Models in lattice QCD computations of scattering amplitudes

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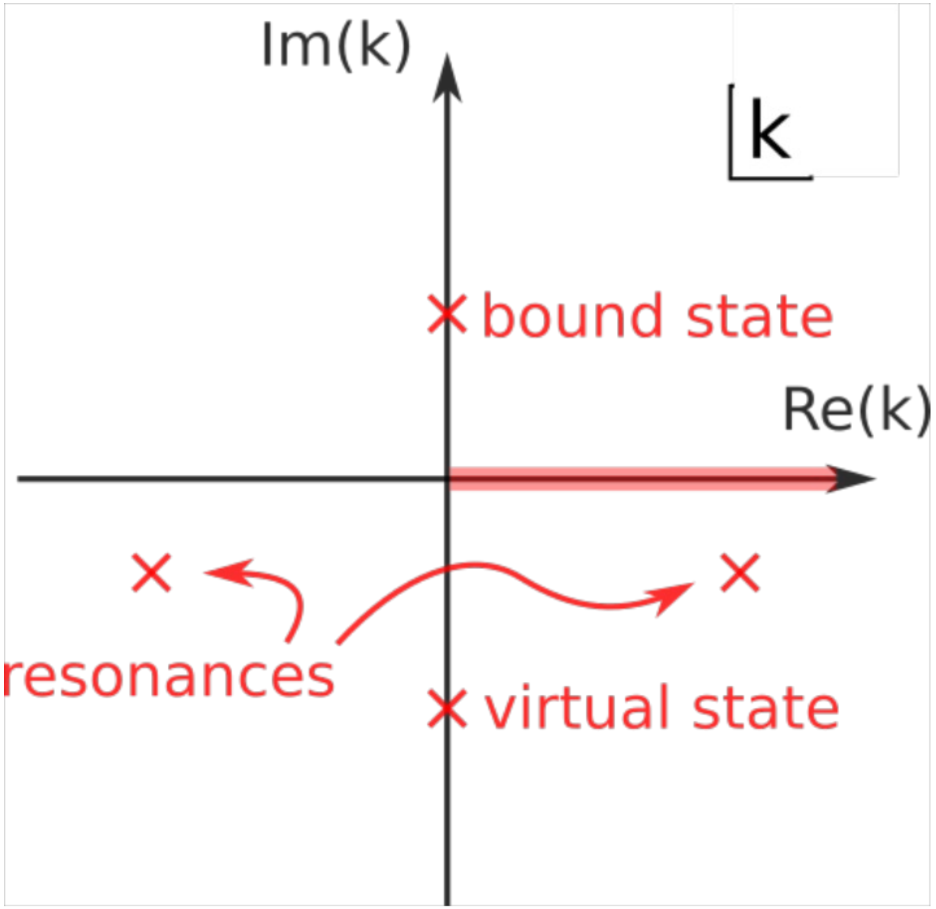
Democratizing Models Workshop RUB Nov. 25-26th, 2024

Introduction:

- Resonances and near-threshold bound-states

- Poles of scattering amplitude in the complex plane

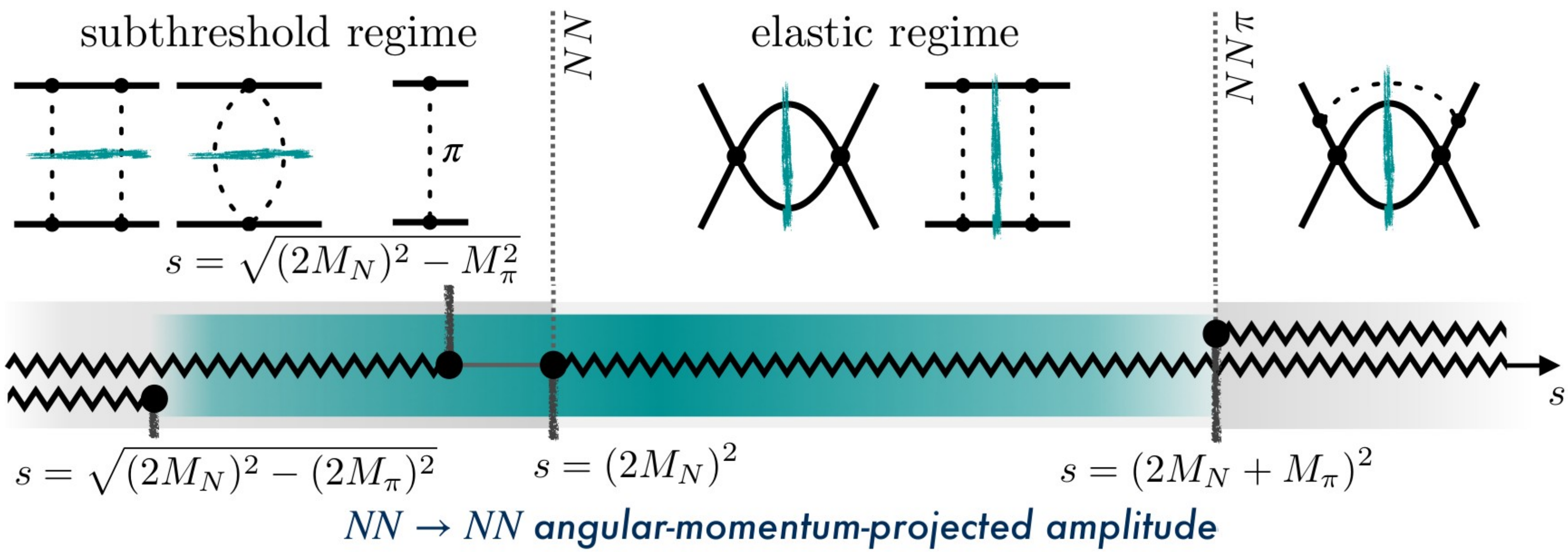
- data on the positive real axis used for analytic continuation



from I. Matuschek, V. Baru, F.-K. Guo, C. Hanhart
Eur.Phys.J.A 57 (2021) 3, 101

Nearby non-analyticities must be treated:

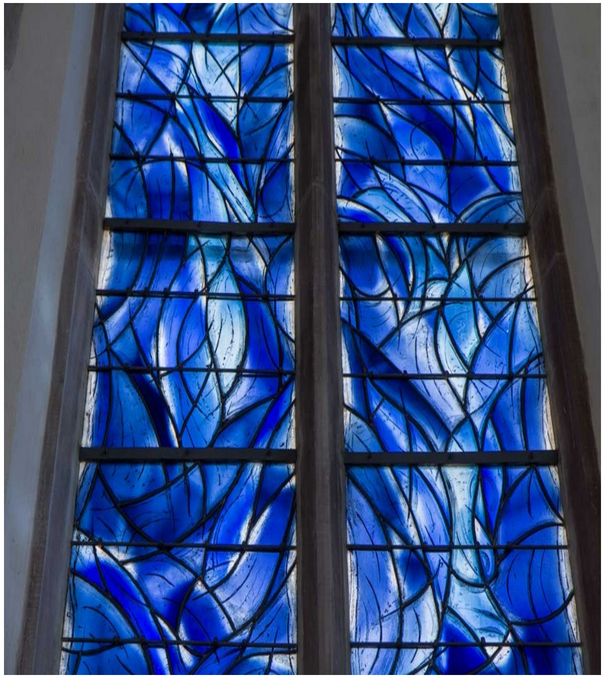
- Right-hand (threshold) cuts
- Left-hand (cross-channel) cuts
- ...



