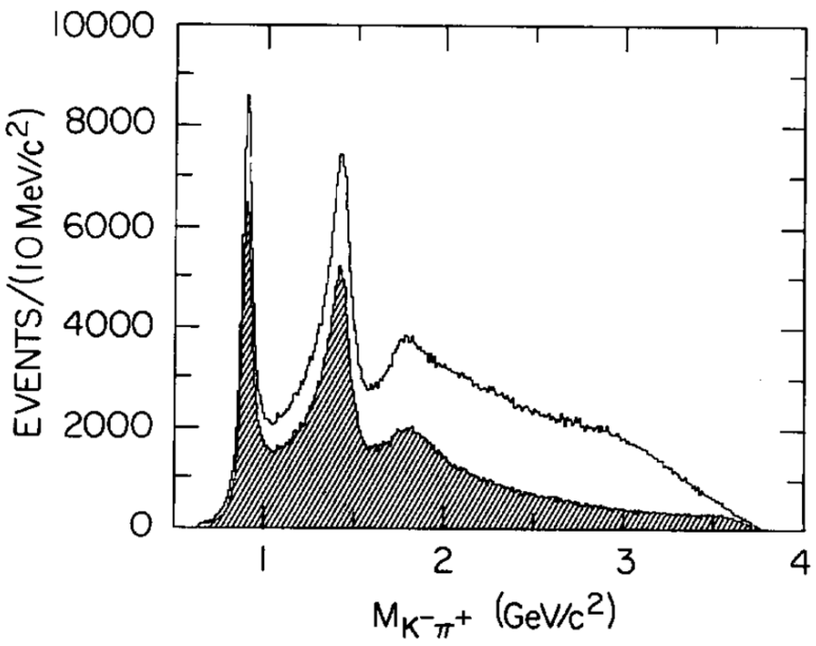
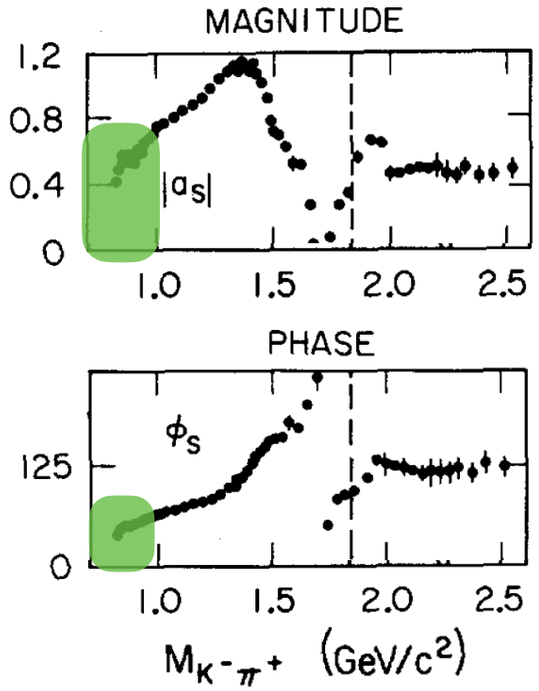
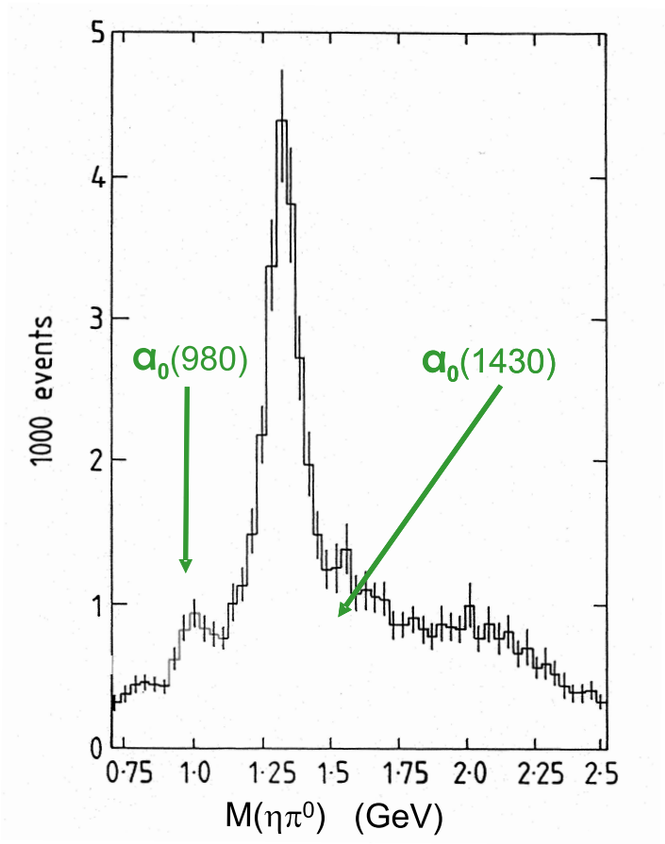
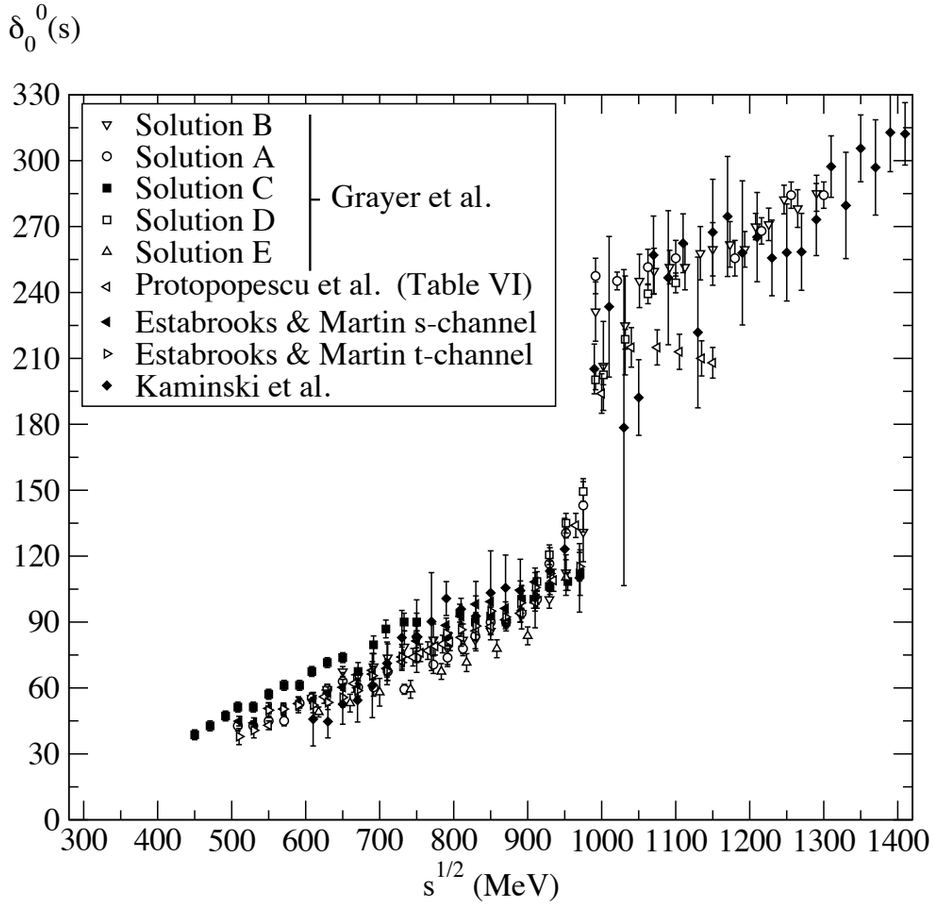
Light scalar mesons - empirically





