LQT4HEP Module 10: Lattice QCD for spectroscopy, resonances & nuclei   Will Detmold

Motivation : QCD in the nonperturbative regime

Does QCD describe nature

- 1970s - now : experiments at high energy vs perturbative QCD
- O(2010) : LQCD calculations of low-energy spectrum vs experiment

Q : How is the proton mass a test of QCD? Aren't there parameters in QCD which can be tuned? What are some of the ways in which these parameters can be tuned?

Q : The proton mass is very precisely known from expt (how many digits?) Can this quantity be used as a test of the Standard Model?

QCD vs the Quark Model

- Quark Model (1960s), MIT Bag model (1970s), large N_c expansion and holographic models (2000s) reproduce eg. spectrum at $\mathcal{O}(10\%)$
- Do these approaches make predictions?
- Yes: predict whole host of excited states of hadrons which we can confront through LQCD calculations
- Also predicts that for some sets of quantum numbers there are no quark model states — <u>exotic channels</u>

- Experimental spectroscopy : major renaissance over last decade
  - LHCb, BES III, Belle 2, ...
  - LHCb's pentaquark state : 5^{th} most cited LHC paper!
  - tetraquarks T_{cc}^{++}
  - doubly charmed baryons Ξ_{cc}^{++}
  - many new (potentially exotic) states defying QM expectations

  Q : How many new states has LHCb discovered?

Nomenclature

- Stable particles

  Q : What are the stable particles?

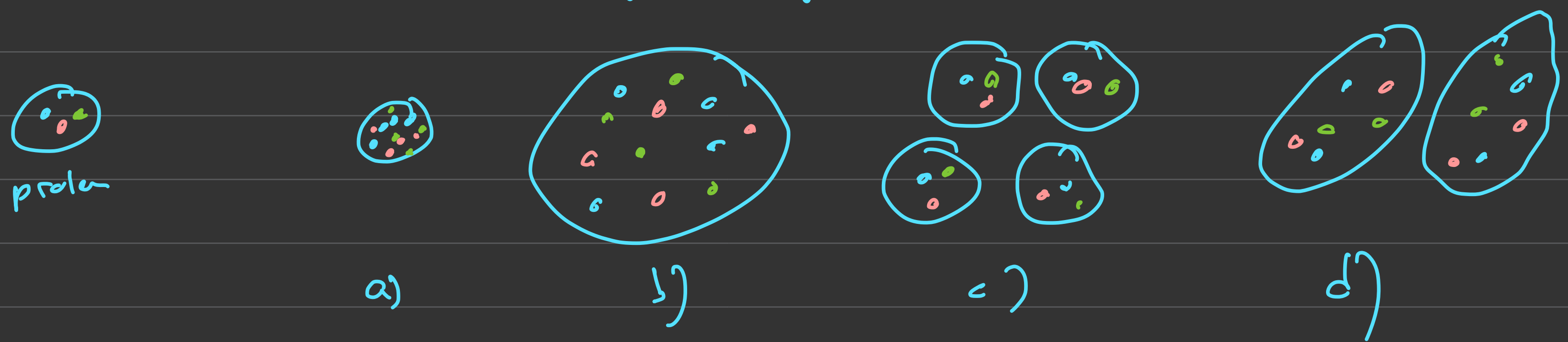
- Strongly-stable particles : stable in pure QCD but may decay in EW
  - π's, K's, p, n, Λ, Σ_b ...
  - depending on quark masses : ρ-meson, Δ baryon stable if quark masses are larger than nature
- Resonances : unstable particles (under strong int) that appear as enhancements in scattering x-sections
- Exotic hadrons : states not allowed in quark model as $\bar{q}q$ or qqq objects

Nuclei: from QCD point-of-view just a tower of hadrons

- have conserved baryon number $B > 1$
- almost everything about nuclear physics determined by

$$\alpha_{EM},\ \alpha_{strong},\ m_e,\ m_u,\ m_d$$

Q: From the QCD Lagrangian, can you tell which of the following pictures is a more accurate depiction of ^4He?



Ex 1: What is the mass of ^{12}C in MeV/c^2?

How does this compare to $6p + 6n + 6e$?

" " " " " $18u + 18d + 6e$?

Q: From $\mathcal{L}_{QCD}$ can you tell that $M(^{12}C)$ is within 1% of $6(m_p + m_n + m_e)$?

- Many pheno reasons to understand nuclei from the St Model
  - Nuclei used as targets in many expts
    1. At intensity frontier (DM searches in lab expts, νA interactions at DUNE) need nuclear targets for bulk since x-secs are so small
    2. Nuclei are useful for testing symmetries and symmetry breaking
       - searches for T-violation through EDMs
       - neutrinoless double β decay (Lepton # violation)

- Some nuclei have properties that a proton cannot have
  - Nuclear gluonometry   Q: what is nuclear gluonometry

- Fine tunings in nuclear physics: eg triple-α process
  How do these depend on the quark masses
  Only LQCD can answer this question

Hyperons: Λ, Σ, Ξ
contain strange quarks

- Nucleon interactions, hyperon-nucleon interactions are important for understanding structure / dynamics of dense matter in neutron stars

