Scattering amplitudes in lattice QCD: thinking inside and outside the box

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“Linking non-perturbative and perturbative approaches to fragmentation”
HEPHY Workshop, May 13th, 2025

Observables from lattice QCD: Euclidean correlation functions

- Large time separation: ground state saturation

$$C_{ij}(\tau) = \langle \mathcal{O}_i(\tau)\bar{\mathcal{O}}_j(0)\rangle_U$$

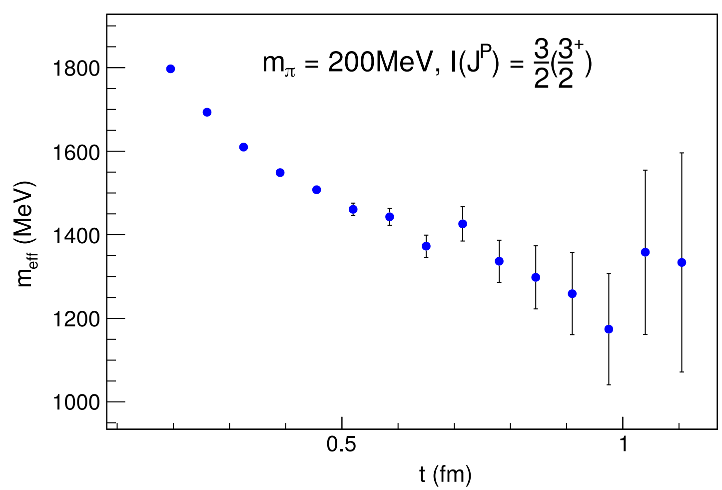
$$\lim_{\tau\to\infty} C_{ij}(\tau) = \langle 0|\hat{O}_i|E_1\rangle\langle E_1|\hat{O}_j^\dagger|0\rangle\, \mathrm{e}^{-E_1\tau}\left\{1 + O(\mathrm{e}^{-(E_2-E_1)\tau})\right\}$$

- Generalized Eigenvalue methods provide a few excited states:

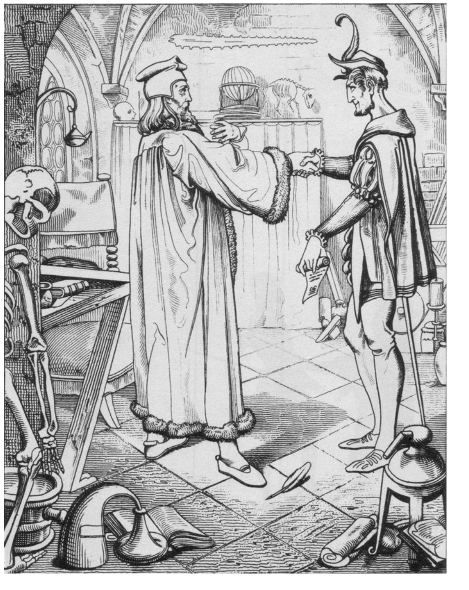
$$C(\tau)v_n(\tau) = \lambda_n(\tau)C(\tau_0)v_n(\tau) \qquad \lim_{\tau\to\infty}\lambda_n(\tau) = \mathrm{e}^{-E_n\tau}$$

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

$$m_{\mathrm{eff}}(\tau) = \log\left[\frac{C(\tau)}{C(\tau+1)}\right]$$



=>



Plot courtesy of C. W. Andersen, apologies to J. W. von Goethe

Real-time scattering in Euclidean lattice QCD

Maiani-Testa No-Go thm. (infinite volume): just threshold amplitudes from $t \to \infty$ limit of Euclidean correlators.

L. Maiani, M. Testa, *Phys. Lett.* **B245** (1990) 585
M. Bruno, M. T. Hansen, 2012.11488 [hep-lat]

Consider $\gamma^* \to \pi + \pi$

$$C(t_2, t_1) = \langle \pi(\boldsymbol{p}, t_2)\pi(-\boldsymbol{p}, t_1)\, J_{\mathrm{em}}(0)\rangle$$

$$\lim_{\substack{t_1, t_2 \to \infty \\ t_2 > t_1}} C(t_2, t_1) = \langle \pi(\boldsymbol{p})|\hat{\pi}(-\boldsymbol{p})|\pi(0)\pi(0)\rangle_{\mathrm{out}} \times$$
$$_{\mathrm{out}}\langle \pi(0)\pi(0)|\hat{J}_{\mathrm{em}}(0)|0\rangle \times \mathrm{e}^{-E_\pi(\boldsymbol{p})(t_2 - t_1) - 2m_\pi t_1}$$

In general: threshold form factor and ‘off-shell’ form factor.

Workaround: finite spatial volume

Finite-volume states give info about infinite-volume scattering amplitudes!

L. Lellouch, M. Lüscher, Comm. Math. Phys. 219 (2001)
H. Meyer, Phys. Rev. Lett 107 (2011)
X. Feng, S. Aoki, Phys. Rev. D91 (2015)
R. Briceno, M. T. Hansen, Phys. Rev. D92 (2015)

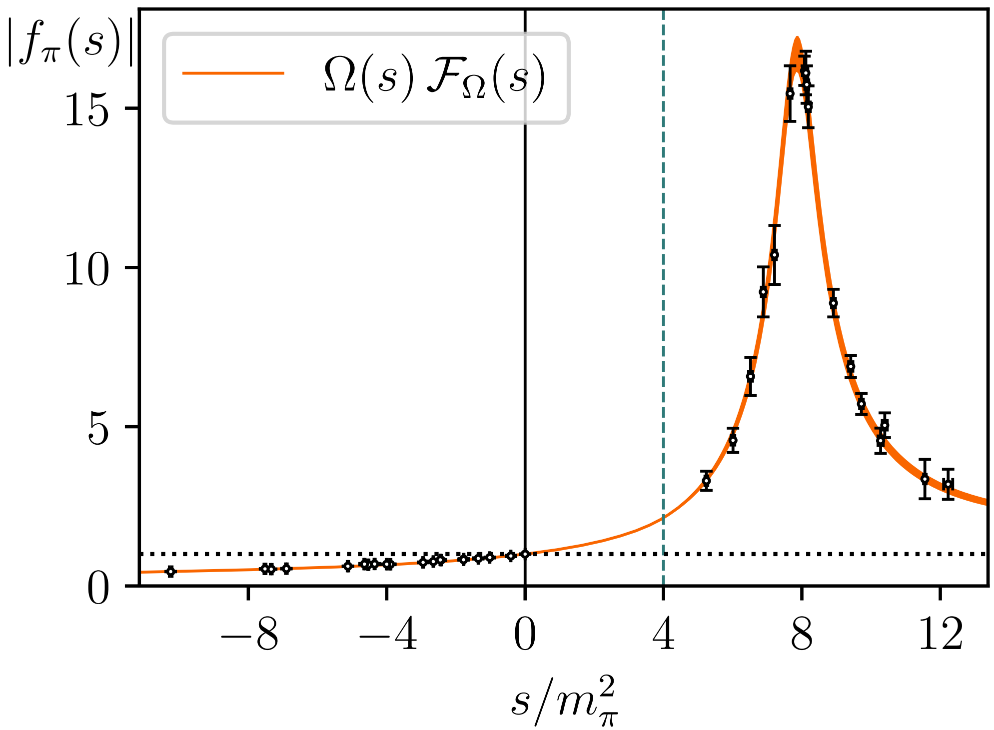
For $E_{\mathrm{cm}} < 4m_\pi$:

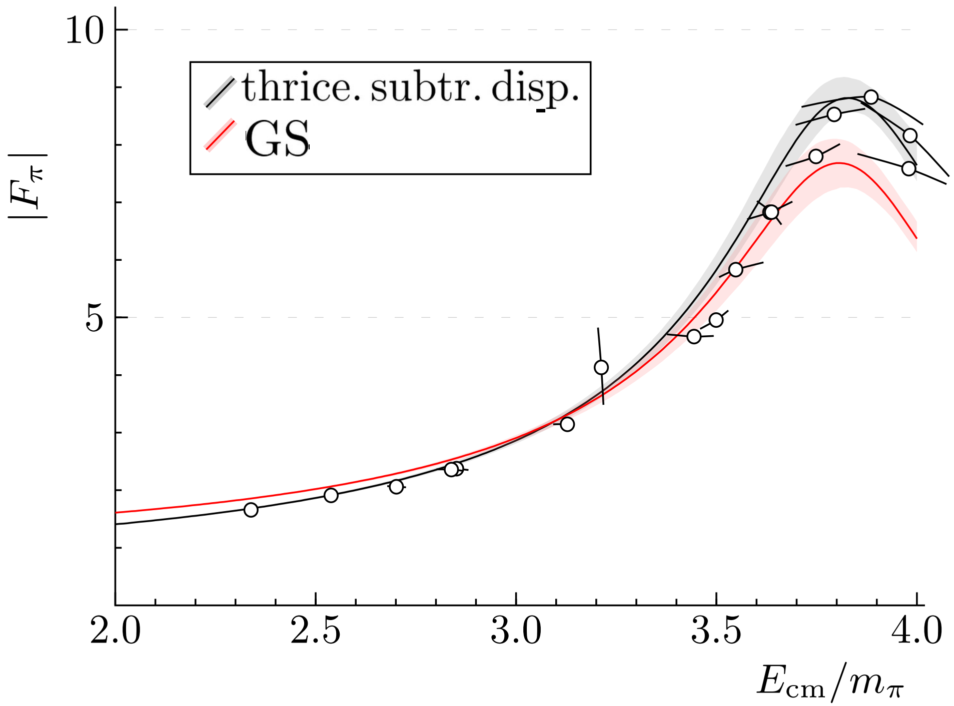
$$|{}_L\langle \pi\pi, E_n, \Lambda(P^2)|\hat{J}_{\mathrm{em}}(0)|0\rangle| = \sqrt{F_{\mathrm{out}}(E_n) R_L(\Lambda) F_{\mathrm{in}}(E_n)} + \mathrm{O}(\mathrm{e}^{-ML})$$

$$F_{\mathrm{out}}(E,\ell) = {}_{\mathrm{out}}\langle \pi\pi, E, \ell|\hat{J}_{\mathrm{em}}(0)|0\rangle$$

- The matrix $R_{L,\ell\ell'}(\Lambda)$ mixes partial waves
- 1-1 relation btw finite-volume and infinite-volume only in leading-partial-wave approx.
- Coupling between $\pi\pi,\ \bar{K}K$ can also be treated.