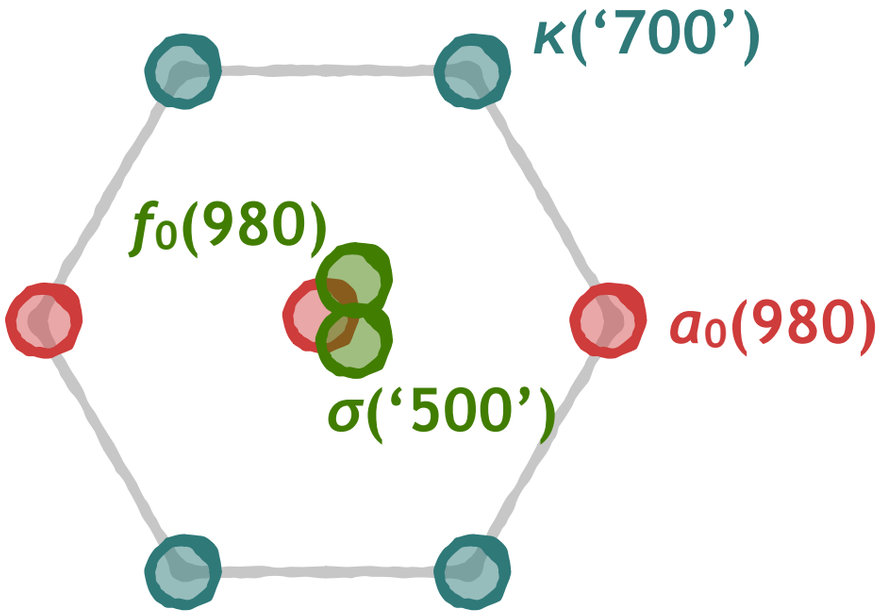




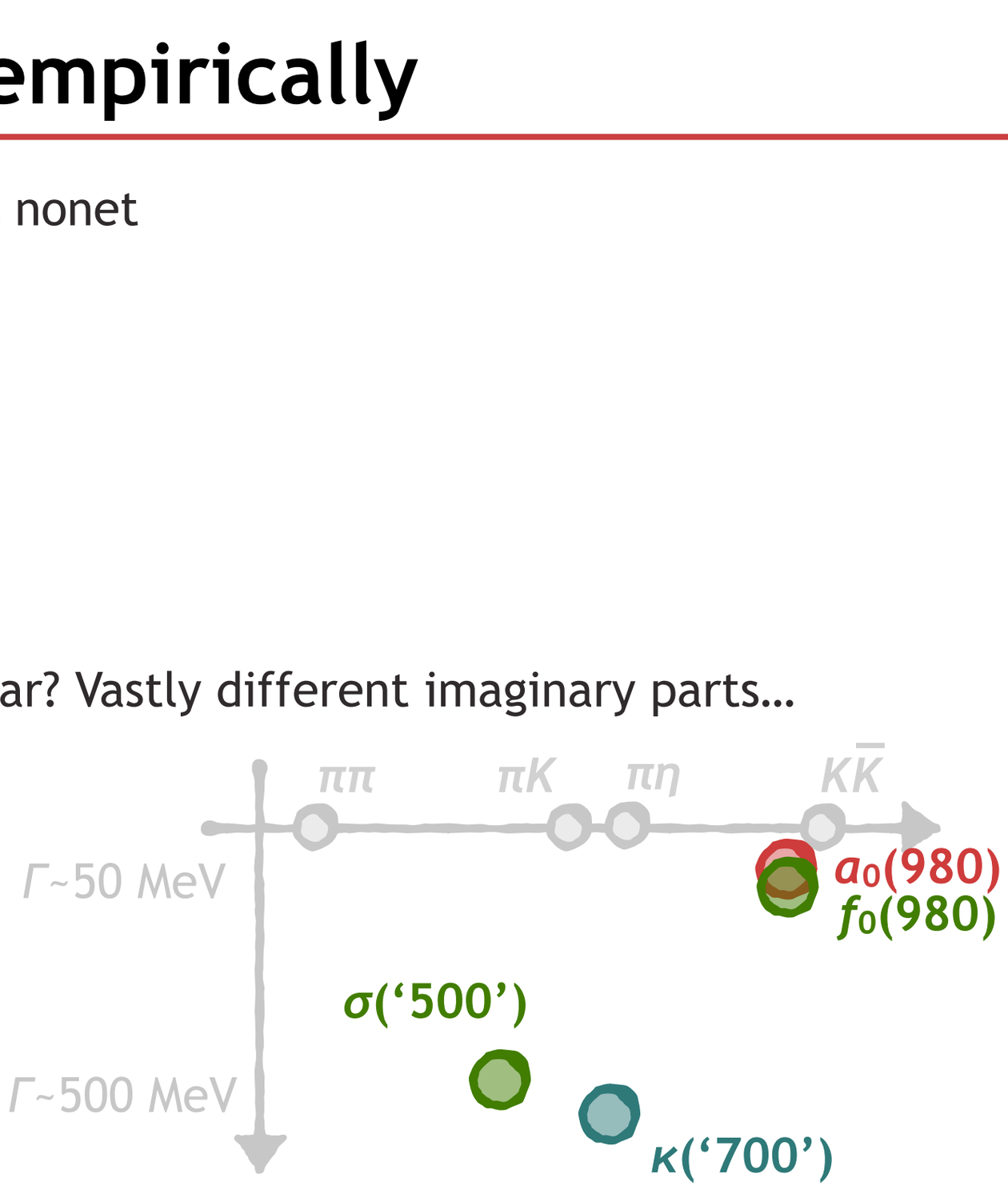


Light scalar mesons - empirically

Conventional wisdom: an ‘inverted’ mass nonet

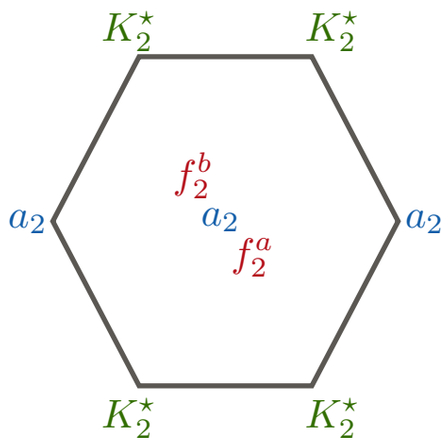


Similar? Vastly different imaginary parts…



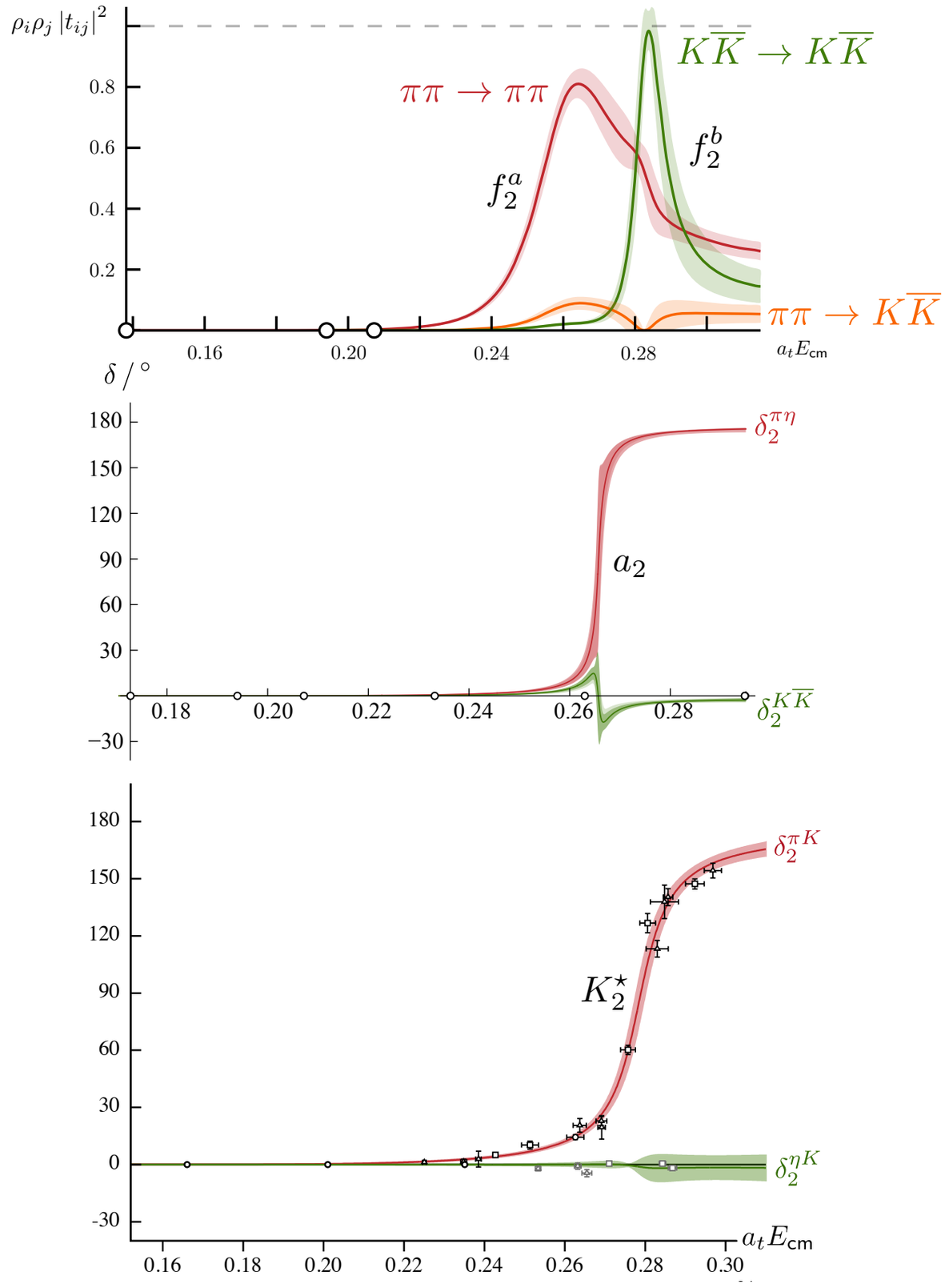
What does QCD have to say?