Lattice QCD spectroscopy

- Eigenstates of QCD Hamiltonian define the QCD spectrum
- LQCD calculations in finite volume : spectrum is discrete
- Phenomenological LQCD calculations use the path integral language and H_{QCD} not directly accessible
- Given certain conditions (Osterwalder-Schrader axioms), a Euclidean field theory action leads to a Hermitian Hamiltonian and a well-defined Hilbert space
- Eigenstates of Hamiltonian

$$\{ |n\rangle \mid \hat{H}|n\rangle = E_n|n\rangle \} \quad \text{with} \quad \hat{I} = \sum_n |n\rangle\langle n|$$

- Time dependence of correlation functions $\Rightarrow$ access to spectrum

$$C_2(t,\vec{p}) = \frac{1}{Z}\int \mathcal{D}\varphi\, e^{-S[\varphi]}\, a^3\sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}}\, \chi_{\underline{\underline{Q}}}(\varphi(\vec{x},t))\, \tilde{\chi}^{\dagger}_{\underline{\underline{Q}}}(\varphi(\vec{x}_0,t_0))$$

quantum numbers

$$= \mathrm{Tr}\Big[e^{-\hat{H}T}\, a^3\sum_{\vec{x}\in\Lambda} e^{-i\vec{p}\cdot\vec{x}}\, \hat{\chi}_Q(\vec{x},t)\, \hat{\tilde{\chi}}^{\dagger}_Q(x_0,t_0)\Big] \Big/ \mathrm{Tr}\big[e^{-\hat{H}T}\big]$$

temporal extent

$$= \sum_m a^3 \sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}} \langle m| e^{-\hat{H}T}\, \hat{\chi}_Q(\vec{x},t)\, \hat{\tilde{\chi}}_Q(\underline{x_0,t_0})|m\rangle \Big/ \sum_m \langle m|e^{-\hat{H}T}|m\rangle$$

set to zero by translational inv.

Use

$$\hat{O}(t) = e^{\hat{H}t}\, O(0)\, e^{-\hat{H}t}$$

Spectral decomposition

$$C_2(t,\vec{p}) = \frac{\sum_m \sum_n a^3 \sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}} \langle m| \overbrace{e^{-\hat{H}T} e^{Ht}}^{e^{-E_m(T-t)}} \overbrace{e^{-i\hat{\vec{p}}\cdot\vec{x}}}^{e^{-i\vec{p}_n\cdot\vec{x}}} \hat{\chi}_a(0) \overbrace{e^{i\hat{p}\cdot x}}^{e^{i\vec{p}_n\cdot\vec{x}}} \overbrace{e^{-\hat{H}t}}^{e^{-E_n t}} |n\rangle\langle n| \tilde{\chi}_a^\dagger |m\rangle}{\sum_m \langle m| \underbrace{e^{-\hat{H}T}|m\rangle}_{e^{-E_m T}}}$$

$E_0 < E_1 \le E_2 \ldots$

set $|\Omega\rangle = |m=0\rangle$

$\hat{H}|\Omega\rangle = 0$

$\hat{p}|\Omega\rangle = 0$

set $E_{m=0} = 0$

take $T \to \infty$

$$= \frac{\sum_n a^3 \sum_{\vec{x}} e^{-i(\vec{p}+\vec{p}_m-\vec{p}_n)\cdot\vec{x}} e^{-E_{m=0}(T-t)} e^{-E_n t} \times \langle\Omega|\hat{\chi}_a|n\rangle\langle n|\tilde{\chi}_a^\dagger|\Omega\rangle}{e^{-E_{m=0}T}}$$

$$= \underbrace{\sum_n a^3 \sum_{\vec{x}}}_{\sum_{E_n,\vec{p}_n}} e^{-i(\vec{p}-\vec{p}_n)\cdot\vec{x}} e^{-E_n(\vec{p}_n)t} Z_n \tilde{Z}_n^\dagger$$

$$= \sum_{E_n} e^{-E_n(\vec{p})t} Z_n \tilde{Z}_n^\dagger \quad *$$

- If $\chi_a = \tilde{\chi}_a \Rightarrow \tilde{Z}_n = Z_n$ so sum over exponentials with positive coefficients
- The overlap factors $Z_n = \langle\Omega|\hat{\chi}_a|n\rangle$ determine which states contribute
  If $|n\rangle$ has q# different from $\hat{\chi}_a|\Omega\rangle$ then it doesn't contribute

Ex1: consider the 3-point correlation function

$$C_3^{Q,Q',Q''} = \sum_{\vec{x},\vec{y}} e^{-i\vec{p}\cdot\vec{x}} e^{-i\vec{p}'\cdot\vec{y}} \, \mathrm{Tr}\left[e^{-T\hat{H}} \hat{\chi}_Q(\vec{x},t) \, \hat{J}_{Q'}(\vec{y},\tau) \, \hat{\chi}^\dagger_{Q''}(\vec{0},0) \right] \Big/ \mathrm{Tr}\left[e^{-T\hat{H}}\right]$$

and derive how it also depends on the spectrum. What additional information (eigenvalues or matrix elements) is needed to describe C_3 ?? What selection rules hold amongst the Q's and $\vec{p}$'s ? How would these change if the correlation function was considered in position space?

