Spectral reconstruction in lattice QCD for inclusive and exclusive scattering amplitudes

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The Baryon Scattering Collaboration (BaSC)

- Goal: computation of baryon scattering amplitudes from lattice QCD
- Members:
 - DESY: JB, J. Green
 - Mainz: H. Wittig, et al.
 - CMU: C. Morningstar, S. Skinner
 - UNC: A. Nicholson, J. Moscoso
 - LBL: A. Walker-Loud
 - BNL: A. Hanlon
 - MIT: F. Romero-Lopez
 - Intel: B. Hoerz
 - Darmstadt: D. Mohler, B. Cid-Mora
- First project: several meson-baryon and baryon-baryon systems on CLS D200

 $N_{\rm f} = 2 + 1, \quad a = 0.065 {\rm fm}, \quad m_{\pi} = 200 {\rm MeV}, \quad 64^3 \times 128$

• Talk yesterday by C. Morningstar: nucleon-pion and Lambda(1405)

<u>Lattice QCD:</u> (without electroweak interactions)

- First-principles computer simulation of quarks and gluons
- Euclidean time: $t \rightarrow it$
- Data outputs: correlation functions

$$\begin{aligned} C(t) &= \langle \mathcal{O}(t)\mathcal{O}^{\dagger}(0) \rangle \\ &= \sum_{n} |\langle n | \hat{\mathcal{O}} | \Omega \rangle|^{2} \mathrm{e}^{-E_{n}} \\ &= \int \mathrm{d}\omega \, \rho(\omega) \, \mathrm{e}^{-\omega t} \end{aligned}$$



• In finite-volume, spectral density is a sum of Dirac-deltas

t

Observables from lattice QCD: Euclidean correlation functions

• Large time separation: ground state saturation

$$\lim_{t \to \infty} C_{\rm N}(t) = A e^{-m_{\rm N} t} \left\{ 1 + O(e^{-m_{\pi} t}) \right\}$$

• Signal-to-noise problem => 'Teufelspakt'

$$\lim_{t \to \infty} \frac{C_{\rm N}(t)}{\sigma_{\rm stat}(t)} \propto e^{-(m_{\rm N} - \frac{3}{2}m_{\pi})t}$$





$$m_{\rm eff}(t+0.5a) = \log\left[\frac{C(t)}{C(t+a)}\right]$$

Dotted lines: result of two-state fit model

Observables from lattice QCD: Euclidean correlation functions

• Large time separation: ground state saturation

$$\lim_{t \to \infty} C_{\rm NN}^{I=0}(t) = A e^{-E_{\rm NN}^{I=0}t} \left\{ 1 + O(e^{-m_{\pi}t}) \right\}$$

• Signal-to-noise problem => 'Teufelspakt'

$$\lim_{t \to \infty} \frac{C_{\rm NN}^{I=0}(t)}{\sigma_{\rm stat}(t)} \propto e^{-2(m_{\rm N} - \frac{3}{2}m_{\pi})t}$$





$$m_{\rm eff}(t+0.5a) = \log\left[\frac{C(t)}{C(t+a)}\right]$$

Dotted lines: 2 x nucleon mass

<u>An alternative to few-state fits at large time:</u>

Goals:

- Use all data, including (precise) early times
- No modeling of excited states

Solution: spectral reconstruction

• From input data

$$C(t) = \int d\omega e^{-\omega t} \rho(\omega), \quad t \in \{2a, 3a, \dots, 25a\}$$

Infer

$$D(\alpha, \tau) = \int d\omega \, \omega^{\alpha} e^{-\omega\tau} \, \rho(\omega), \quad \alpha, \tau \text{ arbitrary}$$
$$= \int d\omega \, \sigma(\omega) \, \rho(\omega)$$

Smeared spectral densities à la Backus-Gilbert:

Hansen, Lupo, Tantalo `19; Pijpers+Thompson `92, Backus+Gilbert `68

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Seek an estimator of the form:

$$\hat{D}(\alpha, \tau) = \sum_{t} g_t C(t) = \int d\omega \left(\sum_{t} g_t e^{-\omega t} \right) \rho(\omega)$$
$$= \int d\omega \,\hat{\sigma}(\omega) \,\rho(\omega)$$

Two competing considerations:

• Accuracy:
$$A[g] = \int d\omega \{\sigma(\omega) - \hat{\sigma}(\omega)\}^2$$

- Precision: $B[g] = \operatorname{Var}[\hat{D}] = \sum_{t,t'} g_t g_{t'} \operatorname{Cov}[C(t), C(t')]$
- Best estimate by minimizing combination:

$$G_{\lambda}[g] = (1 - \lambda)A[g]/A[0] + \lambda B[g]$$

Test: predicting the effective mass

New definition of effective mass:

$$\tilde{m}_{\text{eff}}(\alpha,\beta|\tau) = \left(\frac{D(\alpha,\tau)}{D(\beta,\tau)}\right)^{1/(\alpha-\beta)}$$