Recent finite-volume results





Left: $N_\mathrm{f} = 2+1,\ m_\pi = 280\,\mathrm{MeV}$

F. Ortega-Gama, J. Dudek, R. Edwards (HadSpec), Phys.Rev.D 110 (2024) 9, 094505

Right: $N_\mathrm{f} = 2+1,\ m_\pi = 200\,\mathrm{MeV}$

C. Andersen, JB, B. Hörz, C. Morningstar, Nucl. Phys. B939 (2019)

What about two-to-two amplitudes?:

- Finite volume method: two-hadron energies below $n \geq 3$ hadron thresholds:

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

$$\det[K^{-1}(E^L_{\rm cm}) - B(E^L_{\rm cm})] = 0$$

- Determinant over all partial waves and channels
  - ➔ Truncation at some $\ell_{\rm max}$ → systematic error

For single channel:
$$K^{-1}_{\ell\ell'} = \delta_{\ell\ell'} \cot\delta_\ell$$

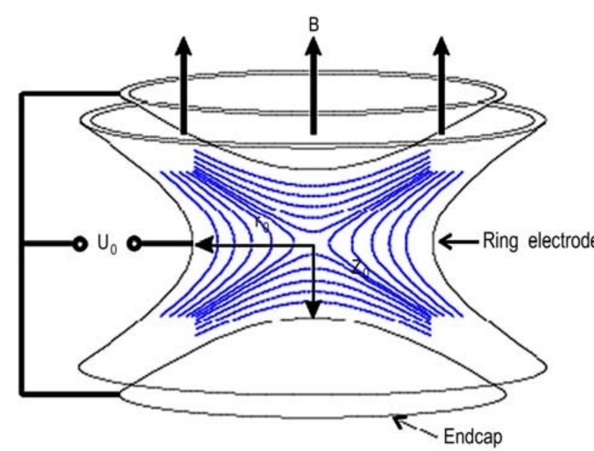
- Signal comes from interaction shift. Large-*L* threshold expansion:

$$\Delta E = E^{I=2}_{2\pi} - 2m_\pi = -\frac{4\pi a_0^{I=2}}{m_\pi L^3} + \mathrm{O}(L^{-4})$$

- For attractive *s*-wave interaction

  → direct constraints in complex plane!

$$E^L_{\rm cm} < E_{\rm thresh}$$



Analogy: two cold atoms in a trap
T. Busch, B.-G. Englert, K. Rzazewski, M. Wilkens, Found. Phys., 28 (1998)

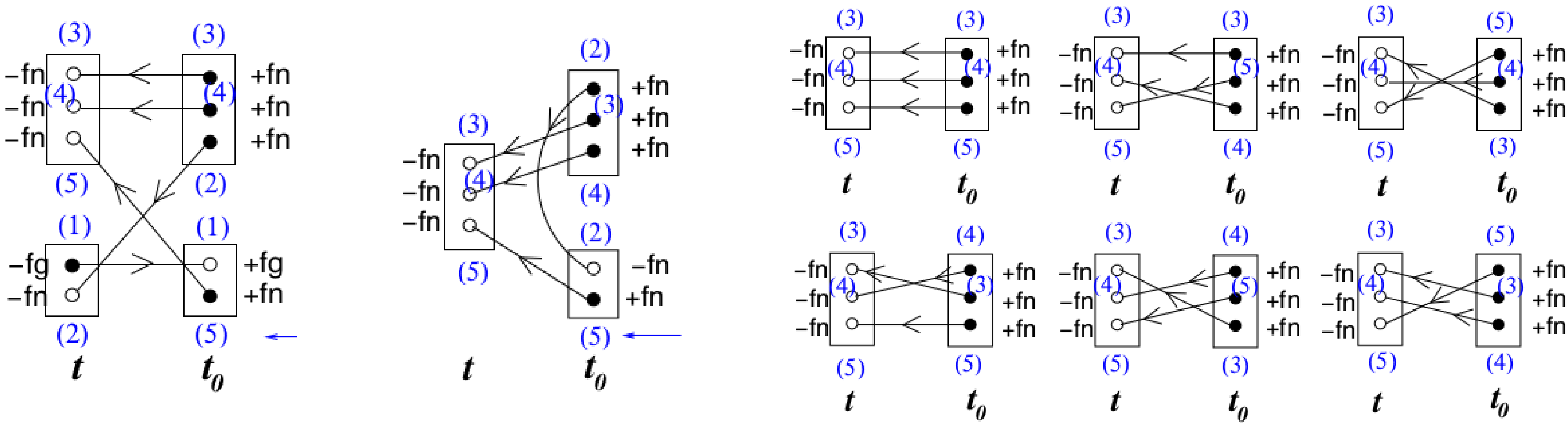
Computing correlation functions: the distillation approach

M. Peardon et al. Phys.Rev.D 80 (2009) 054506; C. Morningstar et al. Phys.Rev.D 83 (2011) 114505

- ‘All-to-all quark propagators are required for complete momentum projection

  → inverse of large sparse Dirac matrix:

$$D\psi = \eta$$



- Factorization enabled by the distillation/stochastic LapH algorithms for quark propagation

- Correlation function computation = tensor contraction

Example of FV formalism

Baryon-Baryon interactions with SU(3) flavor symmetry:

$$8 \otimes 8 = 1 \oplus 8 \oplus 8 \oplus 10 \oplus \overline{10} \oplus 27$$

- Singlet: H-dibaryon
- 10-bar: deuteron
- 27-plet: dineutron

Proof of principle:

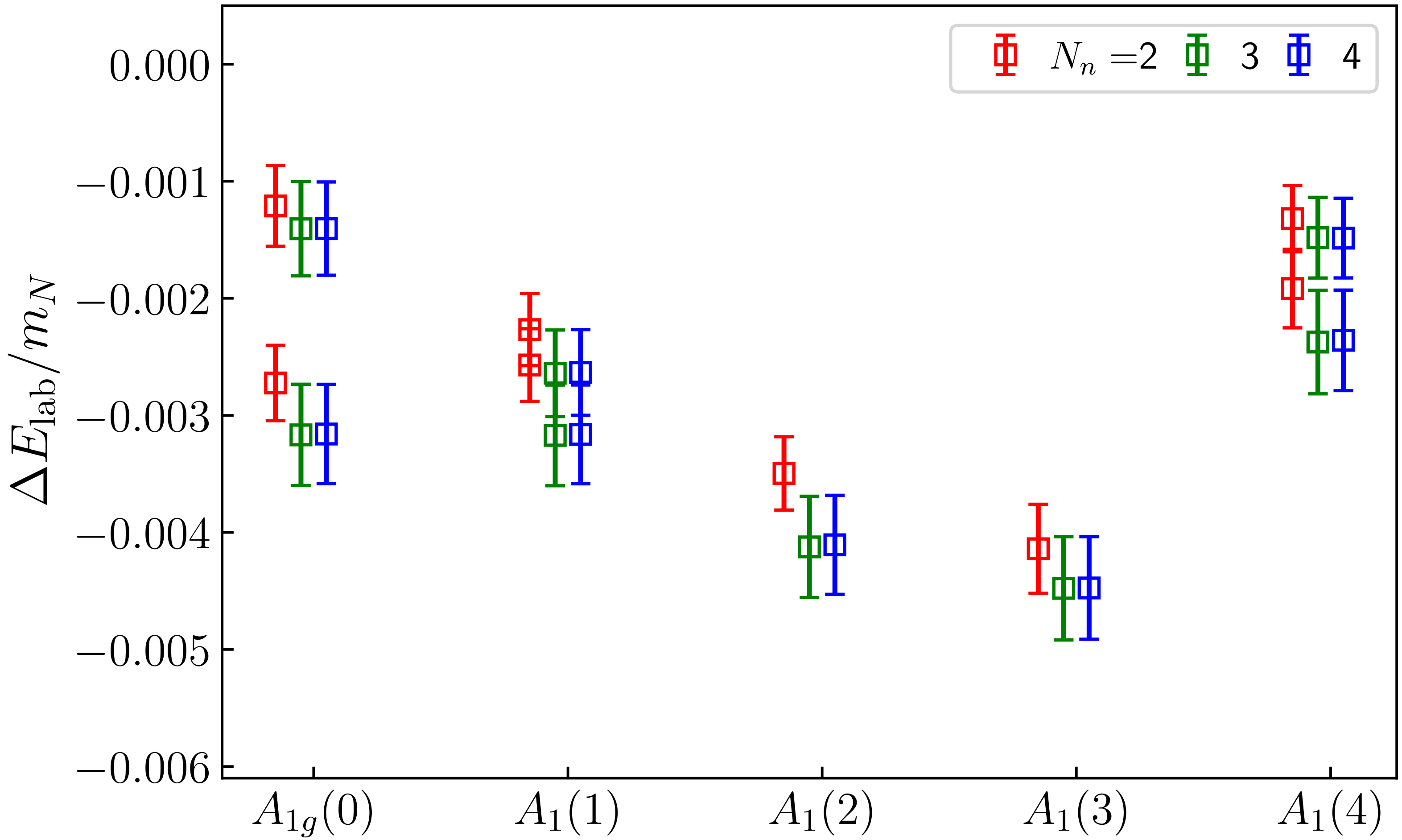
$$N_{\rm f} = 2+1\,, \qquad m_\pi = 700\,{\rm MeV}\,,$$
$$a = 0.09\,{\rm fm}\,, \qquad 48^3 \times 96$$