- The $\sum_n$ is over an infinite tower of states as LQCD Hilbert space is ∞-dimensional. Even on a computer the Hilbert space is VERY large
- LQCD calculations: values of $C_2(\vec{p},t)$ at discrete t evaluated stochastically
  $\Rightarrow$ Even in ∞-statistics it is an ill-posed problem to determine the E_n
- Given stochastic uncertainty at large t, only a finite # of states will give statistically resolvable contributions to $(*)$

Ex2: For the case of $\tilde{\chi}_Q = \chi_Q$, show that the large t behaviour of $C_2^{(Q)}(\vec{p},t)$ provides a rigorous upper bound on $E_0(\vec{p})$ (the lowest energy state with the quantum numbers of χ_Q) assuming $T \to \infty$ and infinite statistics

- Real lattice calcs have a fixed $T \neq \infty$ (periodic (antiperiodic) BCs on bosons (fermions))

$$C_2(\vec{p},t,T) = a^3 \sum_{m,n} \sum_{\vec{q}} e^{-E_m(\vec{q})(T-t)} e^{-E_n(\vec{q}+\vec{p})} |\underbrace{Z_{nm}(\vec{q},\vec{p})}_{\langle m,\vec{q}|\chi_Q|n,\vec{p}\rangle}|^2$$

which can get messy

Multiple correlation functions

- Consider set of operators $\{\hat{\chi}_1, \hat{\chi}_2, \dots, \hat{\chi}_N\}$ all with $q \# Q$ then $(T \to \infty)$

$$\sum_{\vec{p}} \langle \chi_i(t) \chi_i^\dagger(0) \rangle = a^3 \sum_n |Z_{n,i}|^2 e^{-\underbrace{E_n(\vec{p})}_{\text{independent of which operator}} t}$$

- Hermitian matrix of corr funcs $\mathbb{C}^Q(t)$ with matrix elements

$$C^Q_{ij}(t) = \langle \chi_i(t) \chi_j^\dagger(0) \rangle \qquad i,j \in \{1, \dots, N\}$$

$$= \sum_n Z_{n,i} Z^\dagger_{n,j} e^{-E_n t}$$

- In the vector space $\text{span}\{ \hat{X}_i |\Omega\rangle \}$ $\exists$ an operator

$$\hat{\Xi}_a = \sum_{i=1}^{N} v_{a,i} \hat{X}_i$$

such that

$$\hat{\Xi}_a |\Omega\rangle \text{ is closest to eigenstate } |a\rangle$$

ie choose $v_{a,i}$ such that we maximise

$$\frac{\langle a | \hat{\Xi}_a | \Omega \rangle}{| |a\rangle | \, | \Xi_a |\Omega\rangle |}$$

Equivalent to reducing exponential contamination

$$\langle \Omega | \Xi_a(t) \Xi_a^\dagger(0) |\Omega\rangle = \# \Big(e^{-E_a t} + \sum_{n \neq a} \overbrace{|\varepsilon_n|^2}^{\text{hopefully small}} e^{-E_n t} \Big)$$

Write in terms of the $v_{a,i}$ and minimise

$$\sum_{i,j} v_{ai}^* v_{aj} \langle \Omega | X_i(t) X_j^\dagger(0) |\Omega\rangle = \sum_{ij} v_{ai}^* C_{ij}(t) v_{aj} = \vec{v}_a^{\,*} \cdot \underline{C} \cdot \vec{v}_a$$

subject to a normalisation condition (else $\vec{v} = 0$ is a solution!) at t_0

$$\sum_{ij} v_{ai}^* C_{ij}(t_0) v_{aj} = 1$$

Add as a Lagrange multiplier

$$\min_{v_a} \left(\vec{v}_a^{\,*} \cdot \underline{C}(t) \cdot \vec{v}_a - \lambda [\vec{v}_a^{\,*} \cdot \underline{C}(t_0) \cdot \vec{v}_a - 1] \right)$$

require $\frac{\partial}{\partial v_a^*}\left(\quad \right) = 0$

$$\Rightarrow \quad \underline{C}(t) \cdot \vec{v}_a = \lambda_a(t, t_0)\, \underline{C}(t_0) \cdot \vec{v}_a$$

Generalised Eigenvalue Problem (GEVP)

- The eigenvalues $\lambda_a(t, t_0) = \exp\left(-E_a(t, t_0)(t - t_0)\right)$ principle correlators

- The eigenvectors are orthonormal in the sense

$$\vec{v}_a^{\,*}(t, t_0) \cdot \underline{C}(t_0) \cdot \vec{v}_b(t, t_0) = \delta_{ab}$$

- Note that $\frac{\langle a | \Xi_a | \Omega \rangle}{| |a\rangle | \, | \Xi | \Omega \rangle |} < 1$ as $\operatorname{span}\{\chi_1, \dots \chi_N\} \subset \mathcal{H}$

- Convexity of principle correlators guarantees that
$$E_a(t, t_0) \xrightarrow[t \to \infty]{} E_0^+$$

- The <u>Cauchy Interlacing Theorem</u> guarantees that there are at least n true eigenenergies below $E_n(t, t_0)$ for t, t_0

* LQCD spectroscopy in GEVP is <u>variational</u> and strictly only provides upper bounds on the eigenenergies of the lattice theory

Lanczos Iteration Method

- The correlator matrix above corresponds to a set of matrix elements of powers of the transfer matrix $\hat{T} = \exp[-a\hat{H}]$

$$C_{ij}(t) = \langle \chi_i(t)\, \chi_j^{\dagger}(0) \rangle = \langle \chi_i | \hat{T}^{t} | \chi_j \rangle$$

- The Lanczos algorithm gives us a way to use these matrix elts of powers

① Apply Lanczos alg to $\underline{C}(t)$ to determine a Krylov-space approximation $\hat{T}^{(m)}$ to the ∞-dim operator $\hat{T}$ after m iterations