Standard definition is special case:

$$\tilde{m}_{\text{eff}}(1,0|t) = m_{\text{eff}}(t) + O(a^2)$$

• use timeslices [2a,15a]

• predict [16a, 25a]



Test: comparison with two-state fit

• Using all times [2a, 25a], predict times [26a, 35a]



• Long plateau: systematic error changes by factor of 2

Adjusting excited state contamination:

• Different (α, β) have different excited state systematics



• Further confirmation of plateau value

<u>A novel Generalized Eigenvalue Problem (GEVP):</u>

• Two correlation matrices:

$$A_{ij}(t) = D(\alpha_i + \alpha_j, t), \qquad B_{ij}(t) = D(\alpha_i + \alpha_j, t)$$

• Equal-time GEVP: $B(t)v_n(t) = \lambda_n(t)A(t)v_n(t)$



<u>Application to nucleon-nucleon:</u>

• Same setup as single-nucleon, with 2x2 GEVP



• Mild indication for attraction, but not precise enough. :-(

Inclusive processes in lattice QCD



Decay rate from spectral density:

$$C(t) = \int d^3 \boldsymbol{x} \langle \Omega | \hat{V}_z^{\text{cc}}(\boldsymbol{x}) \, \mathrm{e}^{-\hat{H}t} \, \hat{V}_z^{\text{cc}}(0)^{\dagger} | \Omega \rangle$$
$$\propto \int_0^\infty d\omega \, \omega^2 v_1(\omega^2) \, \mathrm{e}^{-\omega t}$$

Smeared spectral densities

• Approximation of Dirac-delta:

$$\lim_{\epsilon \to 0^+} \delta_\epsilon(x) = \delta(x)$$

• Implement $i\epsilon$ -prescription

$$\delta_{\epsilon}(x) = \frac{i}{x + i\epsilon} = \frac{\epsilon}{x^2 + \epsilon^2} + i\frac{x}{x^2 + \epsilon^2}$$

• Cut off high energies (Heaviside approx.):

$$\lim_{\epsilon \to 0^+} \delta_\epsilon(x) = \theta(x)$$

• Dispersion relations, sum rules,

Finite vs. infinite volume

Infinite volume: continuous



Finite volume: sum of Dirac-delta peaks.



Not 'close' to infinite volume at finite L!

Masterfield lattice QCD

• Large volumes needed to saturate ordered double limit:

$$v_1(s) = \lim_{\epsilon \to 0^+} \lim_{L \to \infty} v_{1,\epsilon}^{g}(s), \quad v_{1,\epsilon}^{g}(s) = \int d\omega \, \frac{e^{-\frac{(\omega - \sqrt{s})^2}{2\epsilon^2}}}{\sqrt{2\pi\epsilon}} v_1(\omega^2)$$

- Relevant idea: masterfield simulation paradigm M. Lüscher, `17
 - → Only a few gauge configurations
 - → Accrue statistics from separate space-time regions:
 - \Rightarrow O(1000) gauge configs = 6^4 space time regions of size $~m_\pi L pprox 3$
- Preliminary application: isovector (axial)vector correlators at

$$N_{\rm f} = 2 + 1, \quad L = 18 {\rm fm},$$

 $a = 0.09 {\rm fm}, \quad m_{\pi} = 265 {\rm MeV}$

M. Bruno, JB, A. Francis, P. Fritzsch, J. Green, M. T. Hansen, M. Lüscher, A. Patella, A. Rago, in prep.

Preliminary results

PRELIMINARY



• Comparison to hadronic tau-decay (right)

ALEPH collaboration `05

- No extrapolation to zero-width yet
- Mild indication of four-particle effects.

M. Bruno, JB, A. Francis, P. Fritzsch, J. Green, M. T. Hansen, M. Lüscher, A. Patella, A. Rago, in prep.

Preliminary results



• Comparison to hadronic tau-decay (right)

ALEPH collaboration `05

- No extrapolation to zero-width yet
- Bump from a1(1260), indication of five pions

M. Bruno, JB, A. Francis, P. Fritzsch, J. Green, M. T. Hansen, M. Lüscher, A. Patella, A. Rago, in prep.

Conclusions

- Spectral reconstruction is a promising alternative to standard lattice QCD analysis
- The correlator can be efficiently reconstructed at arbitrary times, with prefactors.
 - →Three-point functions
 - → Thermal effects
- Varying excited state contamination leads to a novel GEVP for spectroscopy.
- Improves nucleon mass, not enough precision for NN
- First lattice QCD computation of inclusive amplitudes are possible!
 - → Large volumes needed for good energy resolution
 - → Masterfield simulation paradigm effective
- Other applications of spectral reconstruction:
 - → SVZ sum rules T. Ishikawa and S. Hashimoto, Phys.Rev.D 104 (2021) 7, 074521
 - → Inclusive semileptonic *B*-decays P. Gambino, et al JHEP 07 (2022) 083
 - Exclusive scattering amplitudes
 JB and M.T. Hansen Phys.Rev.D 100 (2019) 3, 034521