JB, et al. (Baryon Scattering [BaSc] Collaboration), 2502.15546 [hep-lat]

→ Consistency between different groups and methods

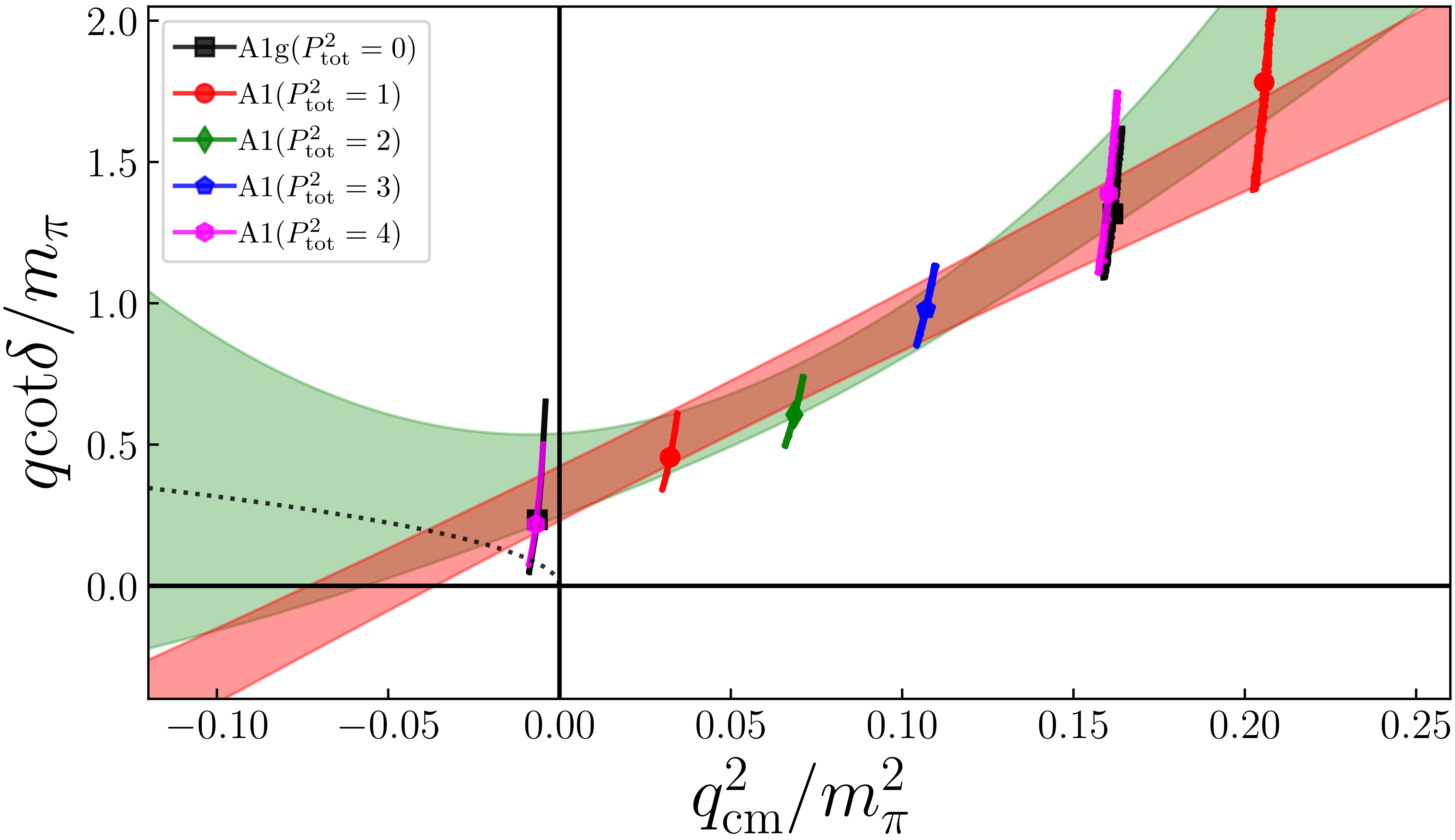
Example of FV formalism

Dineutron: spectrum determination



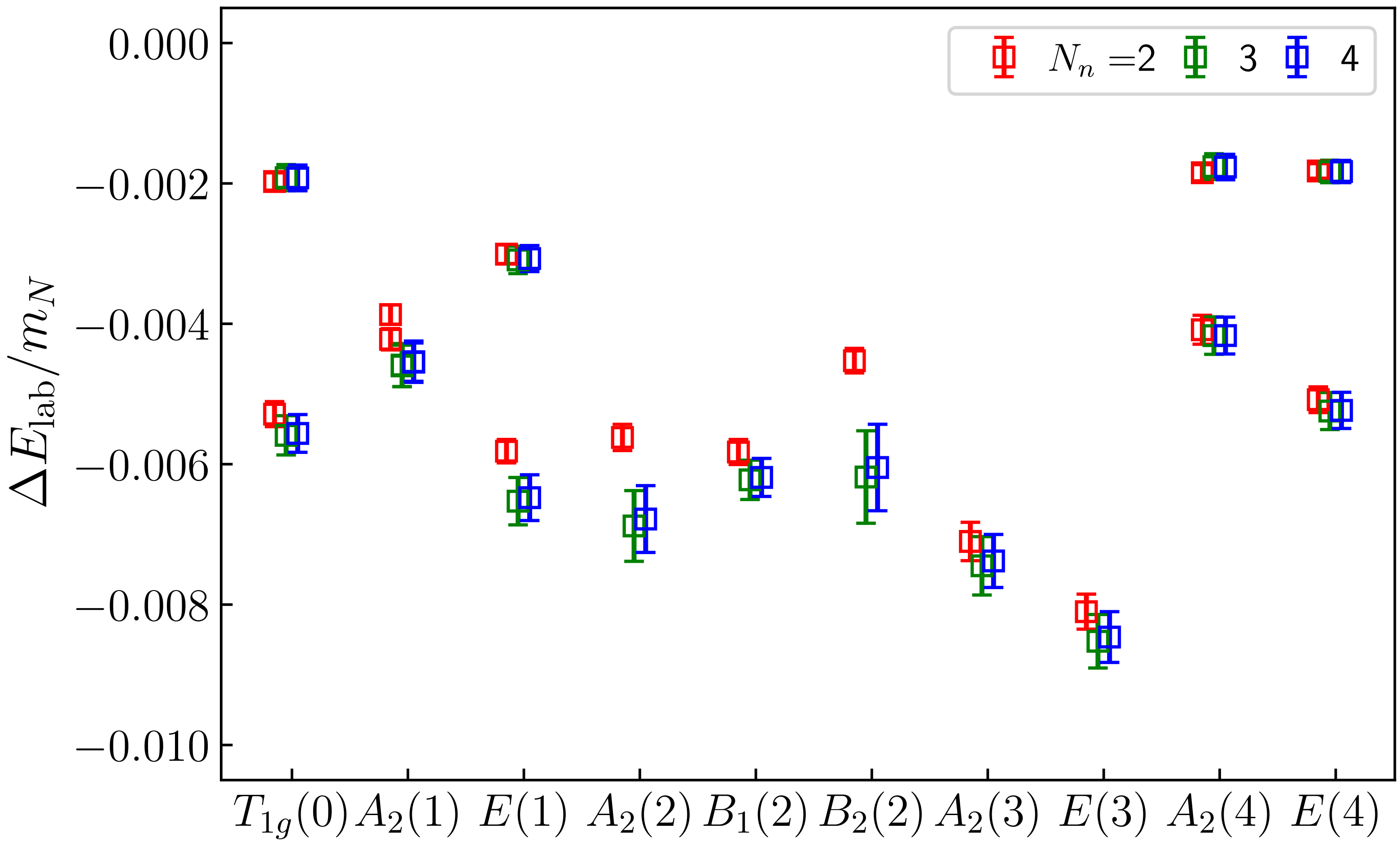
Example of FV formalism

Dineutron: scattering amplitude



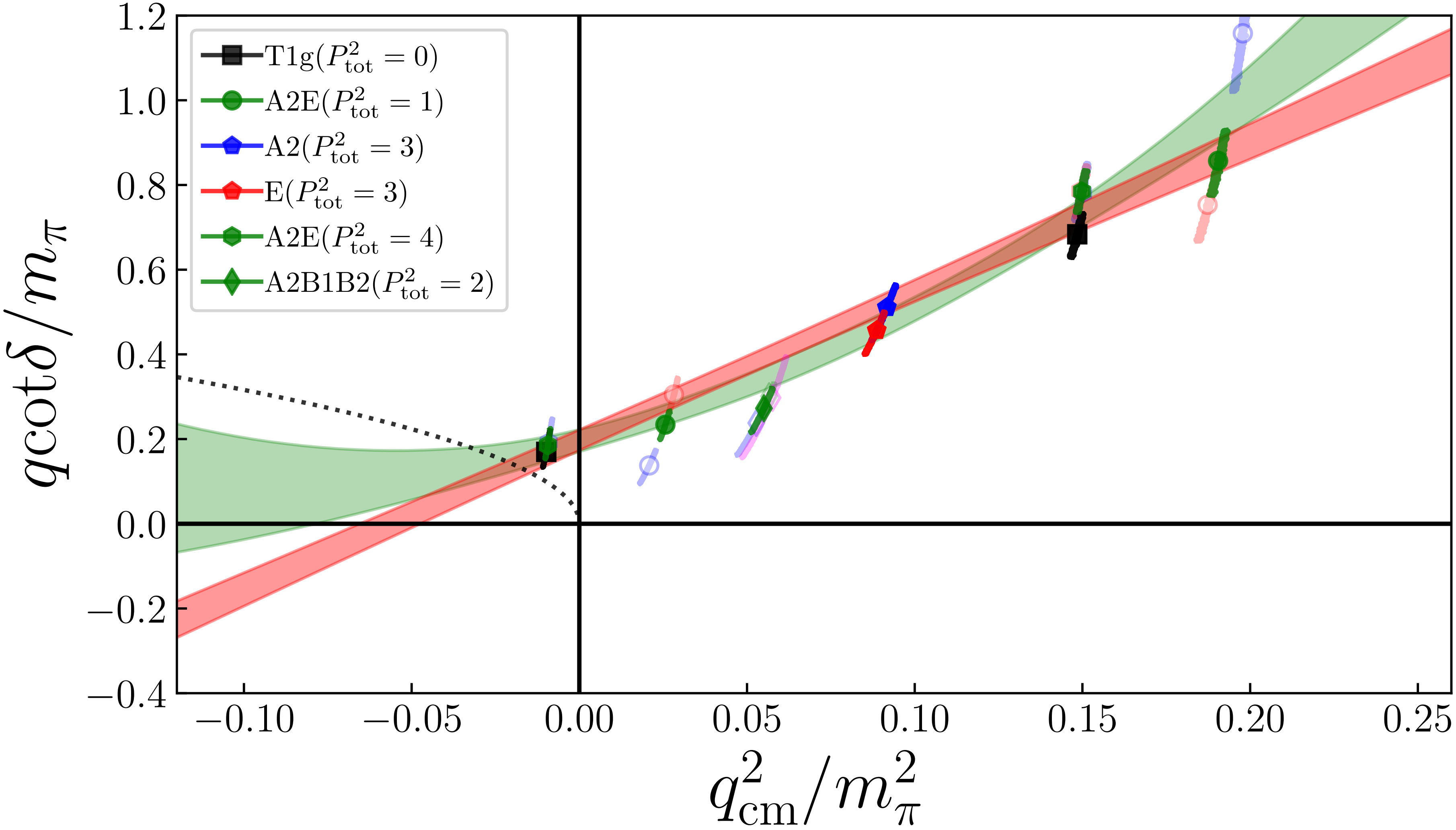
Example of FV formalism

Deuteron: spectrum determination



Example of FV formalism

Deuteron: scattering amplitude

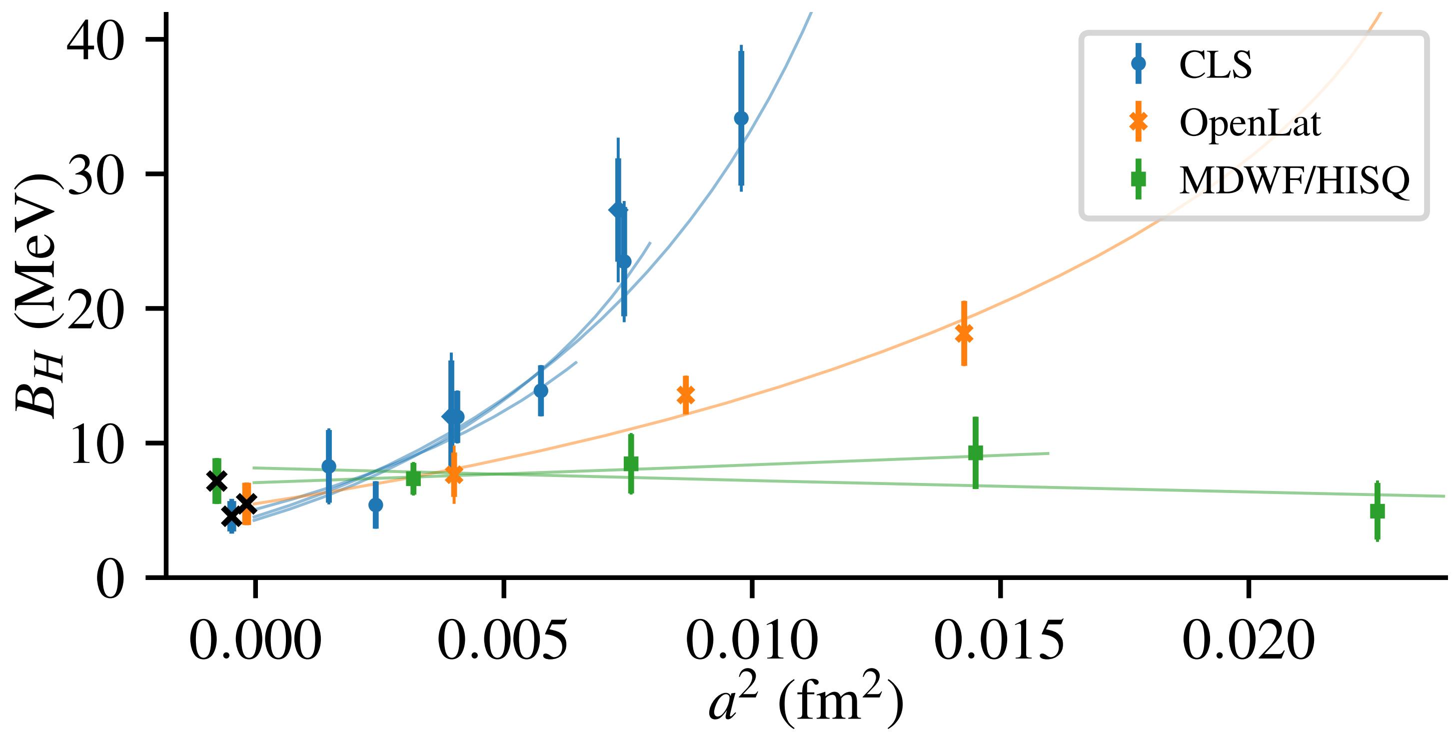


Example of FV formalism

Preliminary SU(3) singlet results: continuum limit

$$N_{\rm f} = 2+1\,, \qquad m_\pi = 420\,\text{MeV}\,,$$
$$a = 0.11 - 0.045\,\text{fm}\,, 3\ \text{discretizations}$$

JB, et al. (Baryon Scattering [BaSc] Collaboration), in preparation



FV formalism: summary

- Limited to two- and three-body amplitudes near threshold
- Current challenges:
  - ➔ cross-channel effects (left-hand cuts)
  - ➔ Three-body amplitudes
  - ➔ (solving integral equations)

=> Works very well for near-threshold amplitudes.

states [8–34] (this allows to study QCD processes in which e.g. a two pion state can rescatter into a two-kaon state) and more recently also to three-particles states [35–71]. The resulting formalism in the case of three-particle states is so involved that it is hard to believe that further generalizations, that would allow to study phenomenologically interesting processes such as e.g. $B \mapsto \pi\pi$ (where the threshold for producing more than 30 pions is open), will ever be obtained or could have practical applicability.