A. Baião Raposo, Lattice ‘23

Lattice QCD:

- Sources of error:
  - Monte Carlo statistics
  - Finite volume and lattice spacing
- Imaginary time (Wick rotation): $t \to i\tau$



Lattice QCD by M. Chagall :-P
(St. Stephen's Church, Mainz)

- Energies/matrix elements from large-time limit of correlation functions:

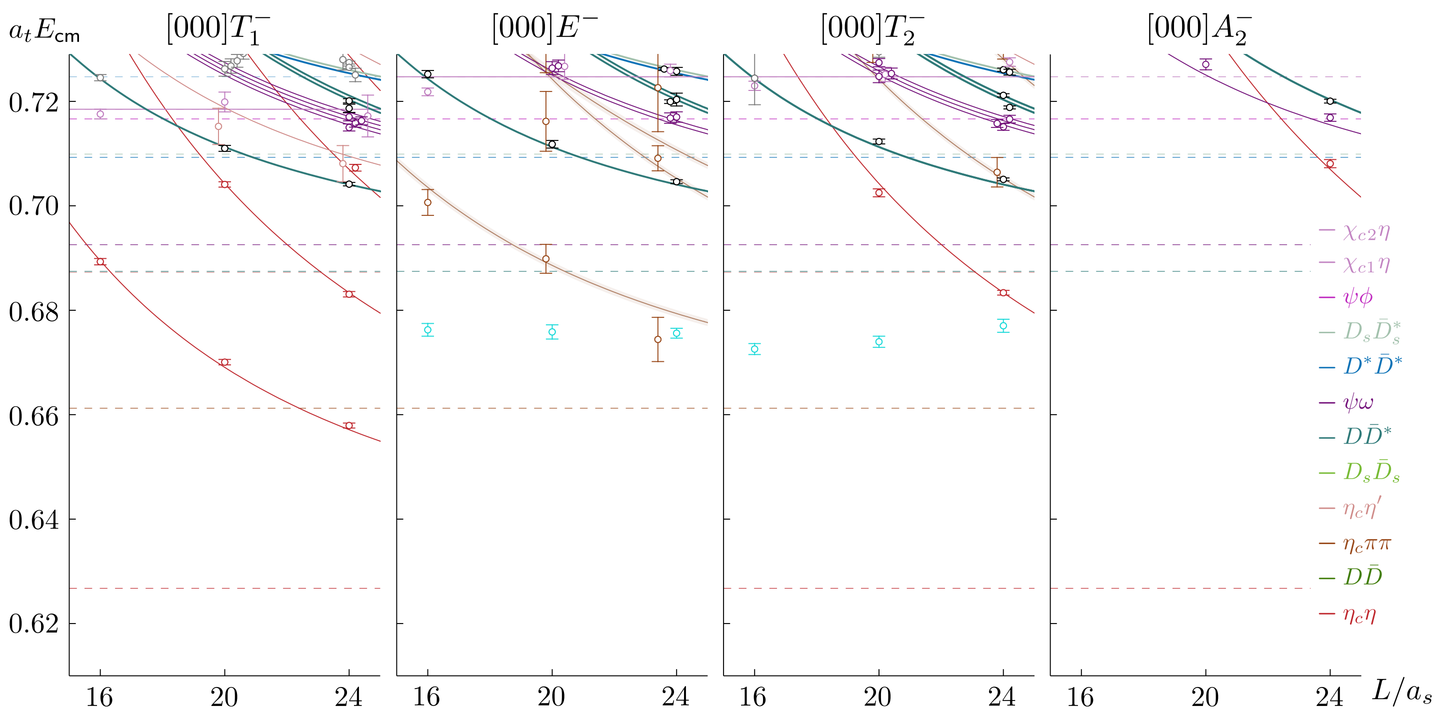
$$C^{2\mathrm{pt}}(\tau) = \sum_n |\langle 0|\hat{O}|n\rangle|^2 \, \mathrm{e}^{-E_n \tau}$$

$$\lim_{\tau\to\infty} C^{2\mathrm{pt}}(\tau) = |\langle 0|\hat{O}|1\rangle|^2 \, \mathrm{e}^{-E_1 \tau}$$

Lattice QCD computations of scattering amplitudes: ingredients

1) Finite-volume multi-hadron energies. Ex: hidden charm (without annihilation)

$$N_\mathrm{f} = 2+1, \quad m_\pi \approx 391\,\mathrm{MeV}, \quad a_\mathrm{s} = 0.12\mathrm{fm} = 3.5 a_\mathrm{t}$$



D. J. Wilson, C. E. Thomas, J. J. Dudek, R. G. Edwards (Hadron Spectrum Coll.), 2309.14071 [hep-lat]

2) Determinant condition relating energies to amplitudes

3) Amplitude parametrizations/fits

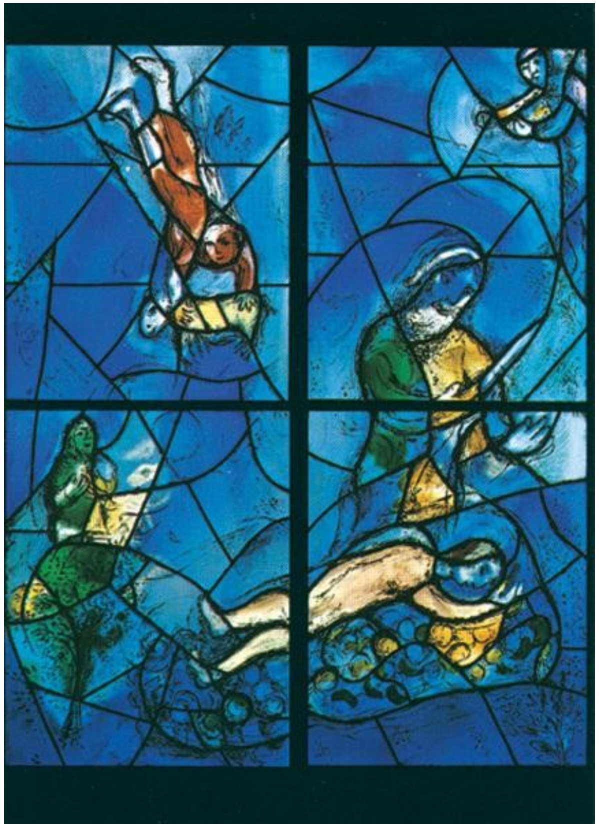
4) Analytic continuation → pole positions/residues

2) Amplitudes from finite-volume energies

$$\det[K^{-1}(E_{\rm cm}^{\rm FV}) - B(\boldsymbol{p}_{\rm cm}^{\rm FV})] = 0$$

M. Lüscher, *Nucl. Phys.* **B354** (1991) 531;...

- Determinant over partial waves and channels
- Direct info below threshold (!) if $E_{\rm cm}^{\rm FV} < E_{\rm thresh}$
- Neglects:
  - Partial waves above $\ell_{\rm max}$
    C. Morningstar, *et al*., Nucl.Phys.B 924 (2017) 477-507
  - Right-hand cuts due to 3+ particles
    Z. Draper, *et al*., JHEP 07 (2023) 226
    S. Dawid, *et al*., Phys.Rev.D 108 (2023) 3, 034016; ...
  - Left-hand cuts
    A. Baiao Raposo, M. T. Hansen, Lattice '22,'23
    M. Habib E Islam, *et al*., Lattice '23
    S. Sharpe, *et al*., Lattice '23
    M.-L. Du, *et al*., 2303.09441 [hep-ph]
  - Exponential finite-volume effects



n-body in a finite volume by M. Chagall :-P
(St. Stephen's Church, Mainz)

- Automated determination of B-matrix elements

C. Morningstar, JB, B. Singh, R. Brett, J. Fallica, A. Hanlon, B. Hörz, Nucl. Phys. **B924** (2017) 477

- For all partial waves $\ell \leq 6$, all total spin $s \leq 7/2$, all irreps, (non-)identical particles.
- Publicly available C++ code for evaluation. (github)
- Example box matrix element:

$$B^{A_1,\mathrm{oa}}(\ell_1 = \ell_2 = 6, n_1 = n_2 = 1) = R_{00} - \frac{2\sqrt{5}}{55} R_{20} - \frac{96}{187} R_{40} - \frac{80\sqrt{13}}{3553} R_{60} + \frac{445\sqrt{17}}{3553} R_{80} + \frac{15\sqrt{24310}}{3553} R_{88} - \frac{498\sqrt{21}}{7429} R_{10,0} + \frac{6\sqrt{510510}}{7429} R_{10,8} + \frac{2178}{37145} R_{12,0} + \frac{66\sqrt{277134}}{37145} R_{12,8}$$