② Diagonalise $\hat{T}^{(m)}$ to get eigenvalues & eigenvectors

③ Evaluate rigorous bounds on eigenvalues

④ Look at what happens as more iterations are applied

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1. Initialise recurrence relations

decompose $\underline{C}(0) = \underline{\beta}_1 \underline{\gamma}_1$ arbitrarily

$$\underline{\alpha}_1 = \underline{\beta}_1^{-1} \underline{C}(1) \underline{\gamma}_1^{-1}$$

$$\underline{A}_1(t) = \underline{\beta}_1^{-1} \underline{C}(t) \underline{\gamma}_1^{-1}$$

decompose residual norm

$$\underline{\Delta}_2 = \underline{A}_1(2) - \underline{\alpha}_1 \underline{\alpha}_1 \equiv \underline{\beta}_2 \underline{\gamma}_2$$

$$\underline{G}_2(t) = \underline{\beta}_2^{-1} [\underline{A}_1(t+1) - \underline{\alpha}_1 \underline{A}_1(t)]$$

$$\underline{B}_2(t) = [\underline{A}_1(t+1) - \underline{A}_1(t)\underline{\alpha}_1] \underline{\gamma}_2^{-1}$$

$$\underline{A}_2(t) = \underline{\beta}_2^{-1} [\underline{A}_1(t+1) + \underline{\alpha}_1 \underline{A}_1(t) \underline{\alpha}_1 - \{\underline{\alpha}_1 \underline{A}_1(t+1) + \underline{A}_1(t+1)\underline{\alpha}_1\}] \gamma_2^{-1}$$

2. Iterate 3 term recurrence

$$\underline{\Delta}_{j+1} = \underline{A}_j(2) - \underline{\alpha}_j \underline{\alpha}_j - \underline{\gamma}_j \underline{\beta}_j \equiv \underline{\beta}_{j+1} \underline{\gamma}_{j+1}$$

$$\underline{G}_{j+1}(t) = \underline{\beta}_{j+1}^{-1} [\underline{A}_j(t+1) - \underline{\alpha}_j \underline{A}_j(t) - \underline{\gamma}_j \underline{B}_j(t)]$$

$$\underline{B}_{j+1}(t) = [\underline{A}_j(t+1) - \underline{A}_j(t)\underline{\alpha}_j - \underline{G}_j(t)\underline{\beta}_j] \underline{\gamma}_{j+1}^{-1}$$

$$\begin{aligned}\underline{A}_{j+1}(t) = \underline{\beta}_{j+1}^{-1} [&\underline{A}_j(t+2) - (\underline{\alpha}_j \underline{A}_j(t+1) + \underline{A}_j(t+1)\underline{\alpha}_j) + \underline{\alpha}_j \underline{A}_j(t) \underline{\alpha}_j \\ &+ \underline{\gamma}_j \underline{A}_{j-1}(t) \underline{\beta}_j - (\underline{\gamma}_j \underline{B}_j(t+1) + \underline{G}_j(t+1)\underline{\beta}_j) \\ &+ \underline{\gamma}_j \underline{B}_j(t) \underline{\alpha}_j + \underline{\alpha}_j \underline{G}_j(t) \underline{\beta}_j] \underline{\gamma}_{j+1}^{-1}\end{aligned}$$

$$\underline{\alpha}_{j+1} = \underline{A}_{j+1}(1) \quad [\underline{\beta}_{j+1} = \underline{B}_{j+1}(1), \ \underline{\gamma}_{j+1} = \underline{G}_{j+1}(1)]$$

Construct block tri-diagonal matrix

$$\hat{T}^{(m)} = \begin{pmatrix} \underline{\alpha_1} & \underline{\beta_2} & & & & & \\ \underline{\gamma_2} & \alpha_2 & \beta_3 & & & 0 & \\ & \gamma_3 & \alpha_3 & \ddots & & & \\ & & \ddots & \ddots & \ddots & \beta_{m-1} & \\ & 0 & & \ddots & \gamma_{m-1} & \alpha_{m-1} & \beta_m \\ & & & & & \gamma_m & \alpha_m \end{pmatrix}$$

② Diagonalise $\hat{T}^{(m)} = \sum_k \lambda_k^{(m)} |\omega_k^{(m)}\rangle\langle\omega_k^{(m)}| \qquad \lambda_k^{(m)} = e^{-E_k^{(m)}}$

- with stochastic $\underline{C}(t)$ you will get spurious eigenvalues (either complex or very small) and some kind of filter is needed

③ Lanczos allows rigorous statements of how close e-vals of $\hat{T}^{(m)}$ are to those of $\hat{T}$ – see [Hackett & Wagman 2412.04444]

A key feature is that Lanczos is not variational and provides two-sided bounds on energies

Ex3: given the attached HDF5 data file containing Monte Carlo results for a 2x2 matrix of correlation functions, use the GEVP or Lanczos method to estimate an energy eigenvalue. Use a resampling method (jackknife or bootstrap) to estimate uncertainties
Note that this exercise will require facility with python/julia/mathematica etc and some careful coding and numerical analysis. If you don't have such experience we'll try to find you a partner who does