From A. Patella, N. Tantalo, JHEP 01 (2025) 091

Another approach: spectral functions

JB, M. T. Hansen, Phys. Rev. D100 (2019)

Consider the spectral function:

$$C(t) = \langle \pi(\boldsymbol{p}_1) | \hat{\pi}(\boldsymbol{p}_2) \mathrm{e}^{-\hat{H}t} \, \hat{J}_{\mathrm{em}}(0) | 0 \rangle$$

$$= \int_0^\infty \mathrm{d}\omega \, \mathrm{e}^{-\omega t} \rho_{\boldsymbol{p}_1 \boldsymbol{p}_2}(\omega)$$

'Smear' with a particular kernel of width ϵ

$$\rho_{\epsilon, \boldsymbol{p}_1 \boldsymbol{p}_2}(E) = \int_0^\infty \mathrm{d}\omega \, K_\epsilon(E - \omega) \, \rho_{\boldsymbol{p}_1 \boldsymbol{p}_2}(\omega)$$

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

Another approach: spectral functions

Apply LSZ reduction:

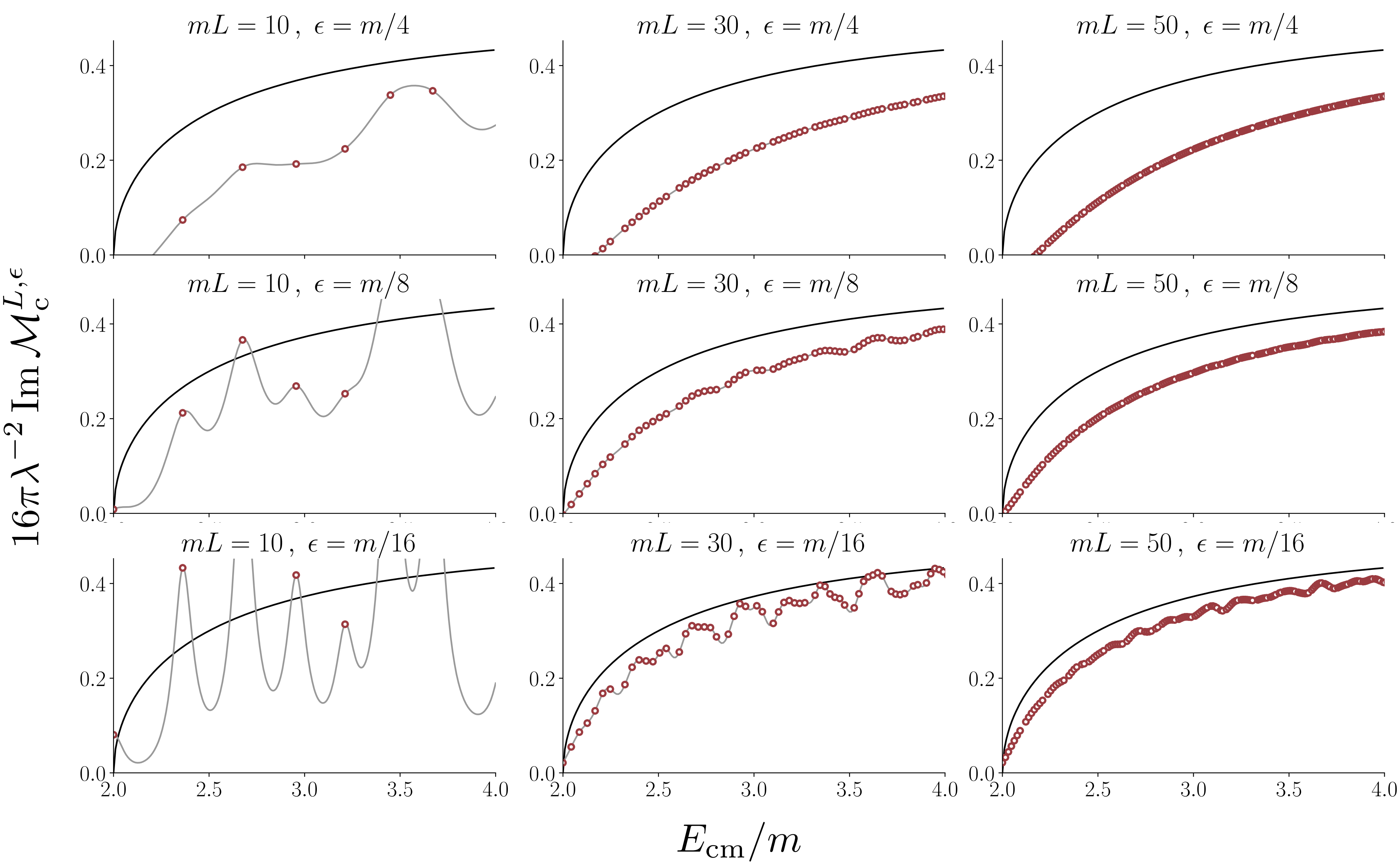
$$ {}_{\text{out}}\langle \pi(\boldsymbol{p}_1)\pi(\boldsymbol{p}_2)|\hat{J}_{\text{em}}(0)|0\rangle = \frac{2E(p_2)}{Z_\pi^{1/2}} \lim_{\epsilon\to 0^+} \epsilon \rho_{\epsilon,\boldsymbol{p}_1\boldsymbol{p}_2}(E(\boldsymbol{p}_2)) $$

Spectral function has an on-shell pole, which must be 'amputated'

- No reliance on finite-volume, applicable above arbitrary thresholds
- Generalizes to arbitrary (inclusive, exclusive) amplitudes (in principle)
- Requires large volume, solution of ill-posed inverse problem

Another approach: spectral functions

Illustrative example: 2-2 scattering in 3+1 dim. $\lambda\phi^4$ (1-loop TOPT)



Another approach: spectral functions

A. Patella, N. Tantalo, JHEP 01 (2025) 091

Recent improvement:

- Based on Haag-Ruelle; Barata-Fredenhagen

- Two types of smearing:
  - ➔ 'interpolator' smearing → only produce single-particle states
  - ➔ **** 'time' smearing → large-t limit = small eps-limit

- Maximum generality in smearing kernels

- TODO: interpolator smearing without compact support

Spectral Reconstruction

Backus, Gilbert ‘68, ‘70
F. Pijpers, M. Thompson ‘92
M. R. Hansen, A. Lupo, N. Tantalo, PRD99 (2019)

Linear ansatz:

$$\hat{\rho}_\epsilon(E) = \sum_{t=a}^{t_{\max}} q_t(\epsilon, E)\, C(t), \qquad \hat{\delta}_\epsilon(E,\omega) = \sum_{t=a}^{t_{\max}} q_t(\epsilon, E)\, \mathrm{e}^{-\omega t}$$

Two criteria when choosing $\{q_t(\epsilon, E)\}$

- Accuracy: $$A[q] = \int_{E_0}^{\infty} \mathrm{d}\omega \left\{ \delta_\epsilon(E-\omega) - \hat{\delta}_\epsilon(E,\omega) \right\}^2$$
- Precision: $$B[q] = \mathrm{Var}\left\{\rho_\epsilon(E)\right\}$$

Optimal coeffs minimize:

$$G_\lambda[q] = (1-\lambda)A[q] + \lambda B[q]$$

Controlled Test

JB, M. W. Hansen, M. T. Hansen, A. Patella, N. Tantalo, JHEP `22

2d O(3)-model: …, M. Lüscher, U. Wolff, Nucl. Phys. B339 (1990),...

$$S[\sigma] = -\beta \sum_{x,\mu} \sigma(x) \cdot \sigma(x+\hat{\mu}), \qquad \sigma(x) \in \mathbb{R}^3, |\sigma(x)| = 1$$

Conserved (global) current:

$$j^a_\mu = \beta \epsilon^{abc} \sigma^b(x) \hat{\partial}_\mu \sigma^c(x)$$

Massive single-particle states. Target process: inclusive rate for $j \to X$

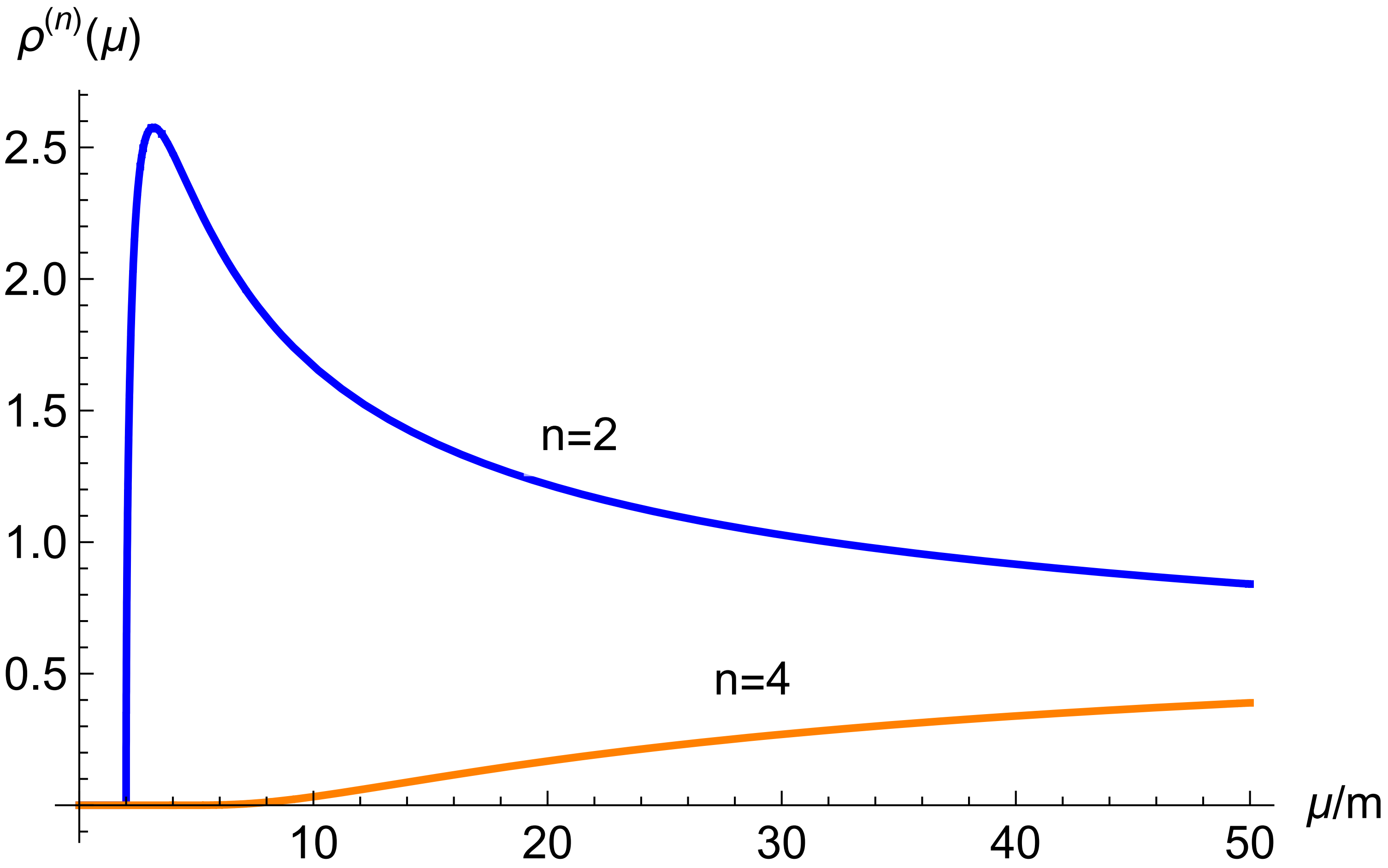
$$\rho(E) = \sum_\alpha \delta(\boldsymbol{P}_\alpha) \delta(E - E_\alpha) \left| {}_{\text{out}}\langle \alpha | \hat{j}(0) | 0 \rangle \right|^2$$