3) Amplitude parametrizations/fits:

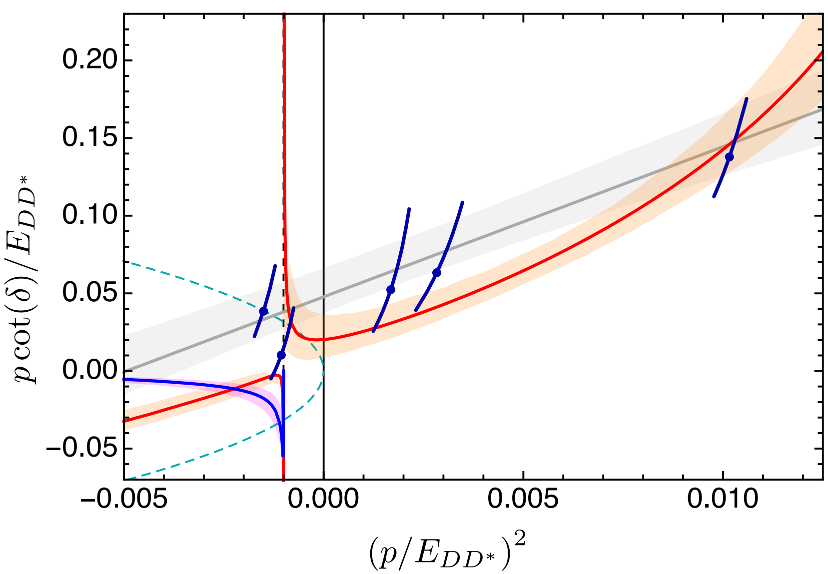
- Typically a variant of the effective range expansion (ERE):

$$p_{\mathrm{cm}}^{2\ell+1}\cot\delta_\ell = \frac{1}{a} + \frac{r}{2}p_{\mathrm{cm}}^2 + \ldots$$

4) Analytic continuation: s-wave pole occurs if

$$p_{\mathrm{cm}}\cot\delta_0 - ip_{\mathrm{cm}} = 0$$

- Radius of convergence limited by nearest cut
  - Ex: $T_{cc}(3875)^+$ in *DD**-scattering
    M.-L. Du, et al., Phys.Rev.Lett. 131 (2023) 13, 131903
  - Points from lattice QCD at $m_\pi = 280\mathrm{MeV}$, gray band is ERE fit
    S. Prelovsek, M. Padmanath, Phys. Rev. Lett. 129, 032002 (2022);
    See also: S. Chen et al., PLB 833, 137391 (2022); Y. Lyu et al., 2302.04505
  - Left hand cut invalidates naive FV formalism
    J. R. Green, et al., Phys.Rev.Lett. 127 (2021) 24, 242003
  - Near left-hand cuts, pole positions from ERE not trustworthy



from M.-L. Du, et al.

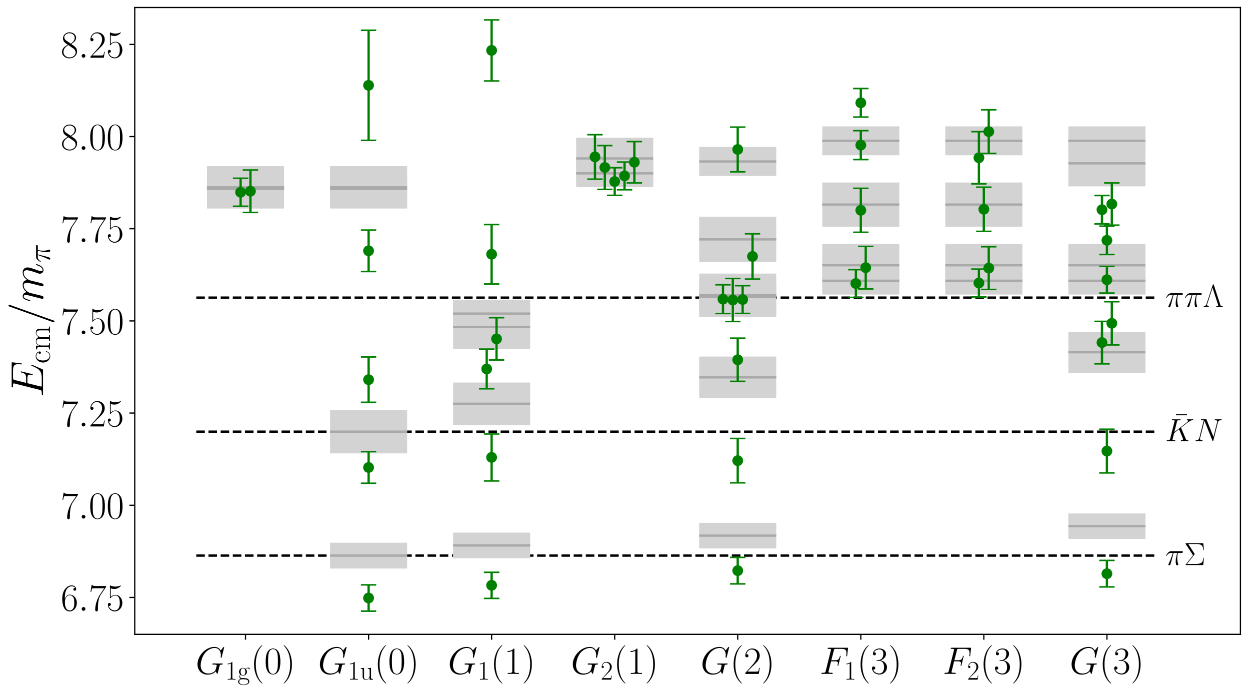
Extended example: recent lattice computation of the Lambda(1405)

JB, B. Cid-Mora, A. Hanlon, B. Hoerz, D. Mohler, C. Morningstar, J. Moscoso, A. Nicholson, F. Romero-Lopez, A. Walker-Loud (For the Baryon Scattering Collaboration BaSC), Phys.Rev.Lett. 132 (2024) 5, 051901 (Editor's Suggestion)

CLS (D200) lattice:

$$64^3 \times 128, \ a = 0.064\text{fm}, \ m_\pi = 200\text{MeV}$$

1) Finite-volume energies:



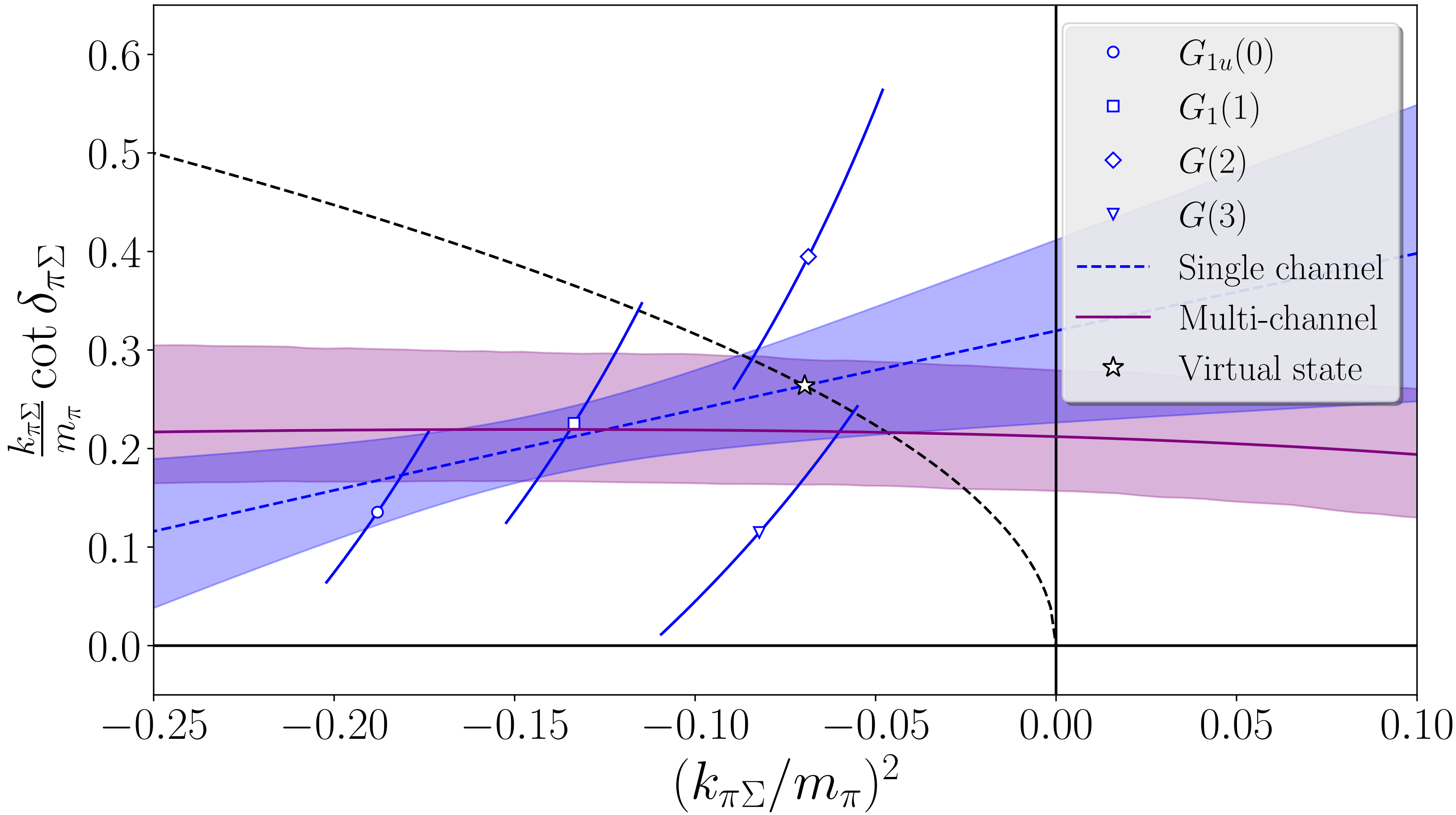
More details in talk of B. Cid-Mora Mon. 4:50pm, Hadron Spectroscopy

Extended example: recent lattice computation of the Lambda(1405)

CLS (D200) lattice:

$$64^3 \times 128,\ a = 0.064\text{fm},\ m_\pi = 200\text{MeV}$$

2) Quantization condition: leading partial wave approximation



Extended example: recent lattice computation of the Lambda(1405)

CLS (D200) lattice:

$$64^3 \times 128,\ a = 0.064\text{fm},\ m_\pi = 200\text{MeV}$$

3) Amplitude parametrization

Variants of:

$$K_{ij}^{-1} = A_{ij} + B_{ij}\Delta(E_{\text{cm}})$$

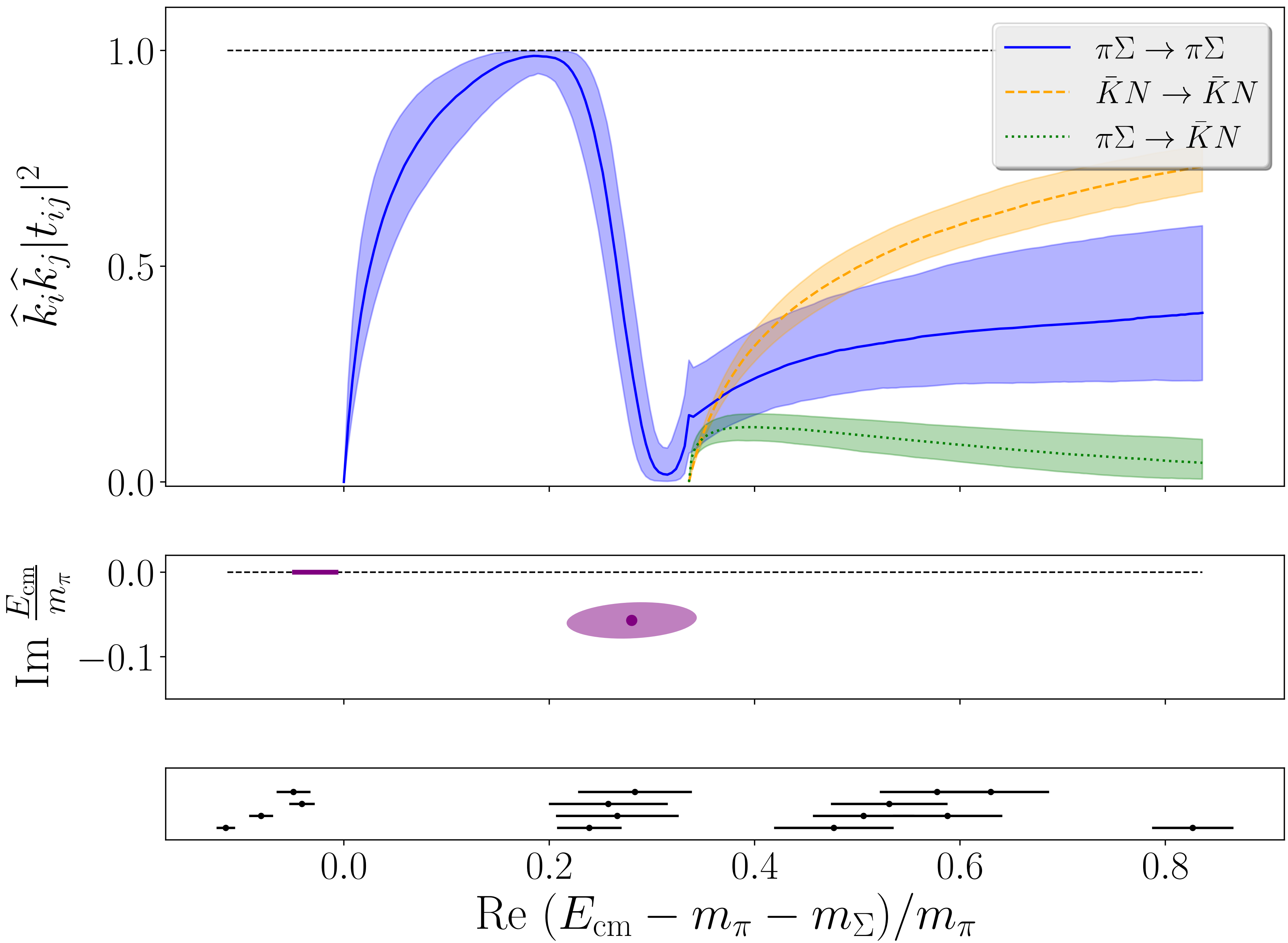
as well as for *K* and Blatt-Biedenharn

4) Analytic continuation: find zeroes of

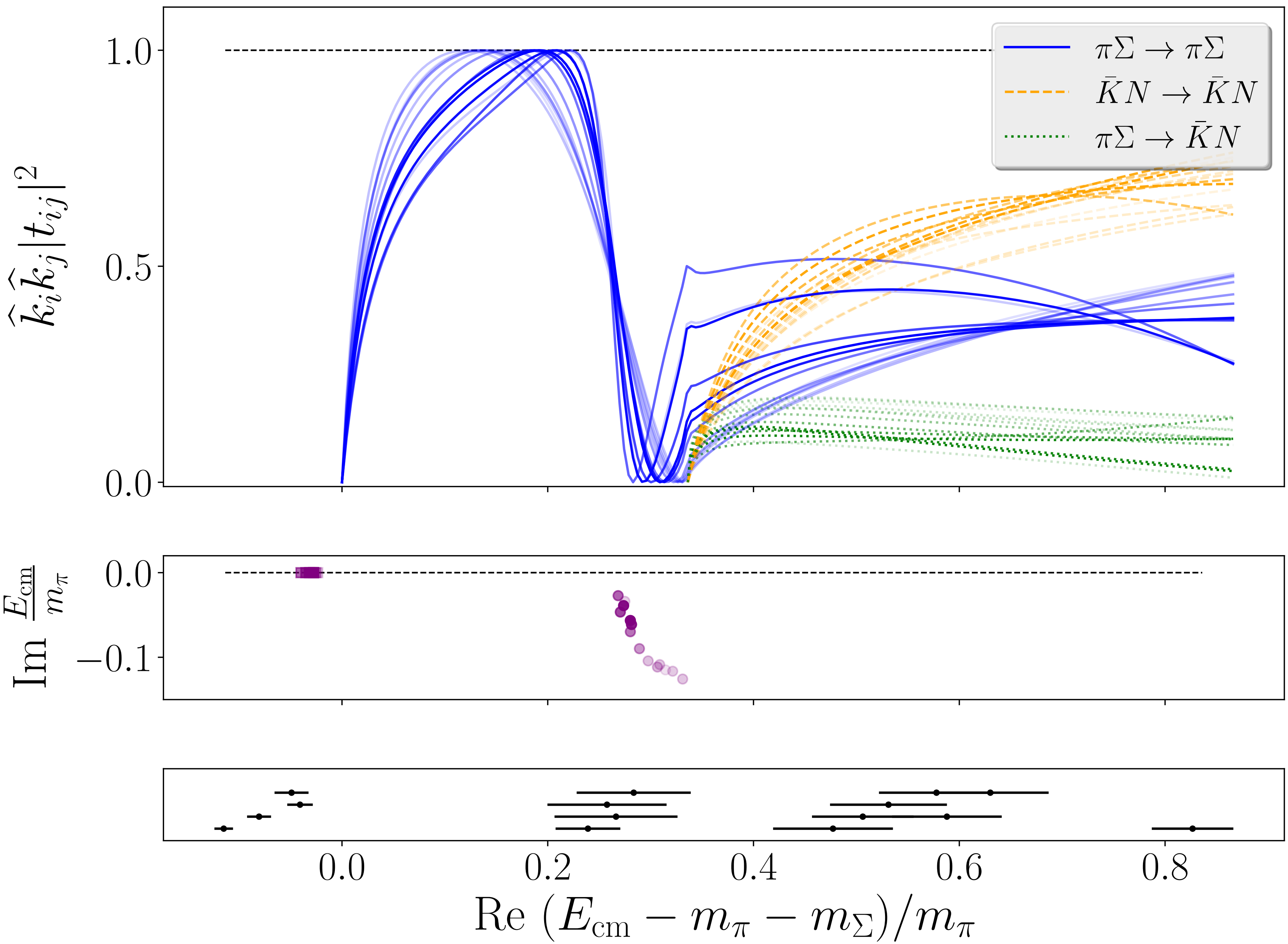
$$t^{-1} = K^{-1} - i\hat{k}$$

No nearby left hand/circular cuts!

Extended example: recent lattice computation of the Lambda(1405)



Extended example: recent lattice computation of the Lambda(1405)



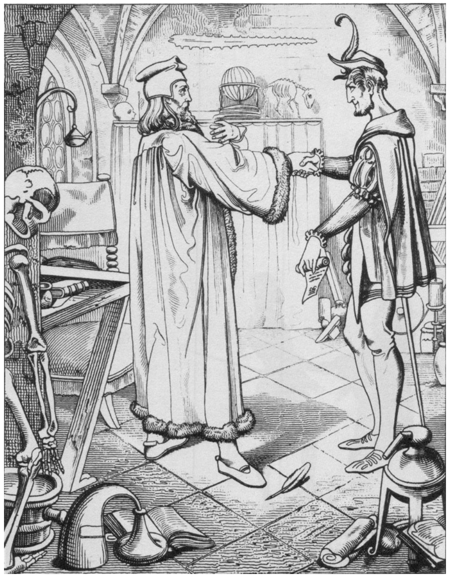
Observables from lattice QCD: Euclidean correlation functions

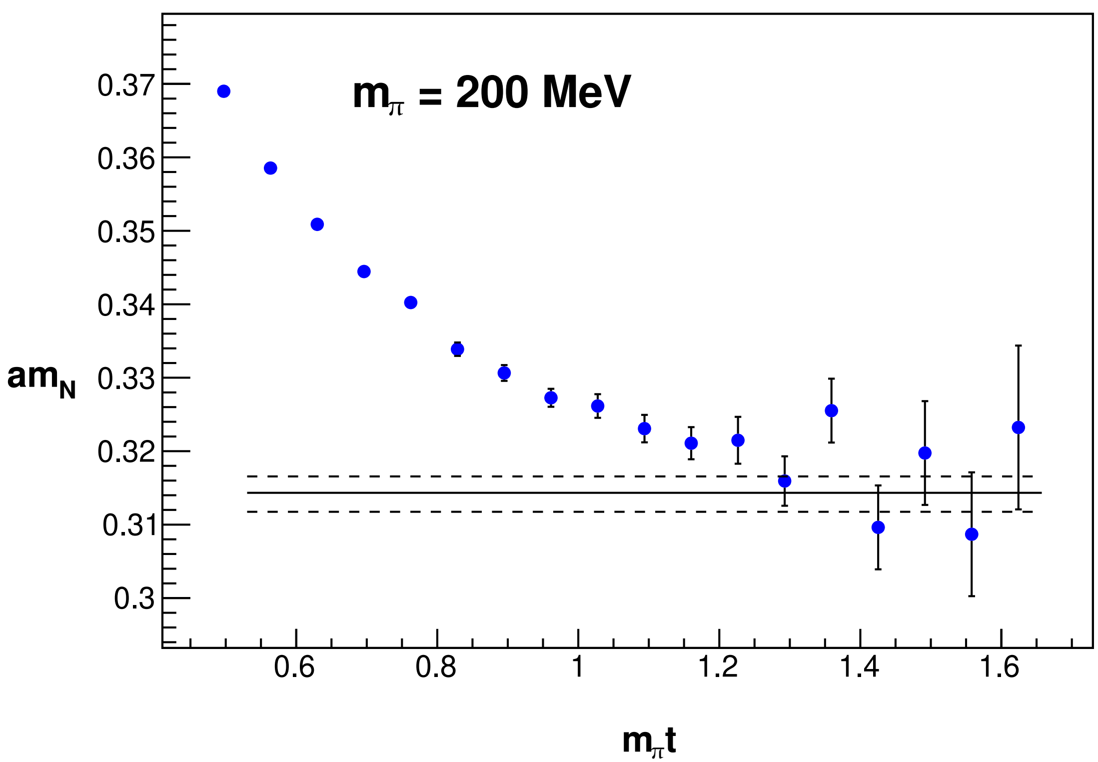
- Large time separation: ground state saturation

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

- Signal-to-noise problem => ‘Teufelspakt’

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





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

Dotted lines: result of two-state fit model

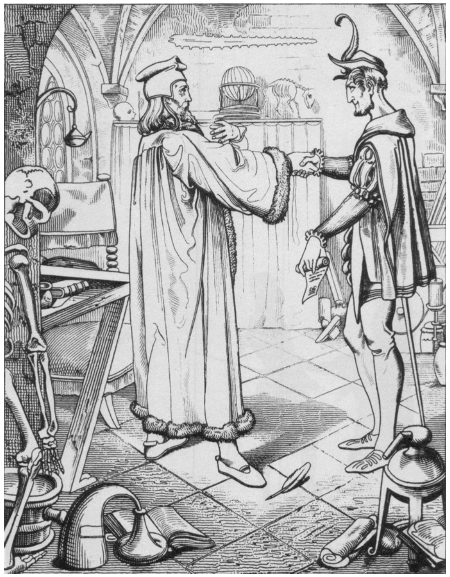
Observables from lattice QCD: Euclidean correlation functions