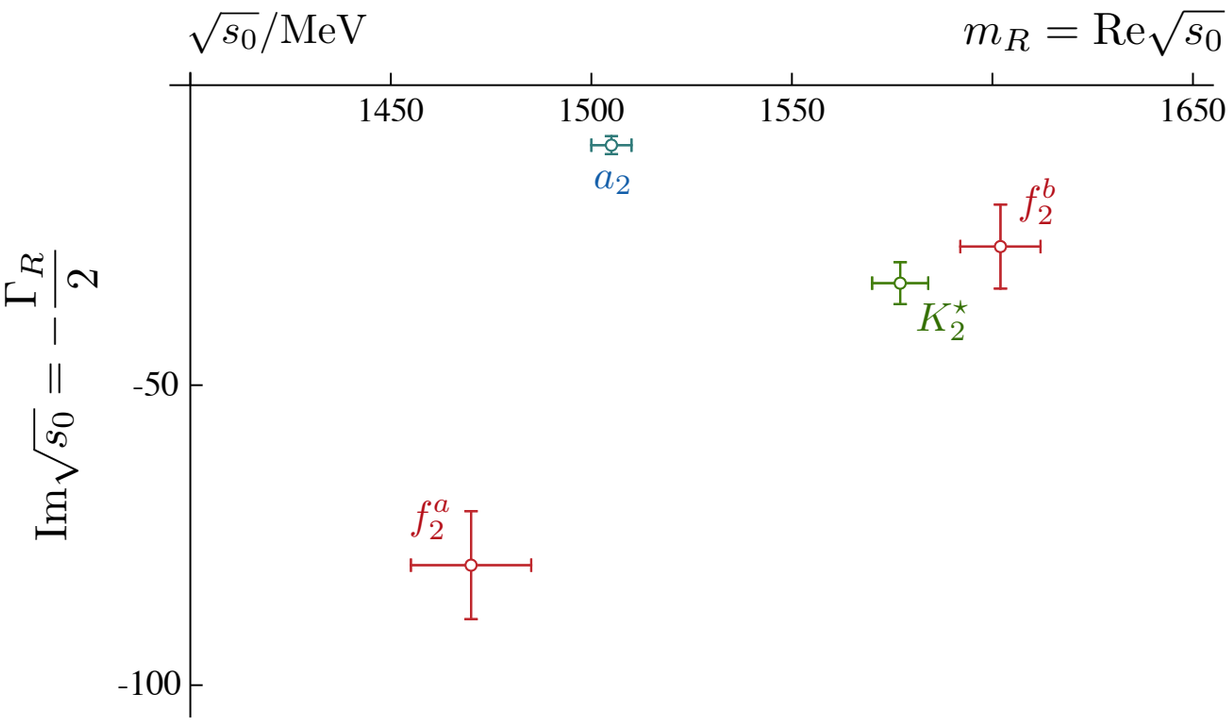
Lightest tensors at m_π=391 MeV



$$t_{ij} \sim \frac{c_i c_j}{s_0 - s}$$

$$\sqrt{s_0} = m_R - i\frac{\Gamma_R}{2}$$





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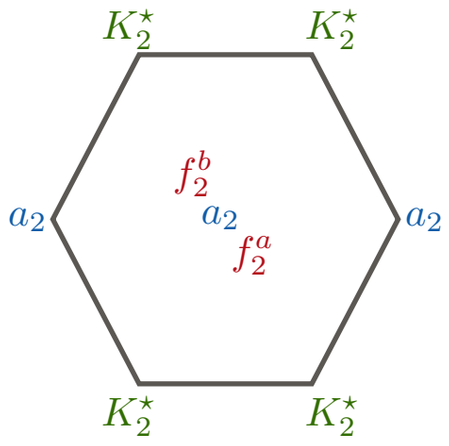
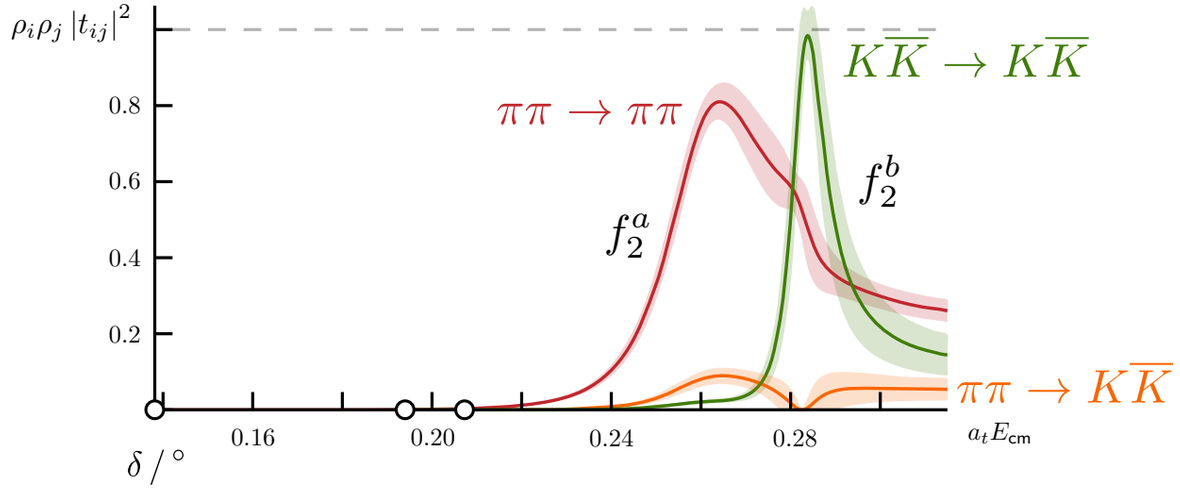
Lightest tensors at m_π=391 MeV