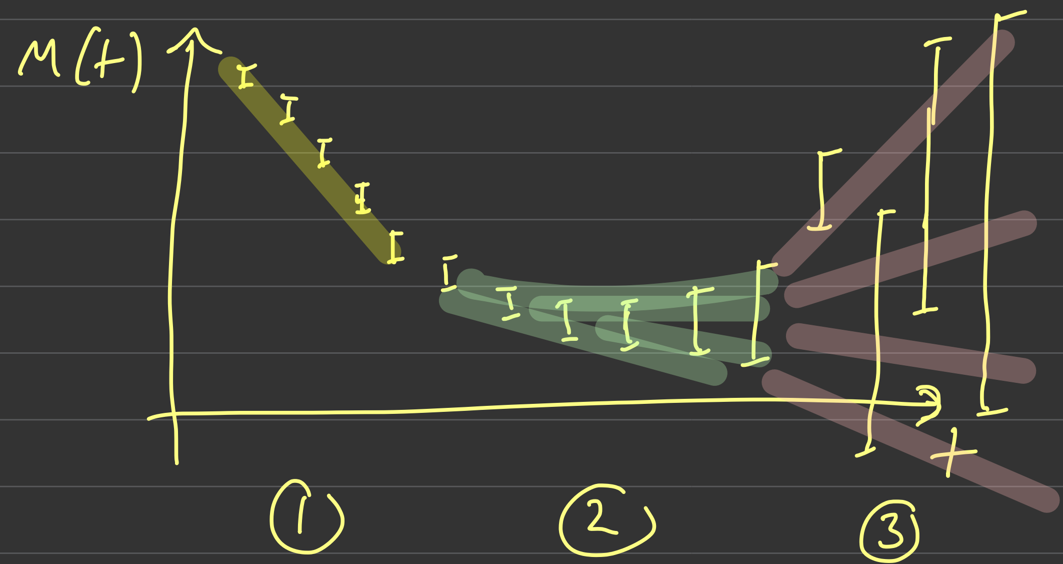
Interpolating operators

- Enormous freedom in what composite operators built from QCD fields that we use

- Key features of QCD correlation functions

Effective mass function

$$M(t) = \ln\left[\frac{C(t+1)}{C(t)}\right] \xrightarrow[t\to\infty]{} M \qquad (T\to\infty)$$



$T \to \infty$

① Strong t-dependence: multiple eigenenergies are contributing significantly

② $M(t)$ independent of t within uncertainties
Uncertainties grow as t increase

③ Very large statistical fluctuations with non-Gaussian distribution

- Choice of operator affects these regions

- Optimise for extraction of energy eigenvalues by
  a) reduce the contributions of high energy states
  b) reduce statistical fluctuations

- Reducing excited states by finding operator that has large overlap onto a single state

$$\hat{\Xi}_a = \sum_i v_{a,i} \hat{\chi}_i \Rightarrow \langle \Xi_a(t) \Xi_a^\dagger(0) \rangle \sim e^{-E_a t} + \text{small}$$

- What about statistical noise?

Given a set of configurations $\{\phi_1, \dots \phi_{N_{cfg}}\}$

$$\bar{C}(t) = \langle \mathcal{C}(t) \rangle = \frac{1}{N_{cfg}} \sum_c \mathcal{C}(t;\phi_c)$$

with variance

$$\text{var}\, C(t) = \frac{1}{N_{cfg}} \sum_c \left(\mathcal{C}(t;\phi_c) - \bar{C}(t) \right)^2 = \langle |\mathcal{C}(t)|^2 \rangle - |\langle \mathcal{C}(t) \rangle|^2$$

if $\mathcal{C}(t) = \chi(t) \tilde{\chi}^\dagger(0)$ then

$$\langle |\mathcal{C}(t)|^2 \rangle = \langle \underbrace{\chi(t) \chi^\dagger(t) \tilde{\chi}^\dagger(0) \tilde{\chi}(0)} \rangle$$

note that $\langle \dots \rangle$ is expectation value over gluon fields after the fermionic integration is performed

$$\xrightarrow[t \to \infty]{} \# \exp[-\tilde{E}_0 t]$$

lowest energy state with q # of $|\chi|^2$: $\langle 0 | |\chi|^2 | \tilde{n} \rangle \neq 0$

Thus the signal-to-noise ratio

$$\frac{\bar{C}(t)}{\sqrt{\mathrm{var}\, C(t)}} \xrightarrow[t\to\infty]{} \# \frac{e^{-E_0 t}}{e^{-\tilde{E}_0 t/2}} = \# \, e^{-(E_0 - \tilde{E}_0/2)t}$$

Parisi, Lepage scaling

If $\tilde{E}_0 \leq 2E_0$ then signal quality degrades (generally the case

Ex 4: Let $C(t)$ be a correlation function built with operators with the following quantum numbers. What states would you expect set the scale $\tilde{E}_0$ that governs the fall off of the variance?

a) pion $\vec{p} = 0$

b) pion $\vec{p} = (1,0,0)$ GeV

c) proton at $\vec{p} = 0$

d) 0^{++} (scalar) glueball

e) ^4He

- Interpolating operators that have small variance are operators Γ such that $|\Gamma|^2$ has small overlaps onto states with energies $\tilde{E}_n < 2E_0$

- How do we choose interpolating operators?
  - a bit of an art - no principled way to do it systematically

① Define the quantum numbers - all properties preserved by QCD
- total momentum $\vec{P}$
- cubic group transformation (little group transformation)
  - representation
  - row of representation

  } lattice analogues of J^2, J_z
- parity, charge conjugation
- baryon number, isospin (I^2, I_z), strangeness, charmness, $SU(3)_f$ rep.