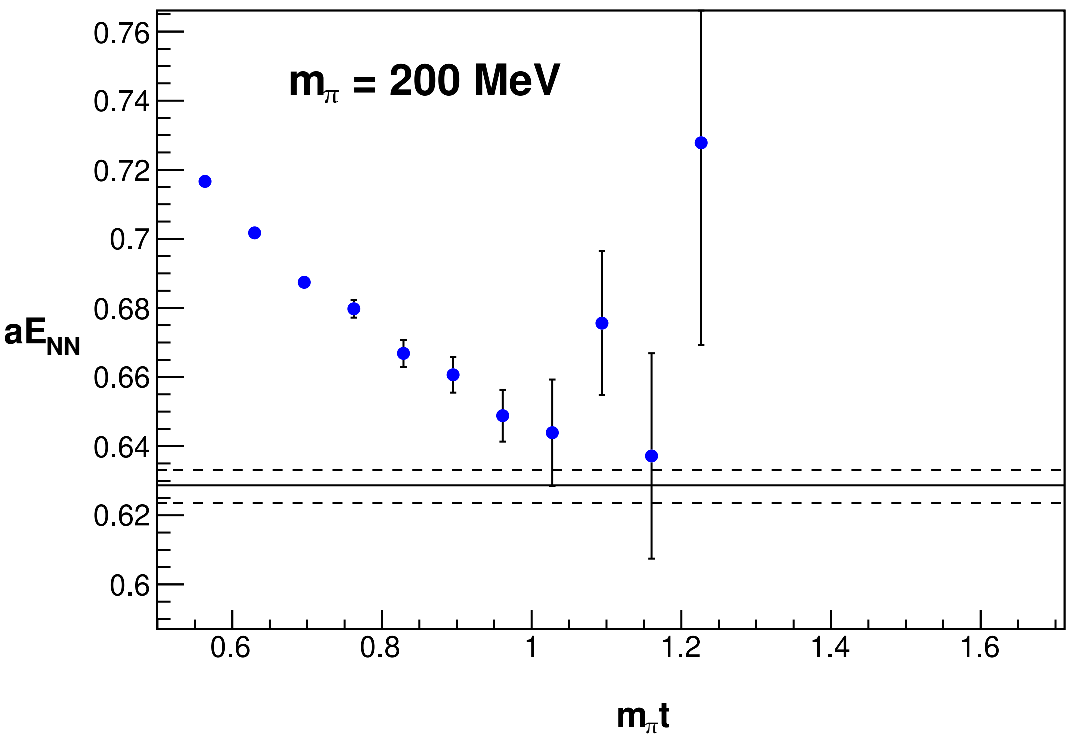
- Large time separation: ground state saturation

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

- Signal-to-noise problem => ‘Teufelspakt’

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





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

Dotted lines: 2 x nucleon mass

An alternative to few-state fits at large time:

Goals:

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

Solution: spectral reconstruction

- From input data

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

- Infer

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

$$= \int \mathrm{d}\omega \, \sigma(\omega) \, \rho(\omega)$$

Smeared spectral densities à la Backus-Gilbert:

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

Seek an estimator of the form:

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

Two competing considerations:

- Accuracy: $$A[g] = \int \mathrm{d}\omega\, \{\sigma(\omega) - \hat{\sigma}(\omega)\}^2$$
- Precision: $$B[g] = \mathrm{Var}[\hat{D}] = \sum_{t,t'} g_t\, g_{t'}\, \mathrm{Cov}[C(t), C(t')]$$
- Best estimate by minimizing combination:

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

Test: predicting the effective mass

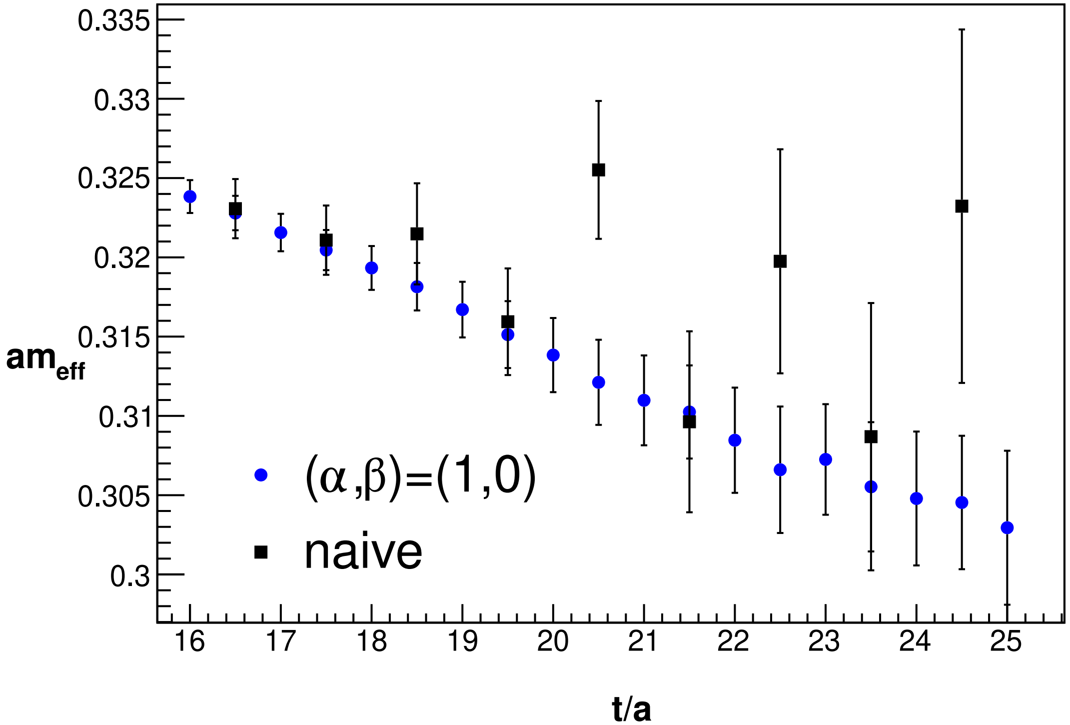
New definition of effective mass:

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

Standard definition is special case:

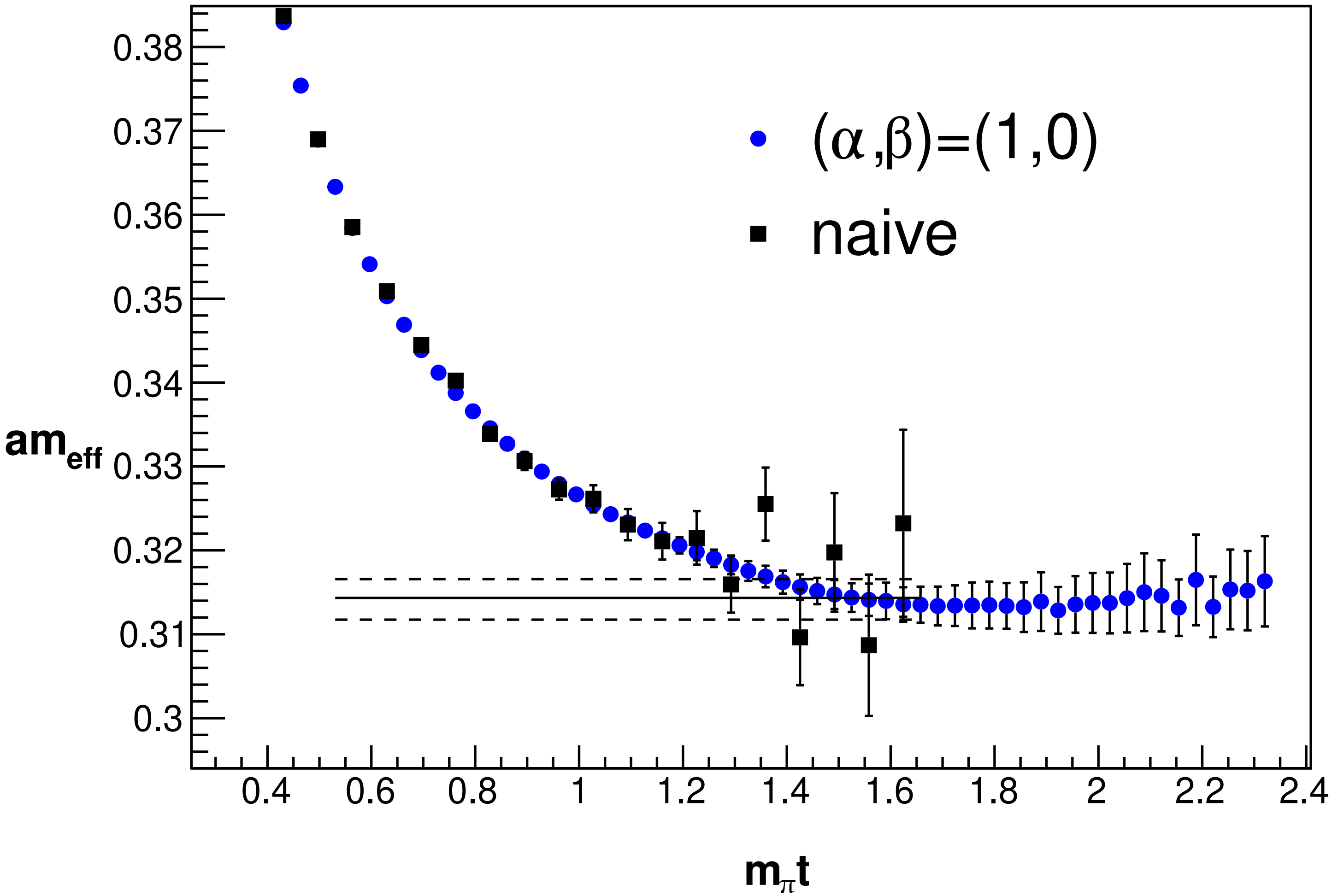
$$\tilde{m}_{\text{eff}}(1, 0|t) = m_{\text{eff}}(t) + \mathrm{O}(a^2)$$

- use timeslices [2a,15a]
- predict [16a, 25a]



Test: comparison with two-state fit

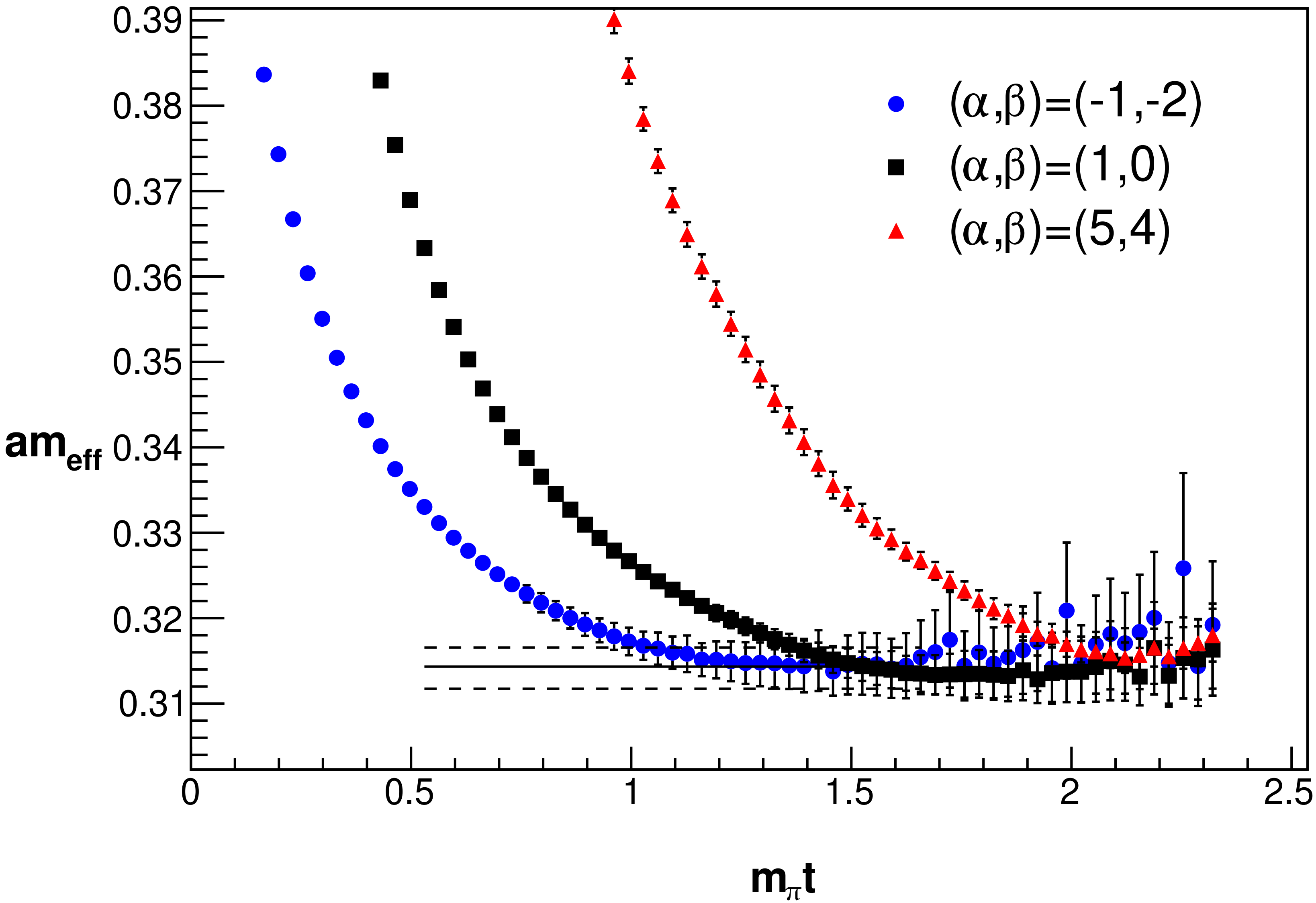
- Using all times [2a, 25a], predict times [26a, 35a]



- Long plateau: systematic error changes by factor of 2

Adjusting excited state contamination:

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



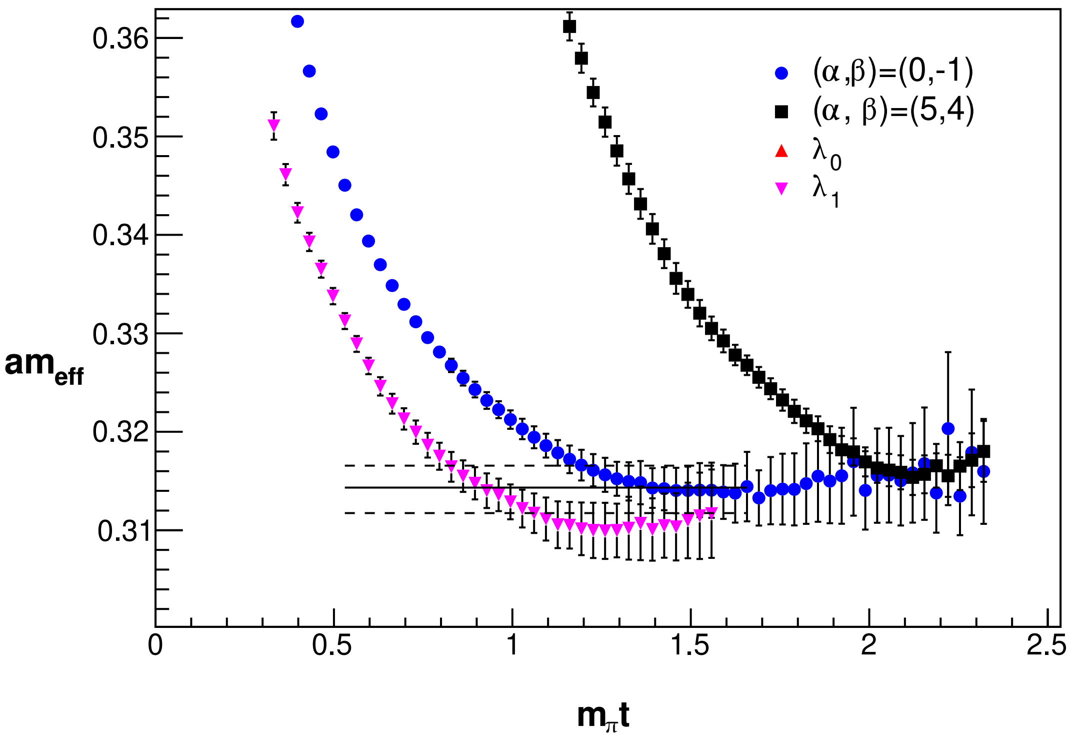
- Further confirmation of plateau value

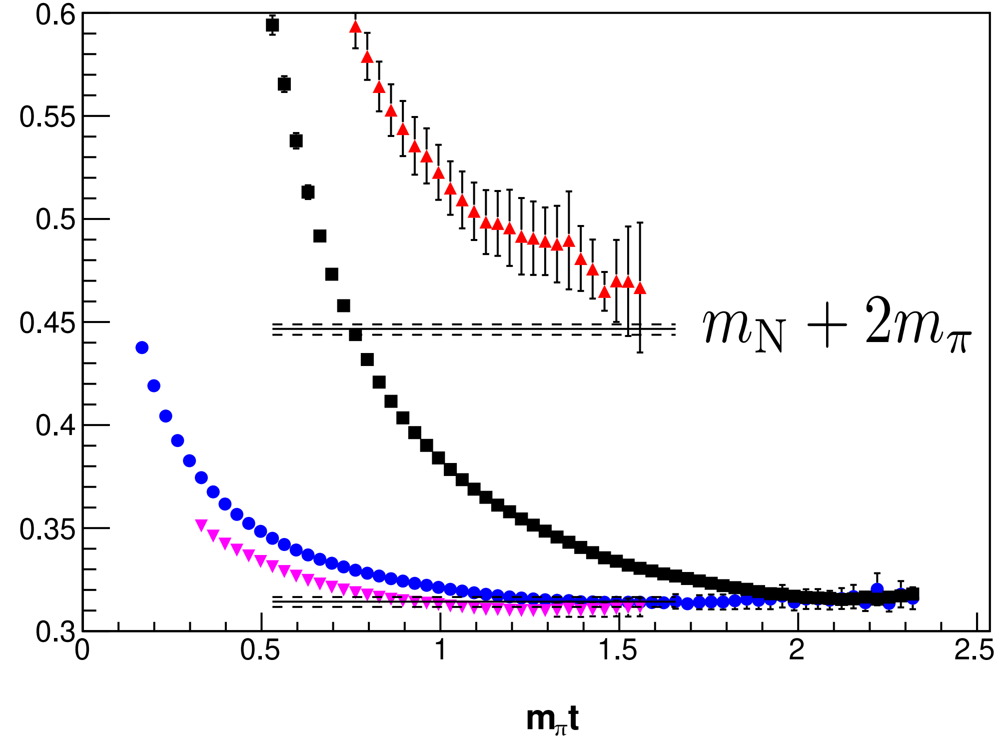
A novel Generalized Eigenvalue Problem (GEVP):

- Two correlation matrices:

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

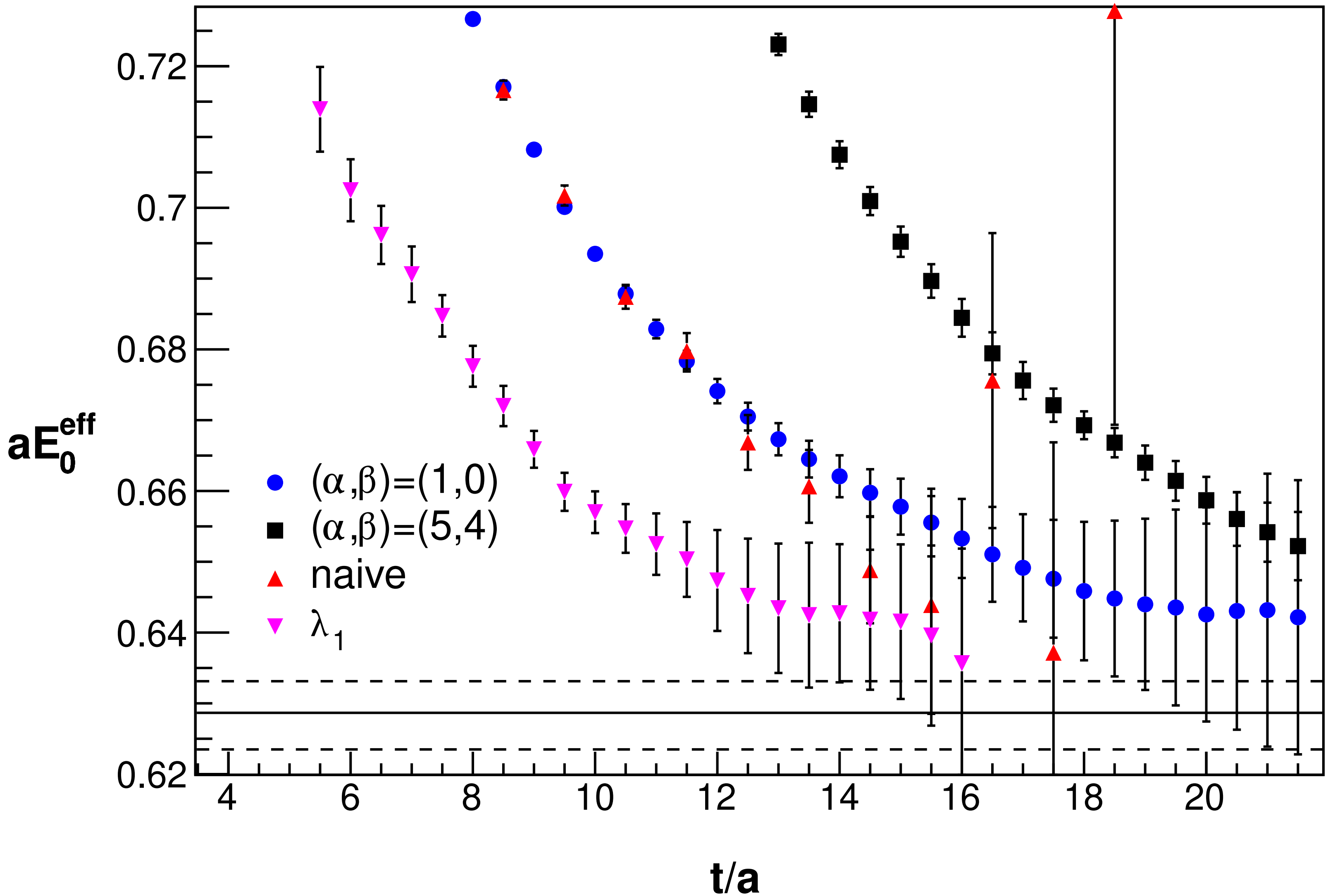
- Equal-time GEVP: $B(t)v_n(t) = \lambda_n(t)A(t)v_n(t)$





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

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



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

Conclusions

- Finite-volume approach to scattering amplitudes requires model parametrizations.

- Near-threshold two-body amplitude parametrizations are rather rudimentary

- Needs:
  - ➔ Three-body amplitude models
  - ➔ Inclusion of cross-channel (left-hand) cuts
  - ➔ Input from effective field theory

- Another source of modelling: correlator fits
  - ➔ Novel parameter-free approach
  - ➔ Equivalent to gaussian processes in ML
  - ➔ Possible integration into a Bayesian framework