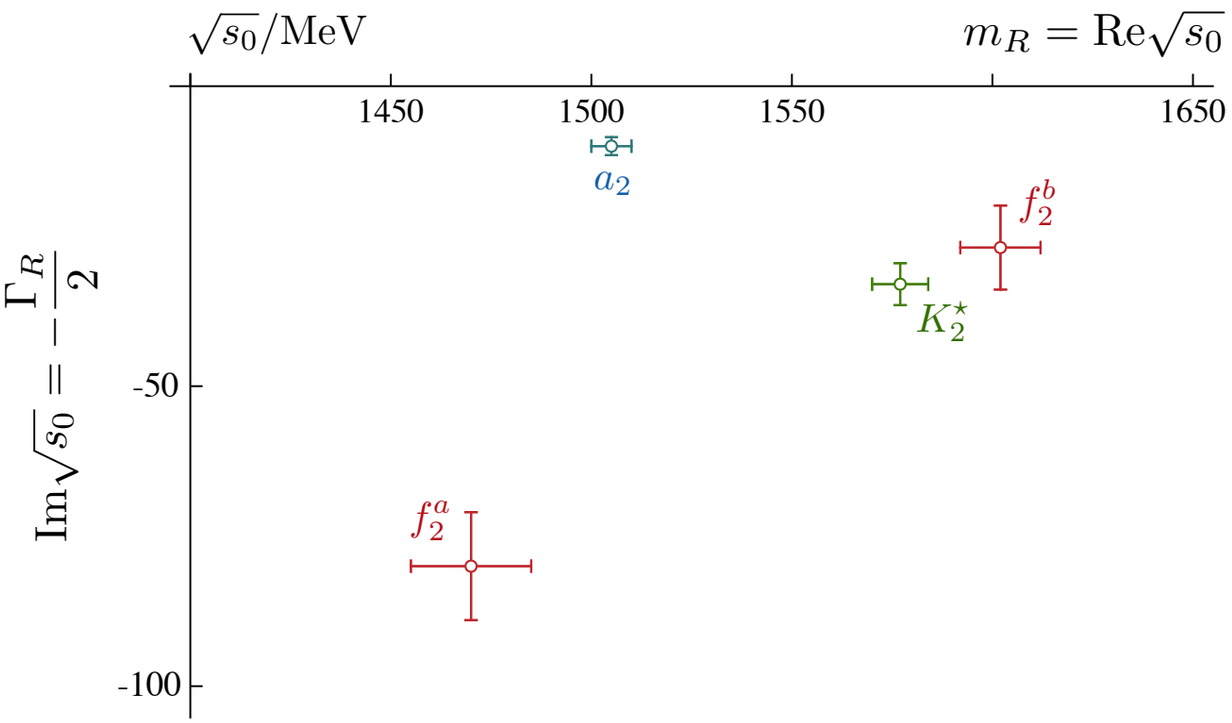


PDG

flavor tagging by decays

$f_2(1270)$ → ππ 84%

$f_2(1525)$ → $K\overline{K}$ 89%



Used as motivation in
GlueX detector upgrade proposal

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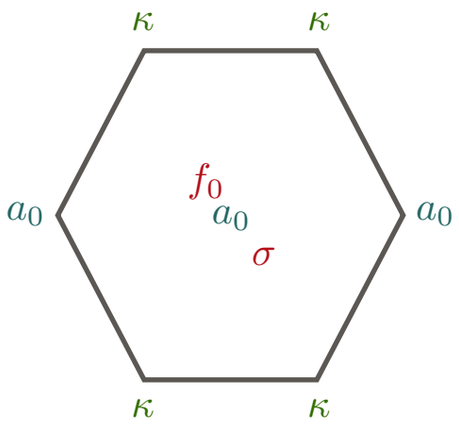
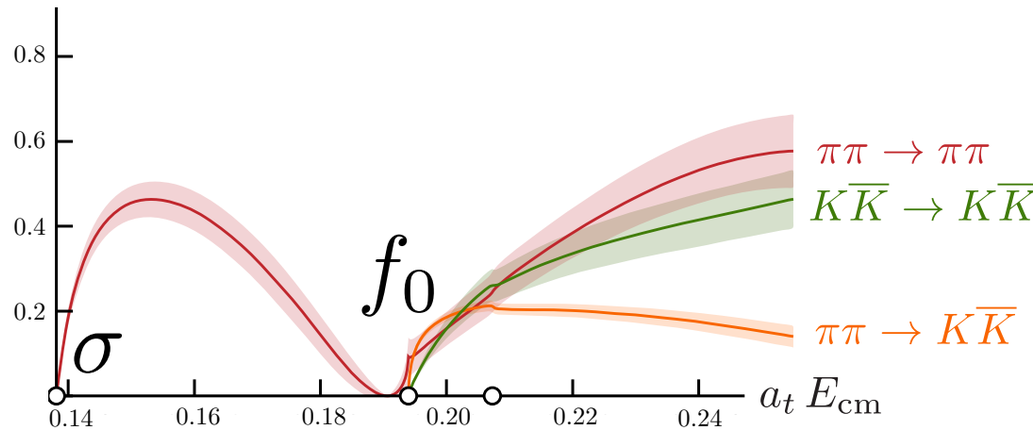
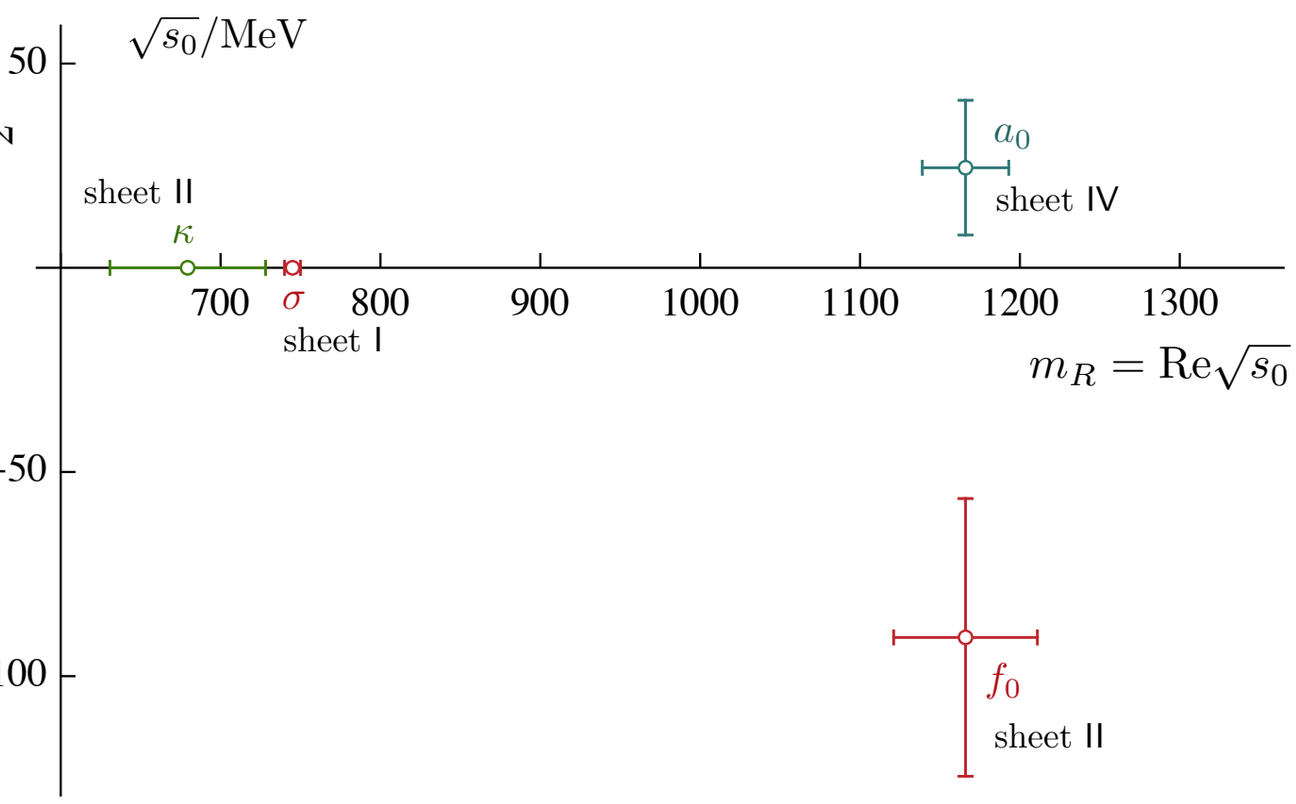
Lightest scalars at m_π=391 MeV