② For q# that corresp. to single hadrons, can use quark model wavefunctions

eg

K^+ $\quad \chi_{K^+}(x) = \bar{u}_a(x)\,\gamma_5\, s_a(x)$

proton $\quad \chi^{\alpha}_{\text{proton}}(x) = \varepsilon_{abc}\,\underbrace{\left(u^T_a(x)\, C\gamma_5\, d_b(x)\right)}_{\text{spin-0 diquark}}\, u^{\alpha}_c(x)$

α: spin index; C: $C = \gamma_0\gamma_2$

Ex 5: construct simple interpolating operators for the octet and decuplet baryons and for the sextet and anti-triplet of singly bottom baryons

(3) Use smeared out version of quark fields with smearing radius ~ 1 fm (the size of the hadron)

(4) Can use (esp. for exotic states) displaced operators

$$\chi_{\pi^+,\mathrm{disp}}(x) = \sum_{\mu=1}^{3} \bar{u}_a(x)\,\gamma_5\, U_\mu(x)\, d_a(x+\hat{\mu})$$

(5) Add any number of gauge invariant gluonic contributions (mult by Wilson loops of various sizes/shapes)

(6) Operators built from multiple colour singlet components eg

$$\chi^{\alpha}_{prot}(x,y) = \varepsilon_{abc}(u^T_a C\gamma_5 d_b)\, u^{\alpha}_c(x)\left(\bar{u}_d(y)\gamma_5 u_d(y) + \bar{d}_d(y)\gamma_5 d_d(y)\right)$$

or in momentum space

$$\chi^{\alpha}_{prot}(\vec{p}_1, \vec{p}_2) = \varepsilon_{abc} \sum_{\vec{x},\vec{y}} e^{-i\vec{p}_1\cdot\vec{x}}\, e^{-i\vec{p}_2\cdot\vec{y}}\, \chi^{\alpha}_{prot}(x,y)$$

with $\vec{P}_{tot} = \vec{p}_1 + \vec{p}_2$ a quantum number (but not $\vec{p}_{rel} = \vec{p}_1 - \vec{p}_2$)

Ex6: Let $\pi^+(\vec{p},t) = \sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}}\, \bar{u}_a(\vec{x},t)\gamma_5 d_a(\vec{x},t)$ and define $\chi_{\pi\pi}(\vec{p}_1,\vec{p}_2,t) = \pi^+(\vec{p}_1,t)\,\pi^+(\vec{p}_2,t)$
Discuss how a calculation of $\langle \chi_{\pi\pi}(\vec{p}_1,\vec{p}_2,t)\, \chi^{\dagger}_{\pi\pi}(\vec{p}_3,\vec{p}_4,0)\rangle$ with $\vec{p}_1+\vec{p}_2 = \vec{p}_3+\vec{p}_4$ would scale with the spatial volume.

- Note that $\chi(t)\tilde{\chi}^\dagger(0)$ containing fermions then this involves evaluating all the Wick contractions from fermion integration

- Computational complexity limits operator construction

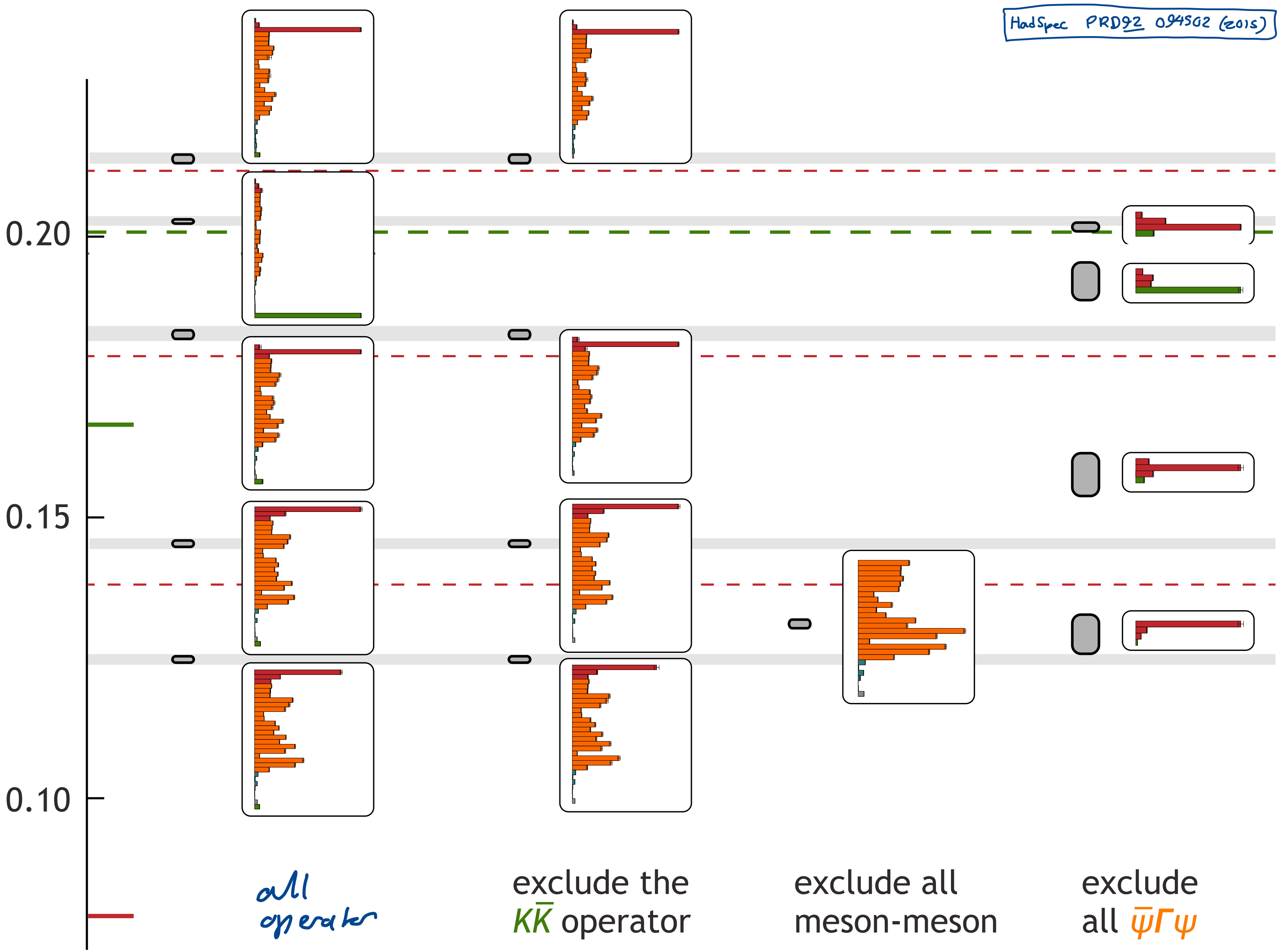
* Cautionary remark: tendency for us to look at operators that are obvious and we know how to make and can afford to compute