$$= \sum_{n=2,4,6,\ldots} \rho^{(n)}(E)$$

Controlled Test

Integrable model => spectral function known exactly:

M. Karowski, P. Weisz, Nucl. Phys. B139 (1978)
A. B. Zamolodchikov, A. B. Zamolodchikov, Nucl. Phys. B133 (1978)
J. Balog, M. Niedermaier, Nucl. Phys. B500 (1997)



Two-particle contribution dominant, four-particle ~2% near E = 10m

Controlled Test

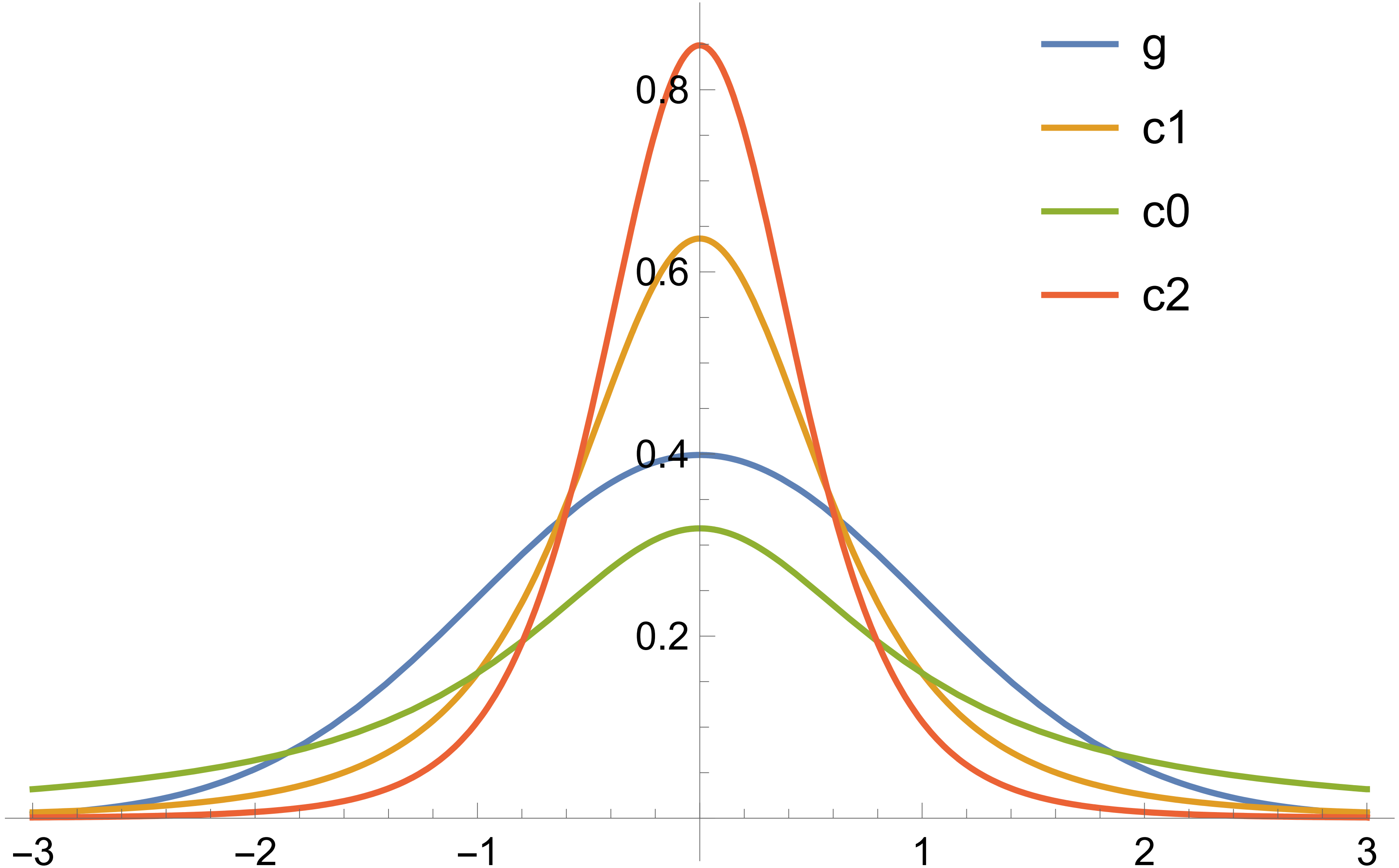
Four smearing kernels $\delta_\epsilon^{\mathrm{x}}(E-\omega)$:

$$\delta_\epsilon^{\mathsf{g}}(x) = \frac{1}{\sqrt{2\pi}\epsilon}\exp\left[-\frac{x^2}{2\epsilon^2}\right], \qquad \delta_\epsilon^{\mathsf{c}0}(x) = \frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2},$$

$$\delta_\epsilon^{\mathsf{c}1}(x) = \frac{2}{\pi}\frac{\epsilon^3}{(x^2+\epsilon^2)^2}, \qquad \delta_\epsilon^{\mathsf{c}2}(x) = \frac{8}{3\pi}\frac{\epsilon^5}{(x^2+\epsilon^2)^3}$$

Controlled Test

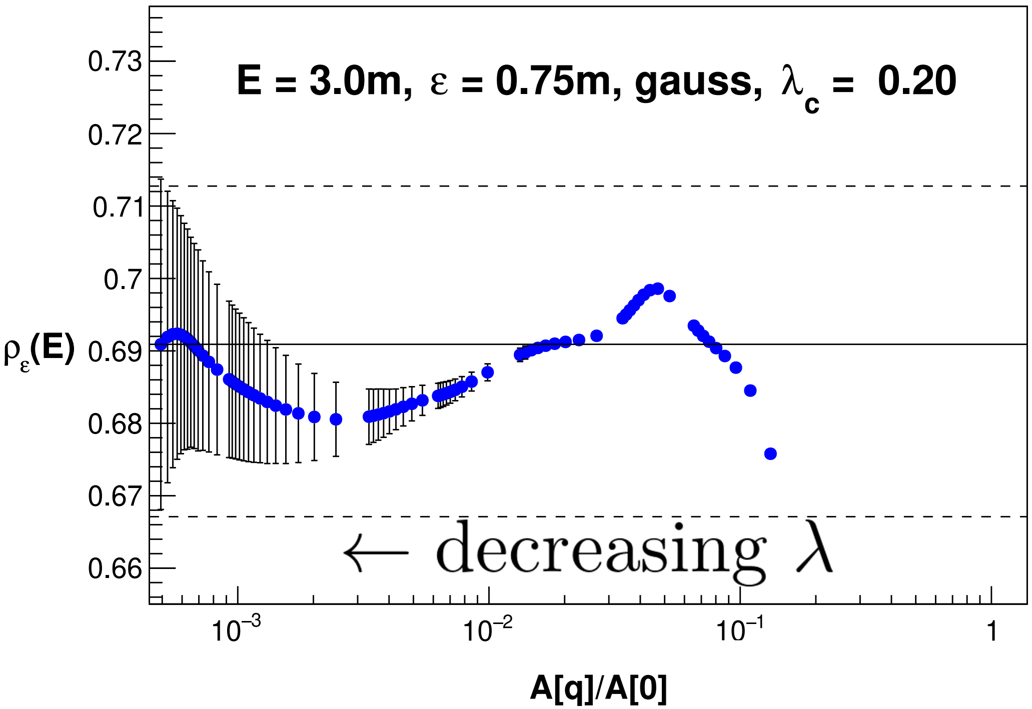
Four smearing kernels $\delta_{\epsilon}^{\mathrm{x}}(E-\omega)$:

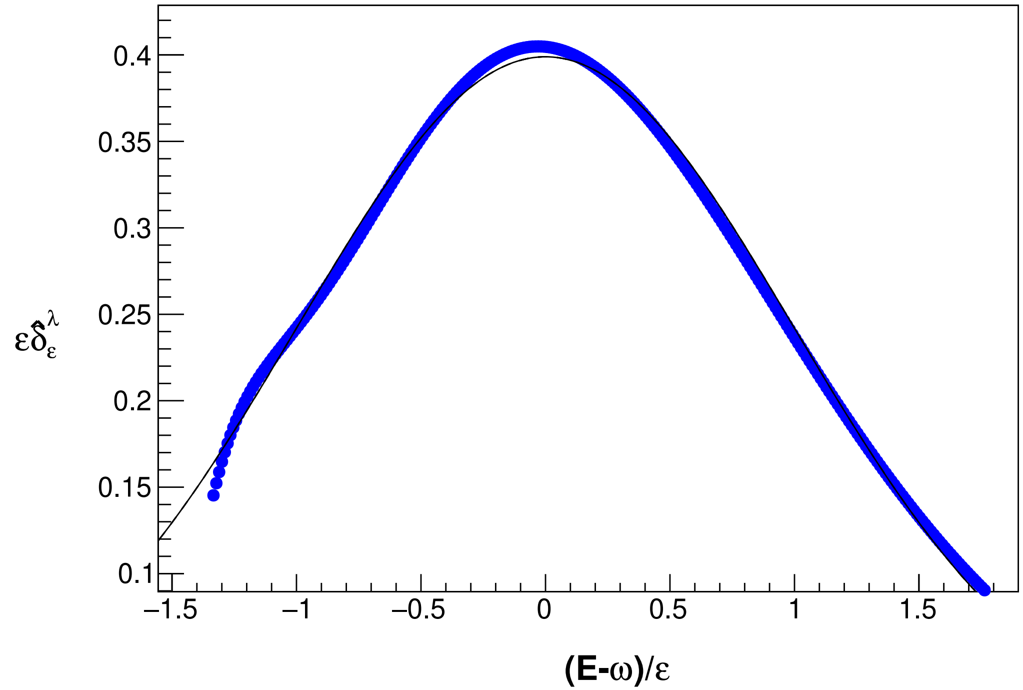


Spectral Reconstruction

$$G_\lambda[q] = (1-\lambda)A[q] + \lambda B[q]$$

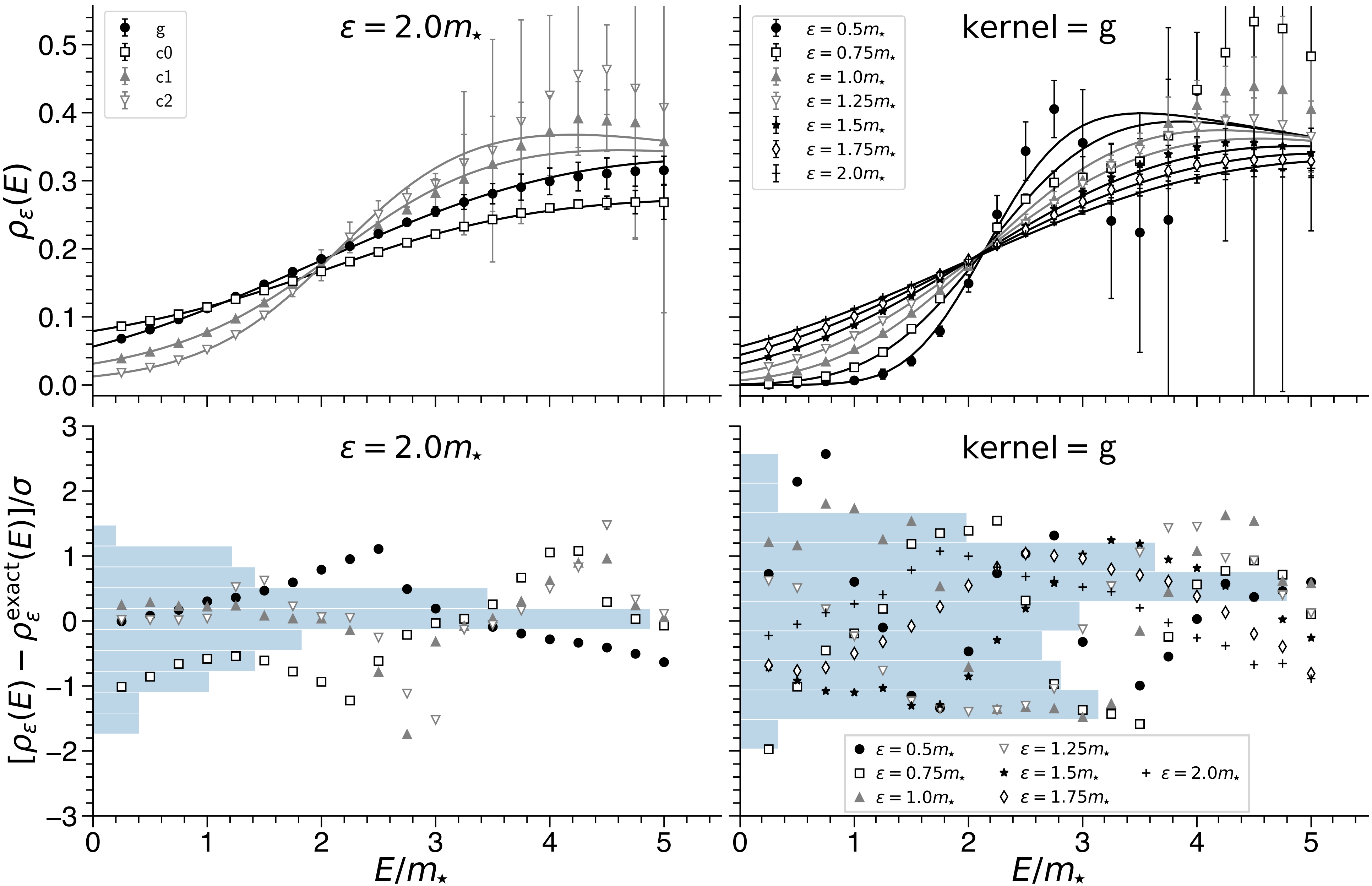
Trade off parameter (λ) balances systematic (A) and statistical (B) error





Plateau indicates statistics-limited regime, automatically selected.

Results: fixed smearing width



Solid lines: exact smeared spectral function, using N=2, 4, 6 particle contributions.

Summary: spectral functions

Many differences wrt to finite-volume approach!

- Cannot use finite-volume momenta → momentum wave packets
- Cannot use quark smearing → smearing in position space (wave packets)
  - ➔ Distillation inapplicable
  - ➔ Sparsening? A. Stump, J. R. Green, PoS LATTICE2024 (2025) 094
    W. Detmold, et al., Phys. Rev. D 104 (2021) 034502
    Y. Li, et al., Phys. Rev. D 103 (2021) 014514
- Large volumes required
  - ➔ Masterfield simulation paradigm M. Lüscher, EPJ Web Conf. 175 (2018) 01002
- All hadrons at different times in correlation function
  - ➔ complicates reconstruction
  - ➔ Complicates correlation function construction

First tests: spectral functions

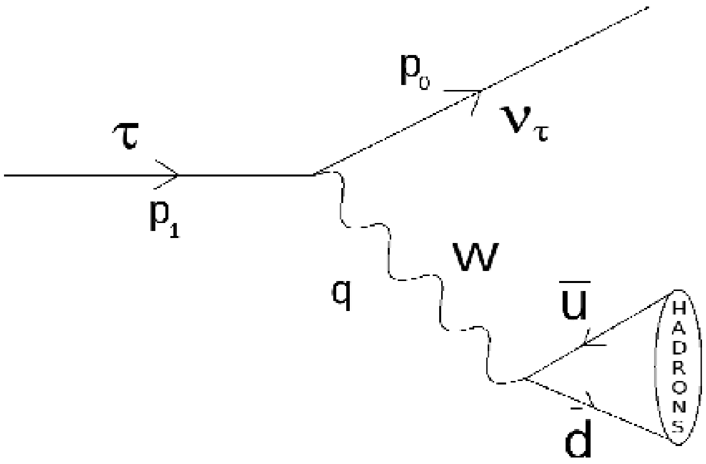
Much work required to implement Tantalo-Patella program

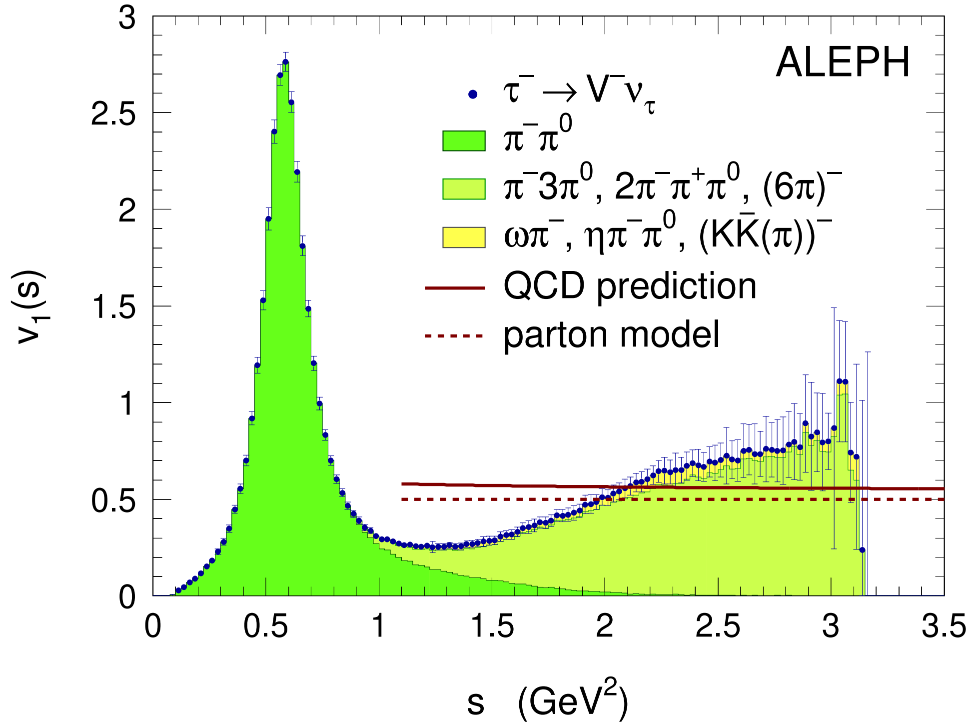
- What can be done now?
  - ➔ ***Inclusive 0→ X : $e^+e^- \to \text{hadrons}$
  - ➔ Inclusive 1 → X : $p + e^- \to X$