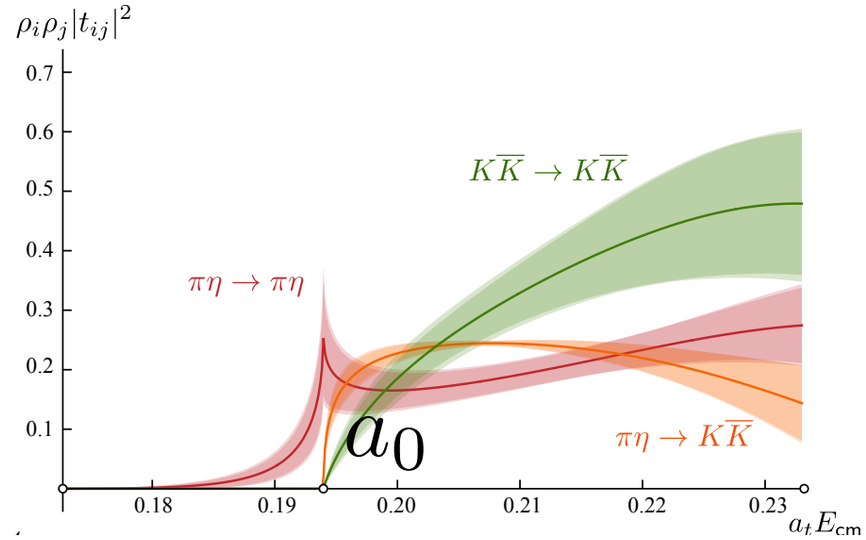


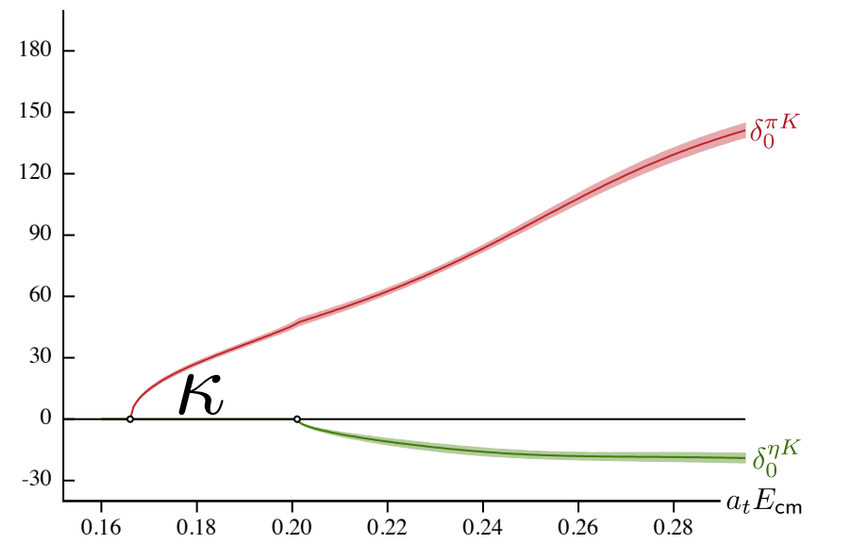
$$t_{ij} \sim \frac{c_i c_j}{s_0 - s}$$

$$\sqrt{s_0} = m_R - i\frac{\Gamma_R}{2}$$









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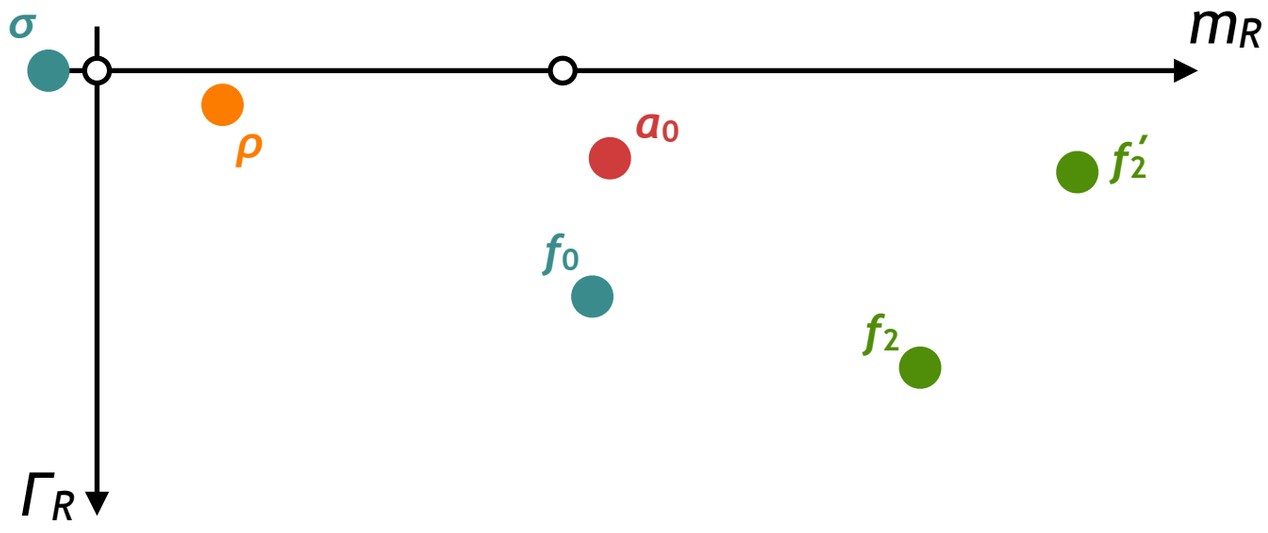
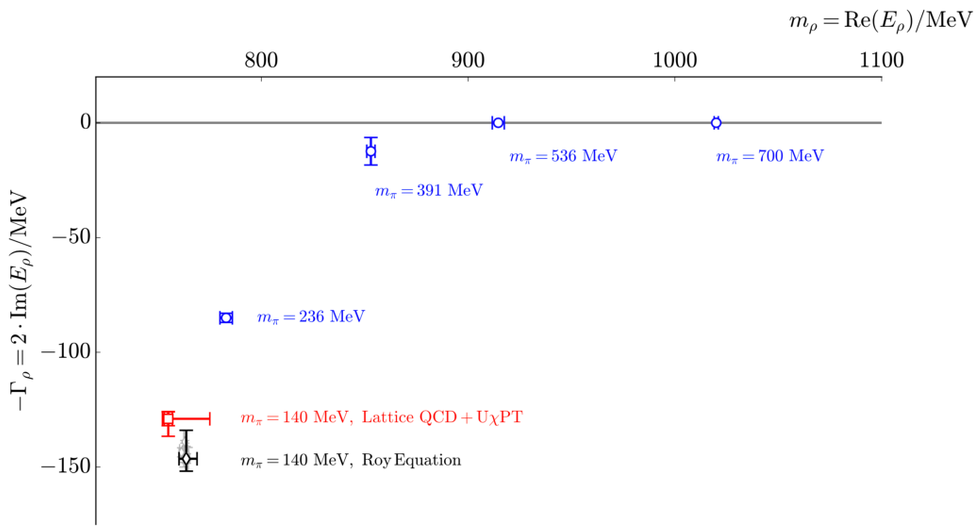
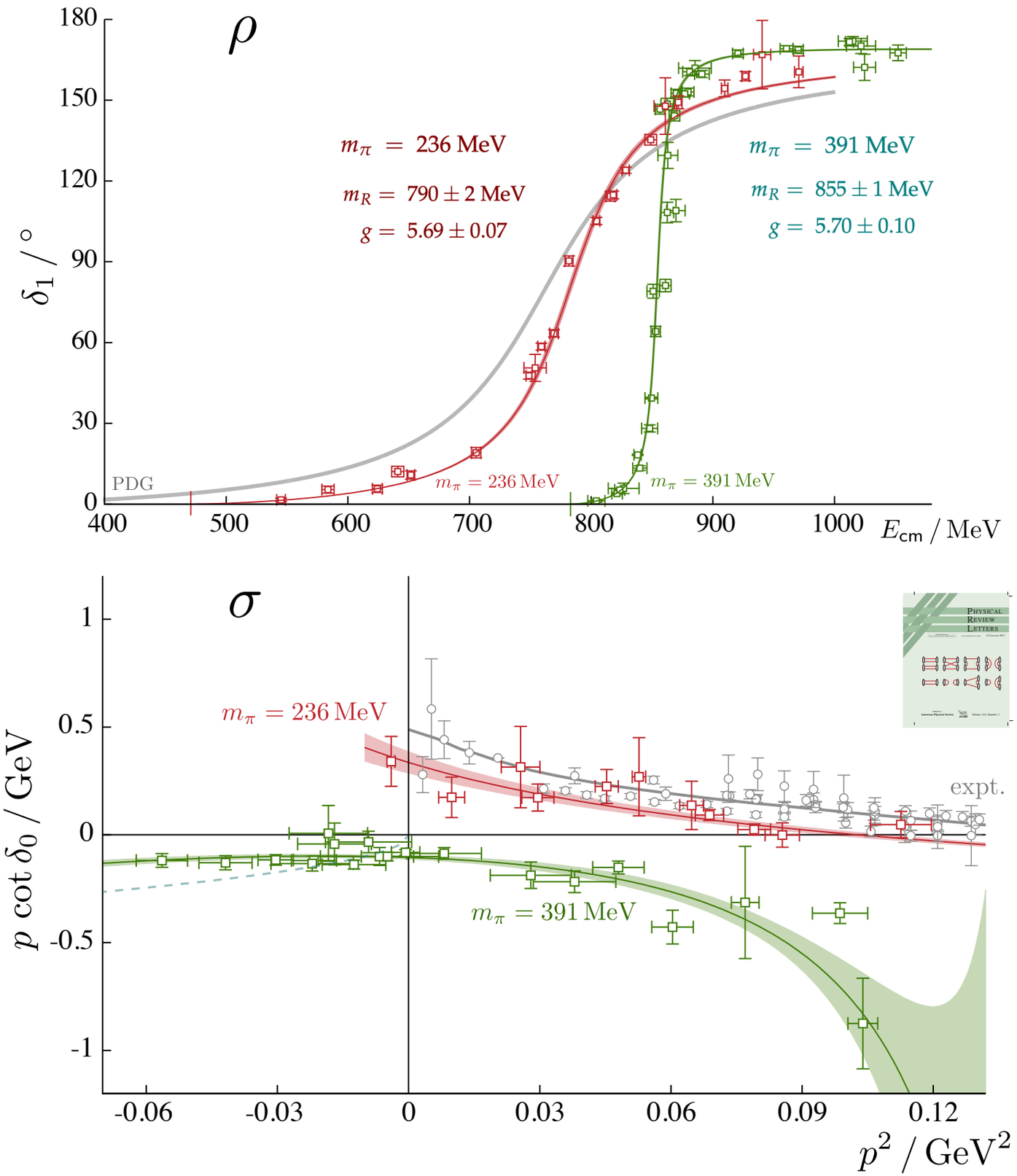
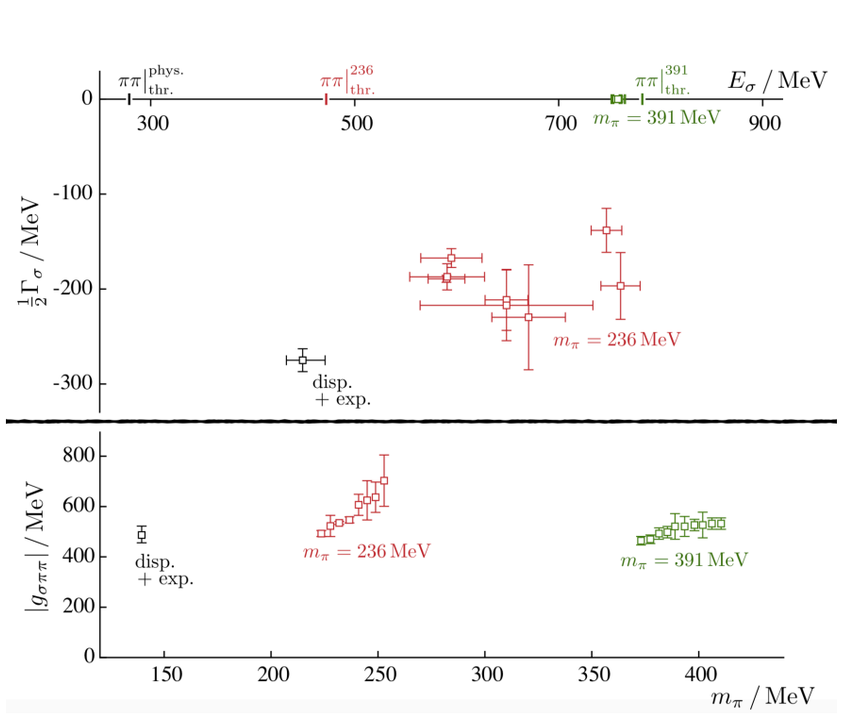
light meson resonances at m_π~391 MeV