- A cautionary tale from HadSpec collaboration for ρ-meson ($I=1$ resonance in $\pi\pi$ scattering) [PRD 92 094502 (2015)]

Operators

- local quark bilinears $\sum_x e^{ip\cdot x}\bar{\psi}(x)\Gamma\psi(x)$ (26 ops)
- π-π-like operators $\sum_x e^{ip\cdot x}\bar{\psi}(x)\gamma_5\psi(x)\sum_y e^{iq\cdot y}\bar{\psi}(y)\gamma_5\psi(y)$ (3 ops)
- $K\bar{K}$-like op $\sum_x e^{ipx}\bar{u}\gamma_5 s(x)\sum_y e^{iqy}\bar{s}\gamma_5 u(y)$ (1 op)

- Spectral bounds depend strongly on operator set



HadSpec PRD92 094502 (2015)
0.20
0.15
0.10
all operator
exclude the $K\bar{K}$ operator
exclude all meson-meson
exclude all $\bar{\psi}\Gamma\psi$

Ex7: what are some other operators you could add to this set?
Do you expect your new operators to significantly change the picture?
How sure are you?

Wick contractions

- Naively for $\langle \chi(t) \tilde{\chi}^{\dagger}(0)$ there are $n_u! \, n_d! \, n_s! \ldots$
  Wick contractions where $n_i = \#$ of quark fields of flavour i in $\chi \tilde{\chi}^{\dagger}$
  - symmetries can reduce this

Ex8: the pion is a spin-zero isotriplet state (π^+, π^0, π^-).
What are the allowed isospins of a two-pion system?
For each total isospin, construct the state with the largest I_z.
Using the simplest possible interpolating operators for each pion, draw diagrams corresponding to all topologies of Wick contractions for correlators built from these operators.
Repeat the exercise for three pions

- Different computational strategies can reduce costs significantly

1. By exploiting symmetry and recursive algorithms for contractions systems of up to 6144 π^+'s have been studied [Abbott et al 2024]

(2) Fermionic nature of quark fields can help

Define a nuclear interpolating operator

$$N_Q = \sum_{\vec{a}} \underbrace{w_{a_1} \dots w_{a_n}}_{\text{complex weights}} q(a_1) \dots q(a_n)$$

multi indices
- spin - colour - flavour - space

$$= \sum_{k=1}^{N_w} w_{(a_1 \dots a_n),k} \sum_{\vec{c}} \underbrace{\varepsilon^{c_1 \dots c_n}}_{\text{n-dim Levi-Civita}} q(a_{c_1}) \dots q(a_{c_n})$$

Corr func

$$\langle N_Q \bar{N}'_Q \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\bar{\Psi} \mathcal{D}\Psi e^{-S} \sum_{k,k'} w^*_{(a'_1 \dots a'_n),k'} w_{(a_1 \dots a_n),k} \sum_{\vec{c},\vec{j}} \varepsilon^{c_1 \dots c_n} \varepsilon^{j_1 \dots j_n}$$

$$\times q(a_{c_1}) \dots q(a_{c_n}) \bar{q}(a'_{j_1}) \dots \bar{q}(a'_{j_n})$$

etc

$$= \frac{1}{Z} \int \mathcal{D}U e^{-S_{eff}} \sum_{k,k'} w^*_{(a'_1 \dots a'_n),k'} w_{(a_1 \dots a_n),k} \det G_{\vec{a},\vec{a}'}[U]$$

with
$$[G_{\vec{a}\vec{a}'}]_{ij} = \begin{cases} S(a'_j, a_c) & \text{if } a'_j \in \vec{a}' \ \& \ a_c \in \vec{a} \\ \delta_{a'_j a_c} & \text{otherwise} \end{cases}$$