Quark mass dependence: I=0 & 1







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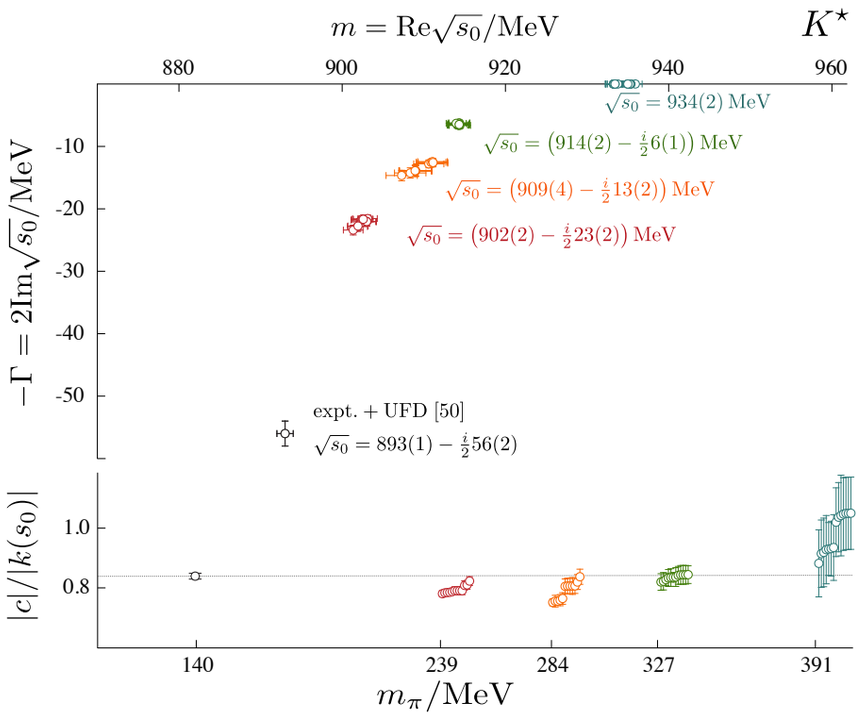
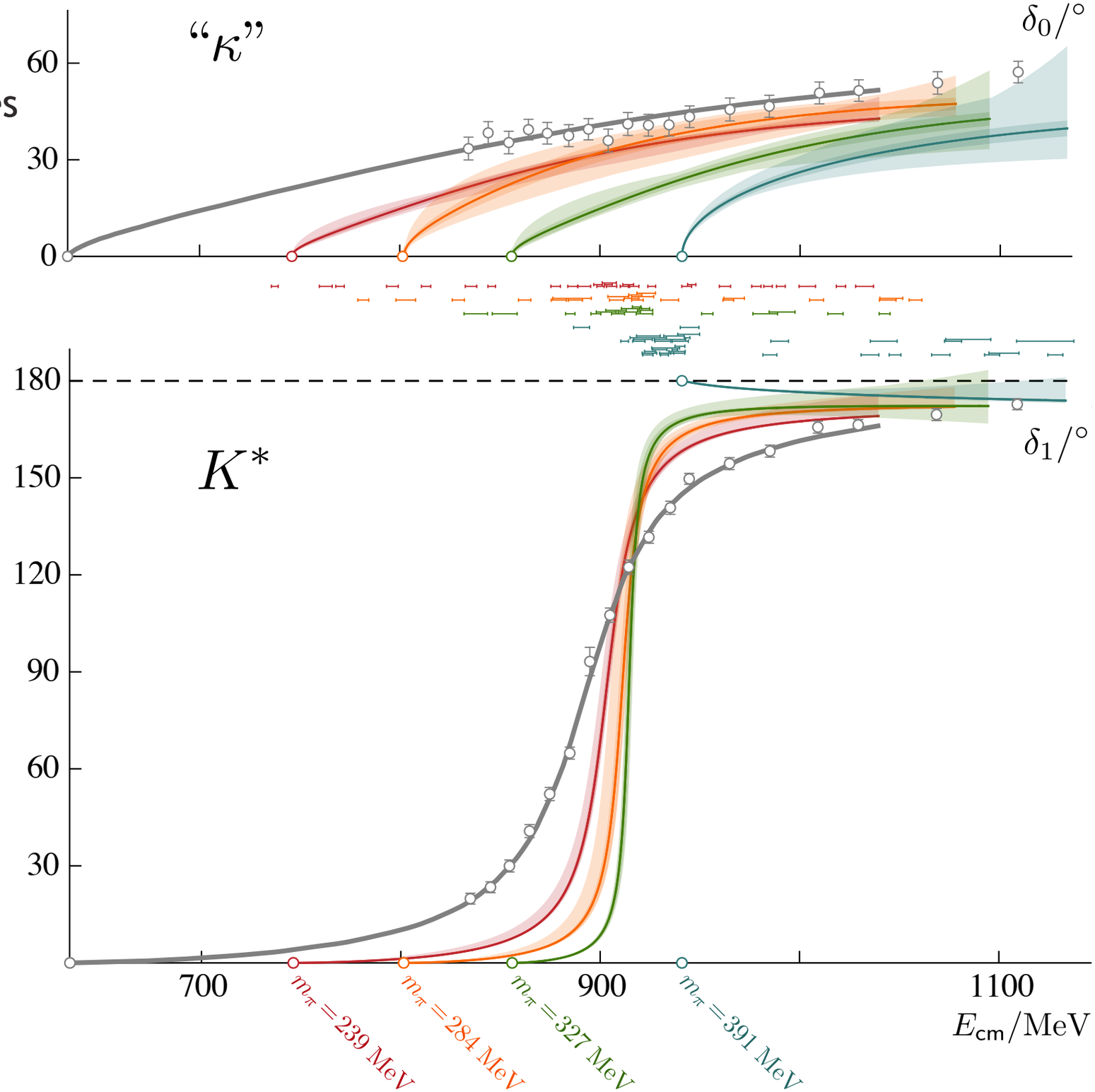
Quark mass dependence: I= 1/2

arXiv:1904:03188

A more complicated story…
need “t” & “u”-channel amplitudes





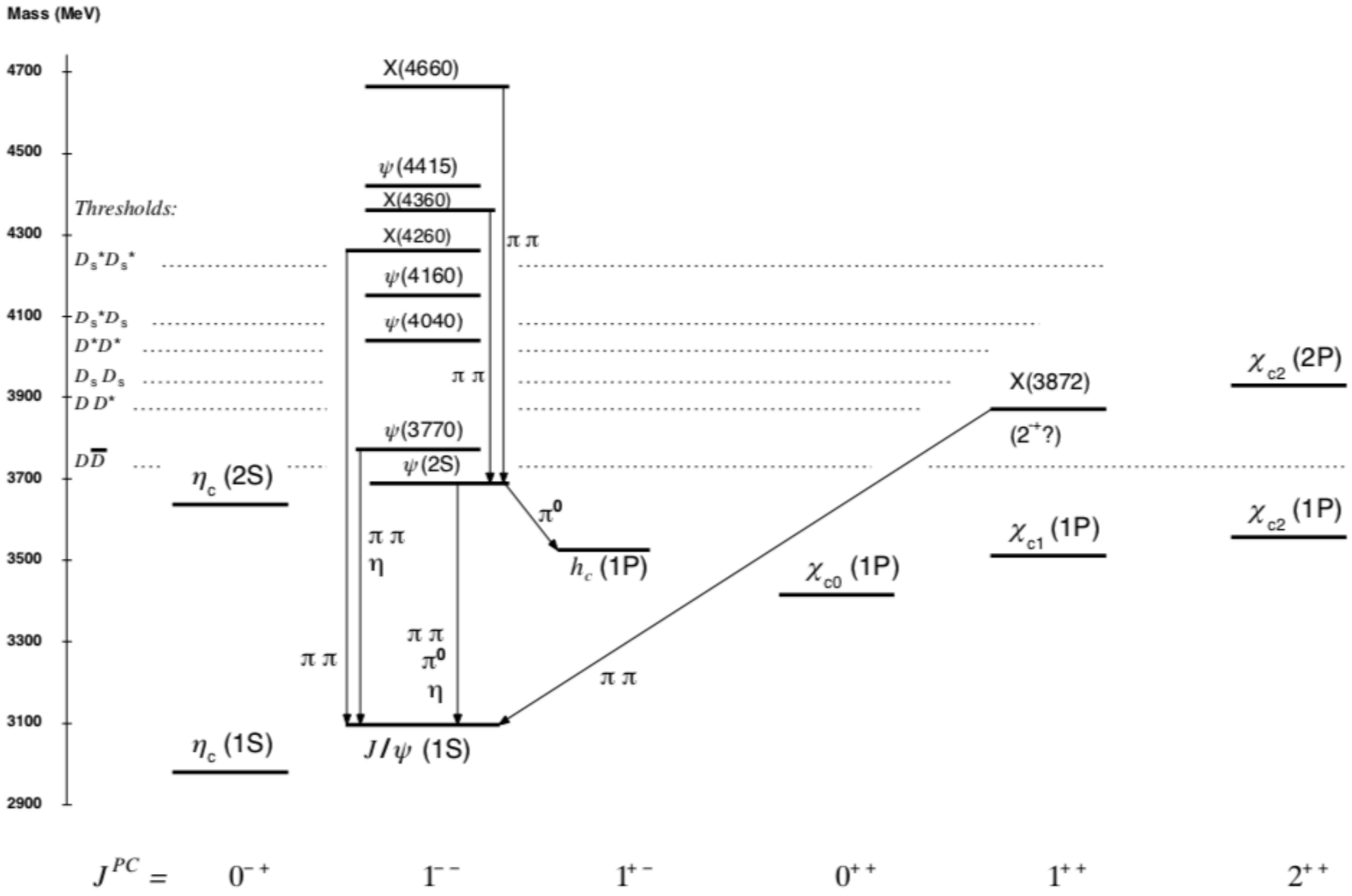
Added new dynamical ensembles

Jefferson Lab

Charmonium resonances

PDG

Several resonances reported near $D\bar{D}$ thresholds



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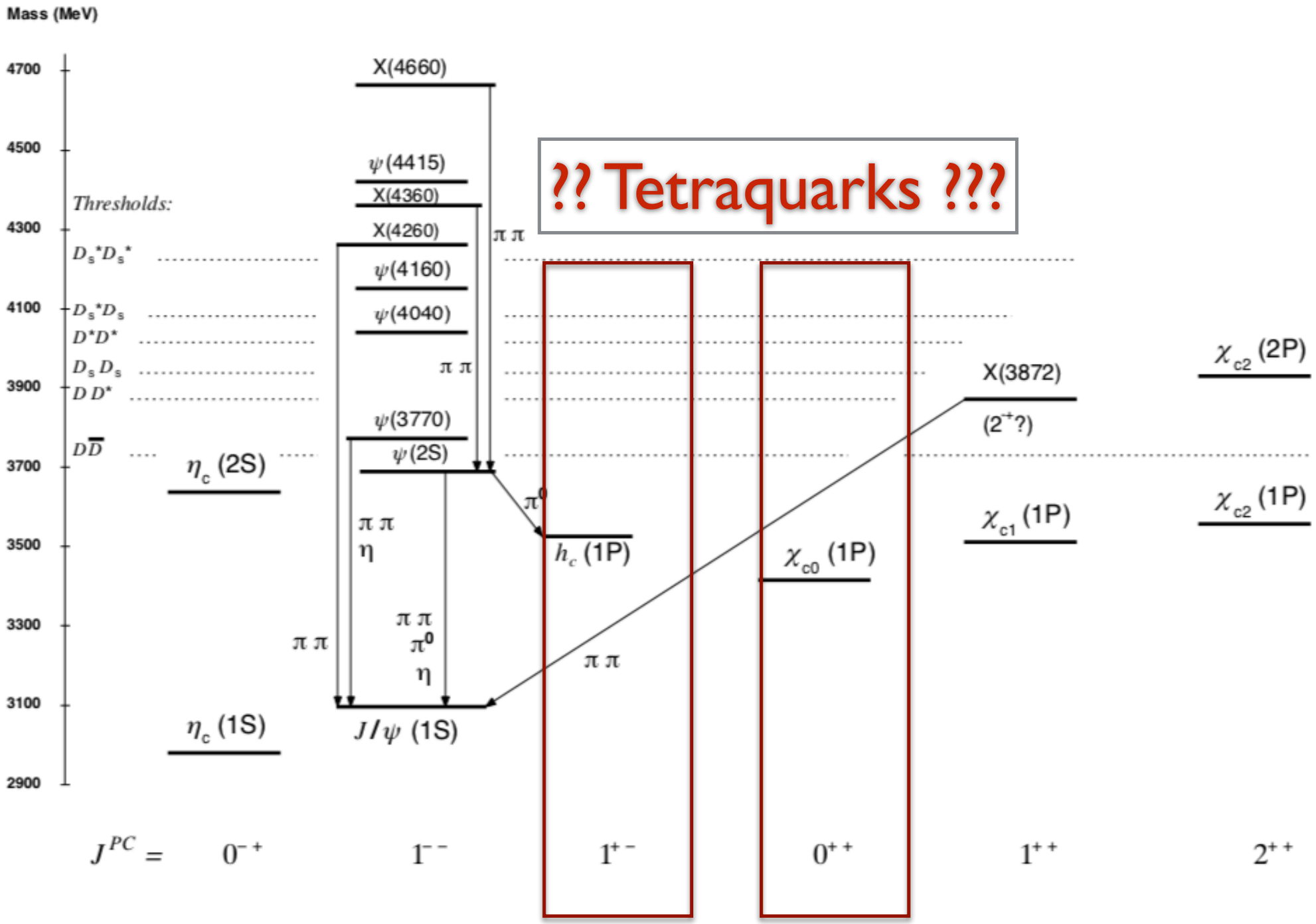
Charmonium resonances

PDG

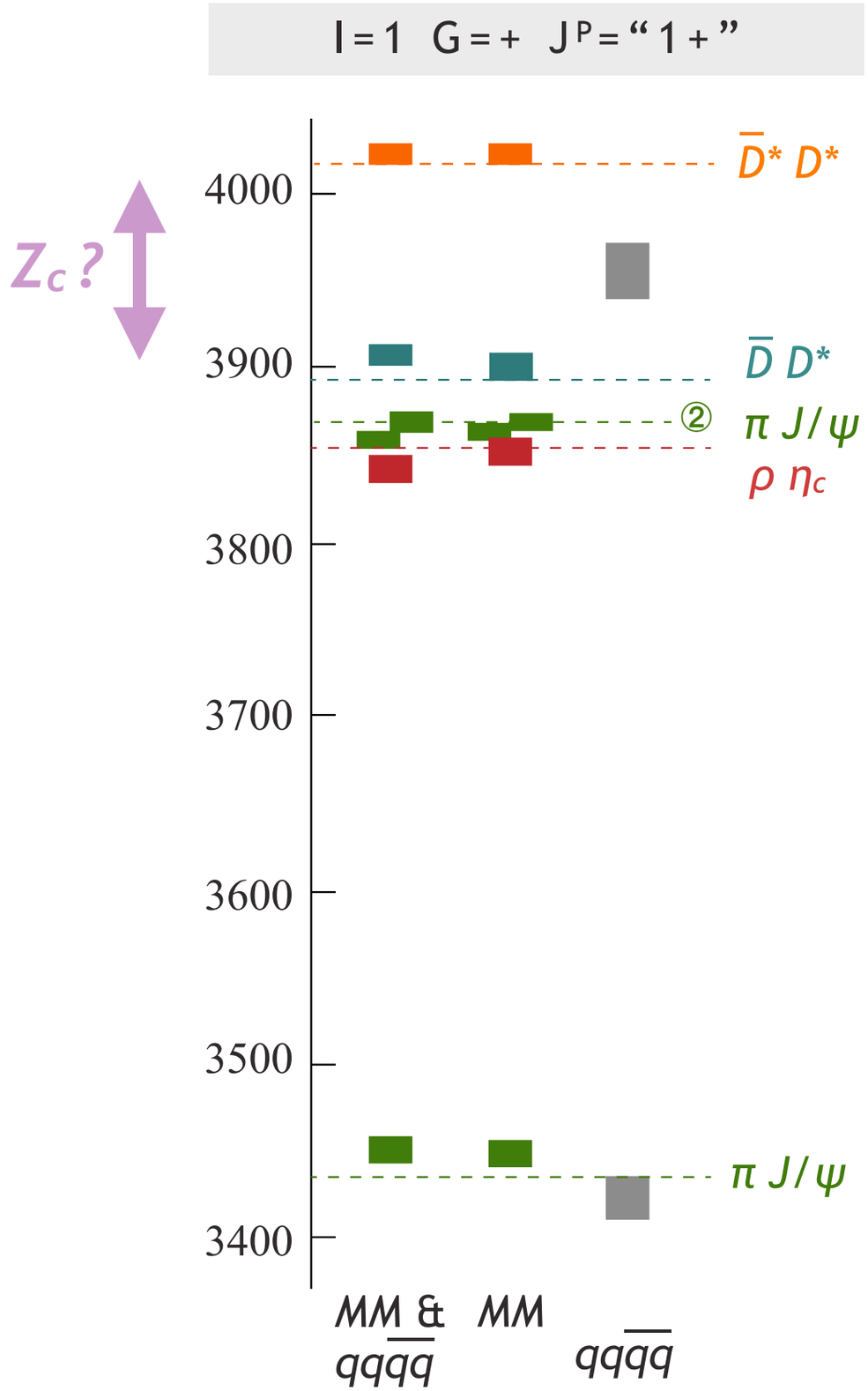
Isospin 1 charmonium?

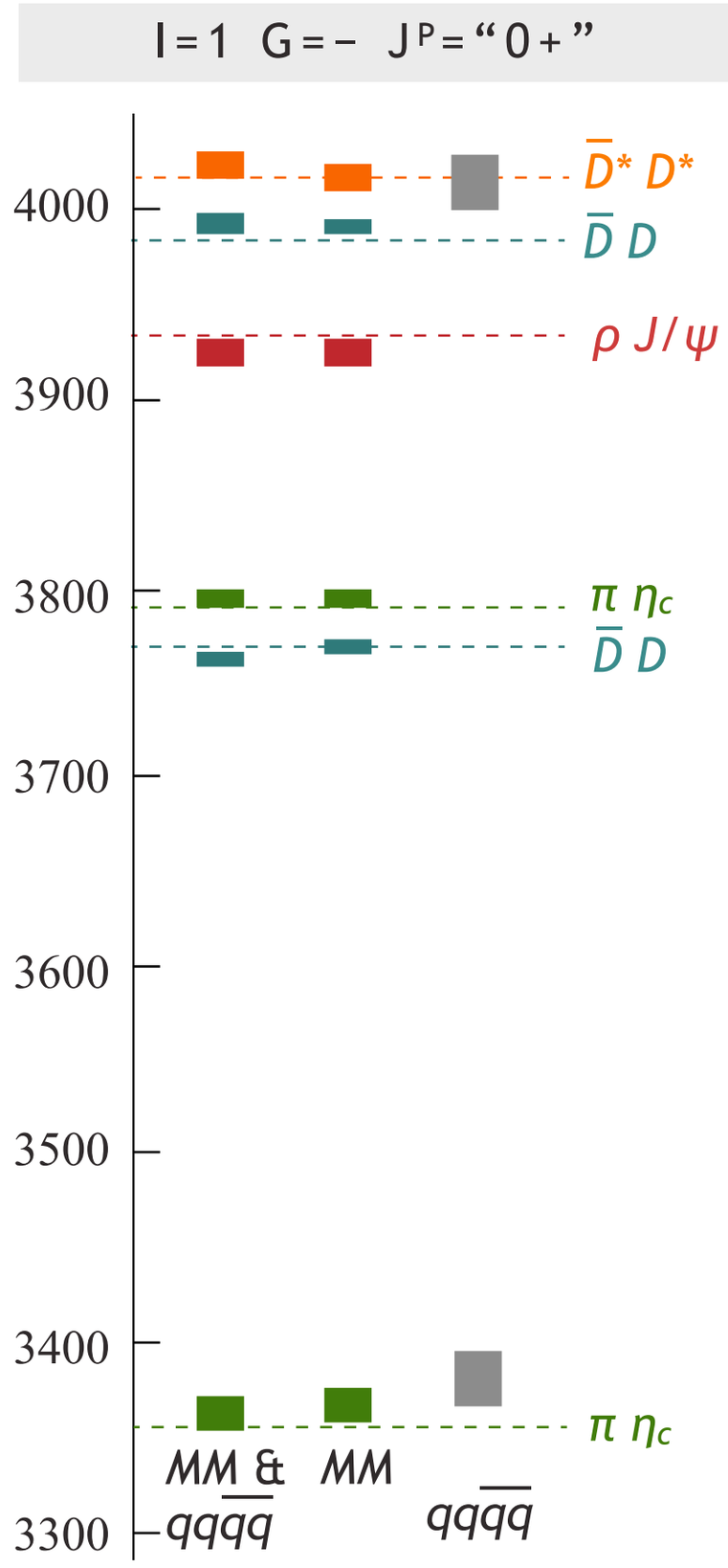


Tetraquarks ?