cost : $N_w N_{w'} (n_u^3 + n_d^3 + n_s^3)$ using LU-decomposition

$\ll n_u! \, n_d! \, n_s!$ typically

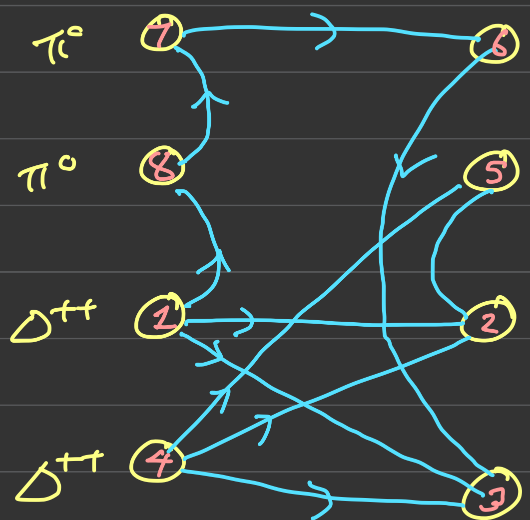
- A given Wick contraction

$$\sum_{i_1} \cdots \sum_{i_N} \sum_{j_1} \cdots \sum_{j_N} T_{i_1 \ldots i_N j_1 \ldots j_N} \; S_{i_1 j_1} \cdots S_{i_N j_N}$$

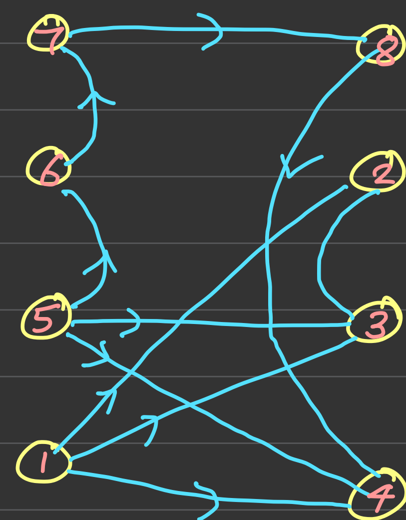
care needed in evaluation order

Ex: $\Delta^{++}\Delta^{++}\pi^0\pi^0$ correlator

- <u>Memory used</u>

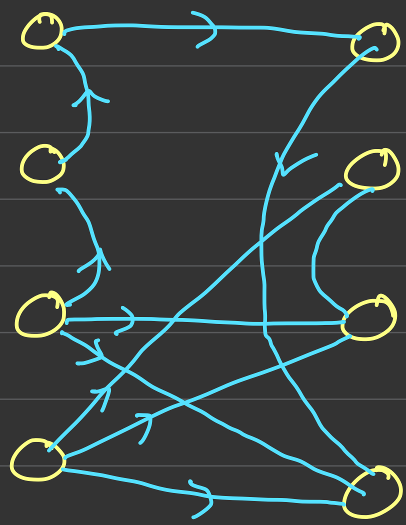


step	1	2	3	4	5	6	7	8
indices	3	4	5	4	2	2	2	0



1	2	3	4	5	6	7	8
3	3	2	3	2	2	2	0

- Work needed (redundant work)

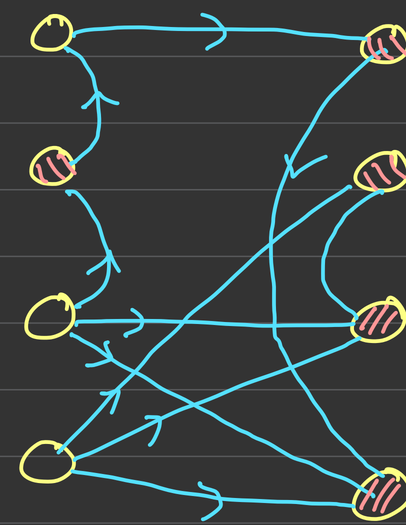


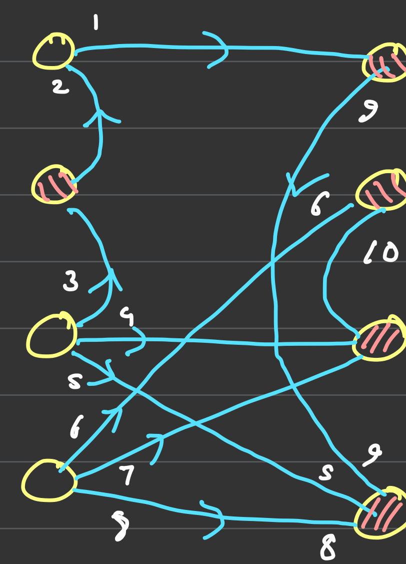
work required : $(\text{rank})^{20}$

$T_{12} S_{23} T_{34} S_{45} T_{567} S_{28} T_{8910}$

$\times S_{911} T_{111213} S_{1314} T_{1415} S_{1516} S_{912}$

$\times S_{617} T_{161718} S_{1819} T_{1920} S_{201}$





precompute

$B_{14} = \;{}^{1}_{4} = S_{12} T_{23} S_{34}$: rank^2

$B_{145} = \; = T_{123} S_{24} S_{35}$: rank^3

work required : $(\text{rank})^{10}$

$T_{12} B_{23} T_{345} T_{678} B_{19} B_{610} B_{1047} B_{958}$

- Graph theoretic methods to consider

Summary

- Spectroscopy is a powerful tool for understanding QCD and learning about bound states, resonances and nuclei

- Many ways to build correlation functions to access spectrum

- Many ways to extract energy bounds from them

- Computational cost increase with # hadrons $\longrightarrow$ nuclei
  a big challenge

- Lots of room for innovation

- Lots of ways to impact phenomenology