m_π ~ 391 MeV

JHEP 1711 033 (2017)





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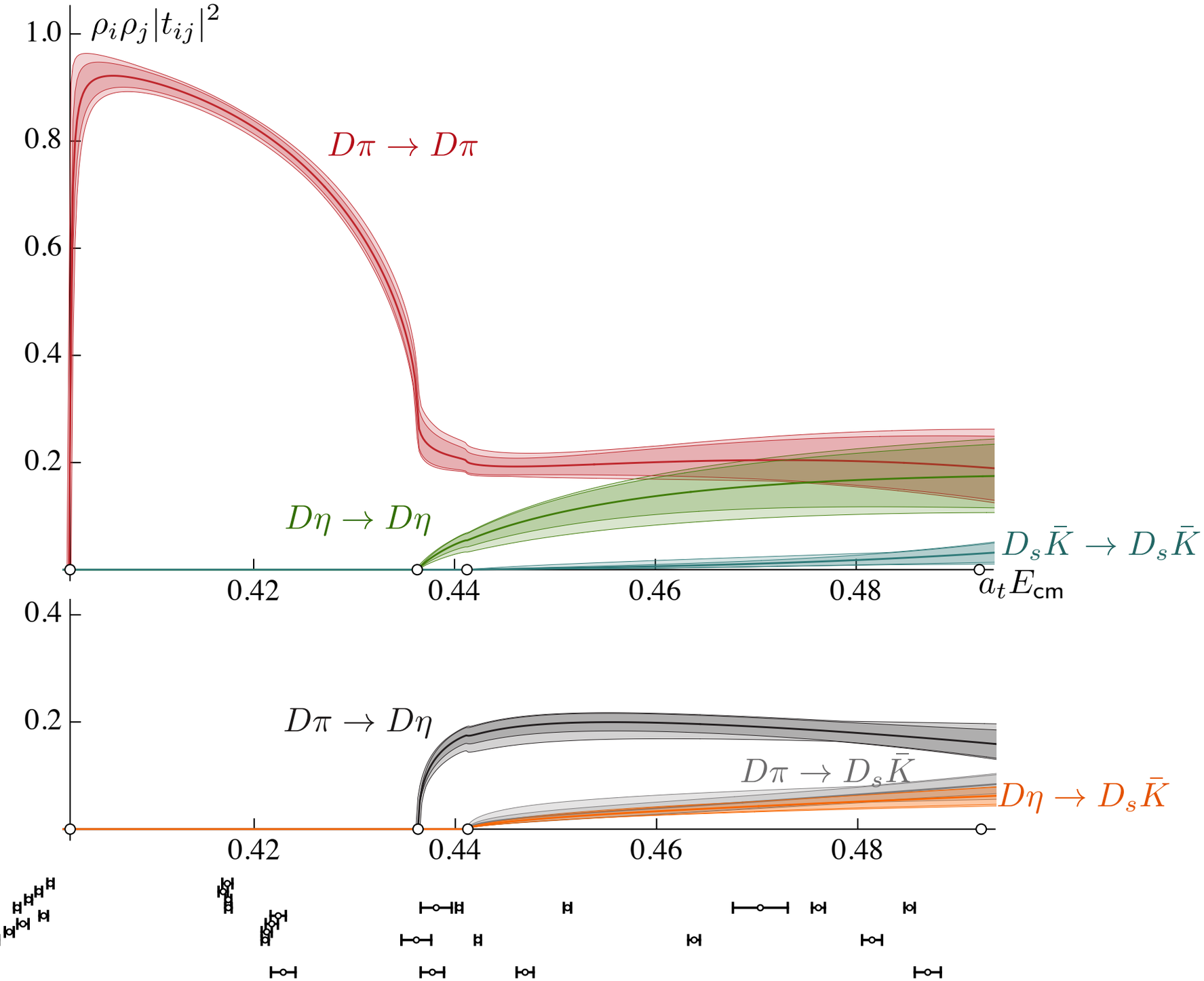
S-wave D decays

Moir et al, JHEP 1610 (2016) 011

Sharp threshold behavior in D & D_s



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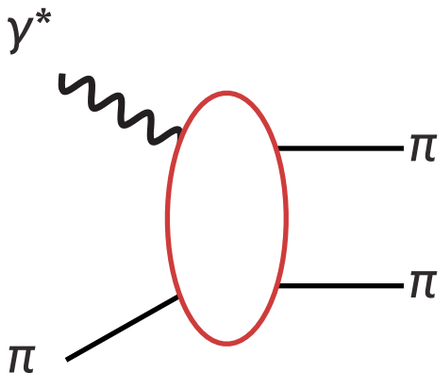
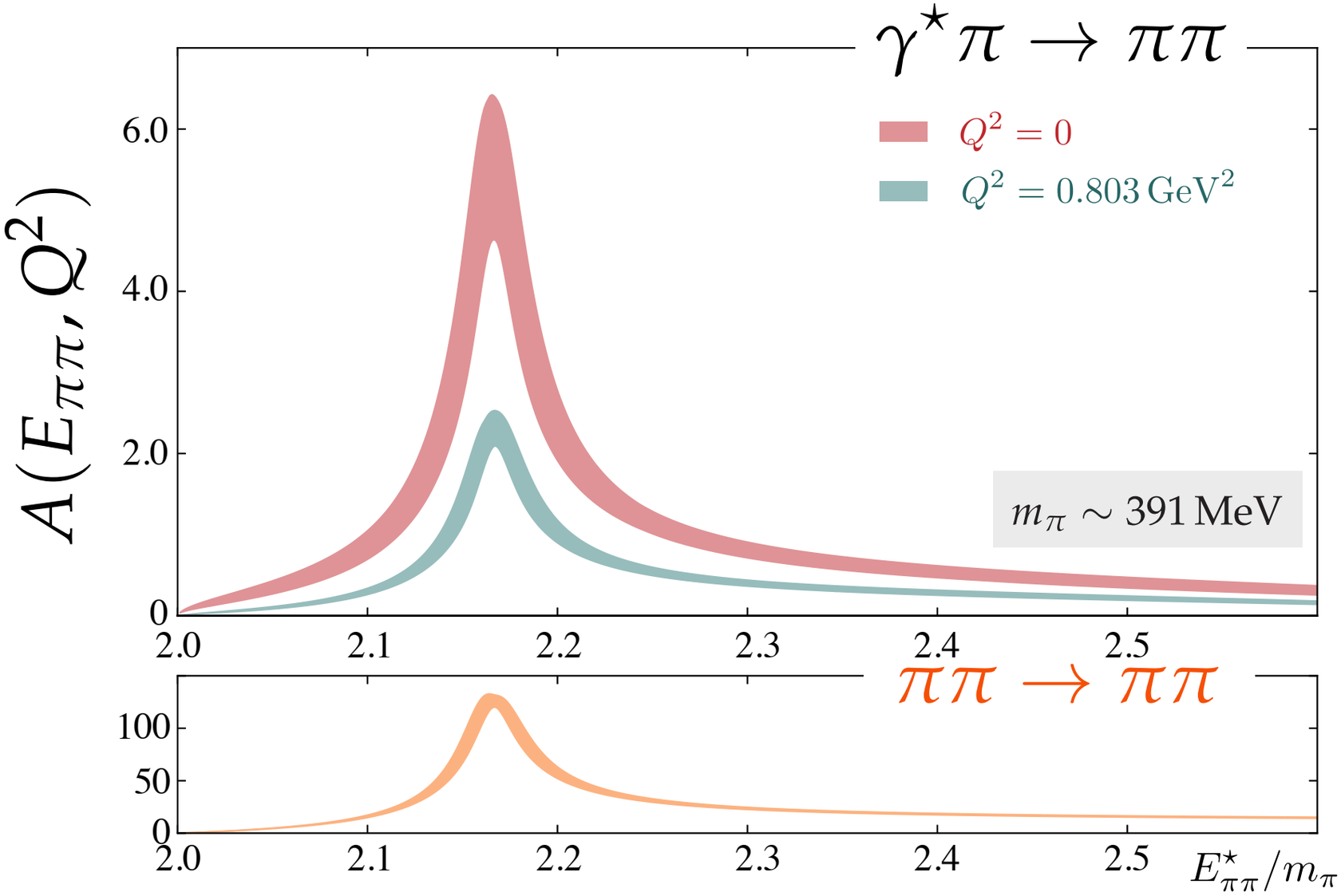
Coupling resonances to currents

- Production mechanisms - e.g., photo-production





PRL 115 242001 (2015)
arXiv: 1604.03530