M. T. Hansen, H. B. Meyer, D. Robaina, Phys.Rev.D 96 (2017) 9, 094513

Inclusive processes in lattice QCD

Hadronic Tau decays:





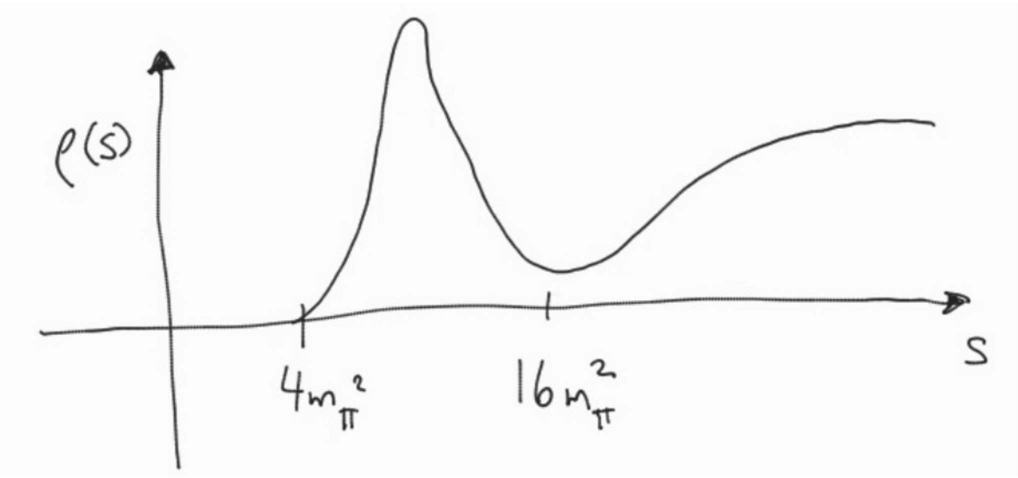
Decay rate from spectral density:

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

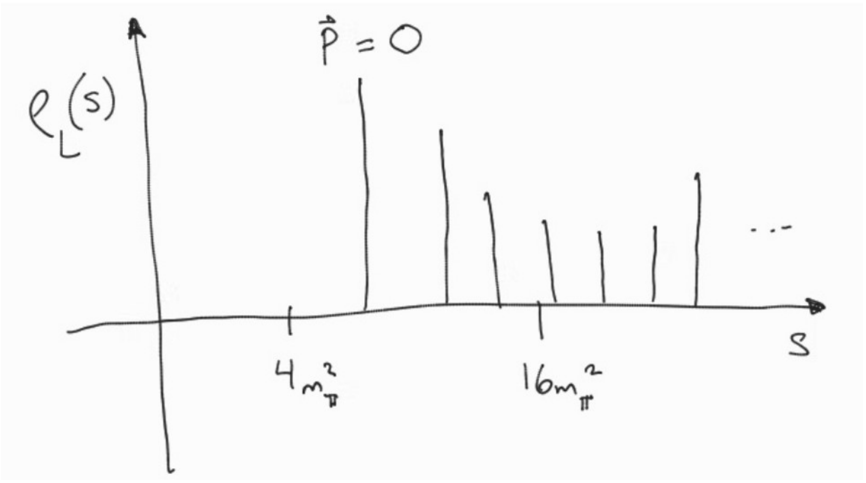
$$\propto \int_0^\infty d\omega\, \omega^2 v_1(\omega^2)\,\mathrm{e}^{-\omega t}$$

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:

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

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

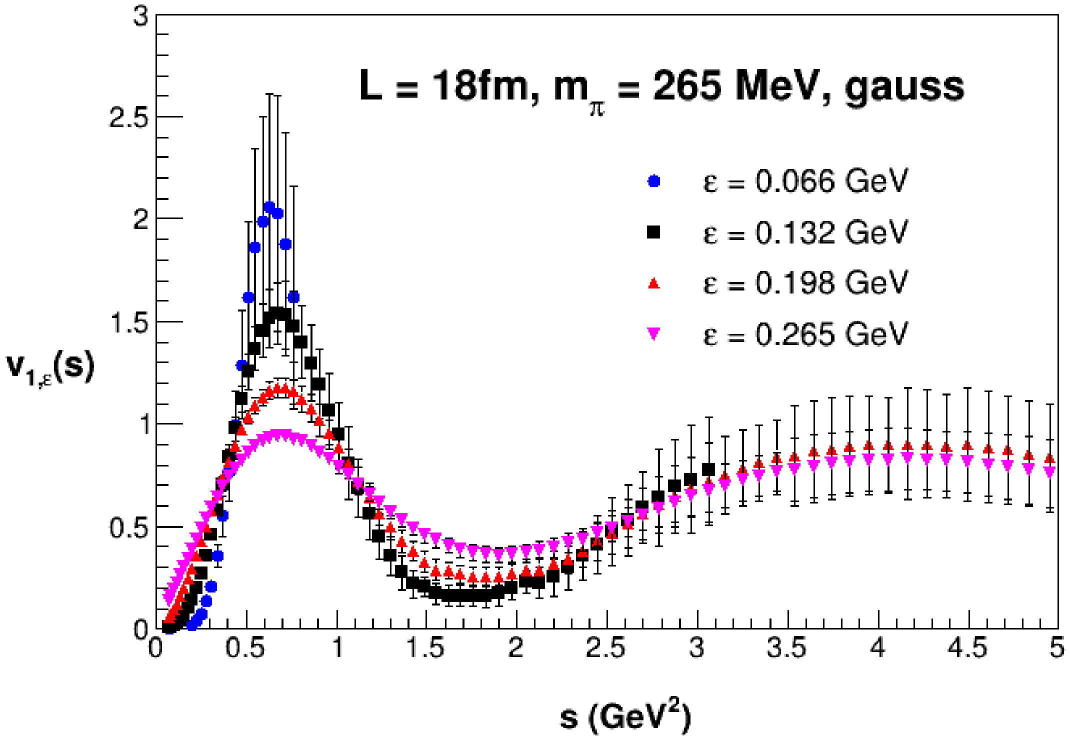
$$N_{\rm f} = 2+1, \quad L = 18{\rm fm},$$

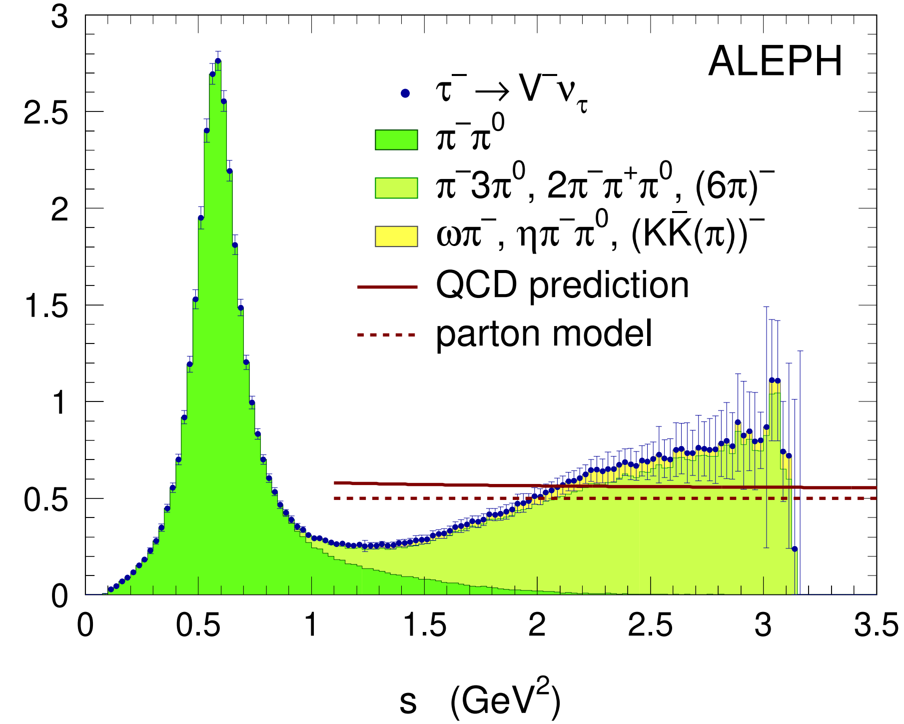
$$a = 0.09{\rm fm}, \quad m_\pi = 265{\rm MeV}$$

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

Preliminary results

PRELIMINARY





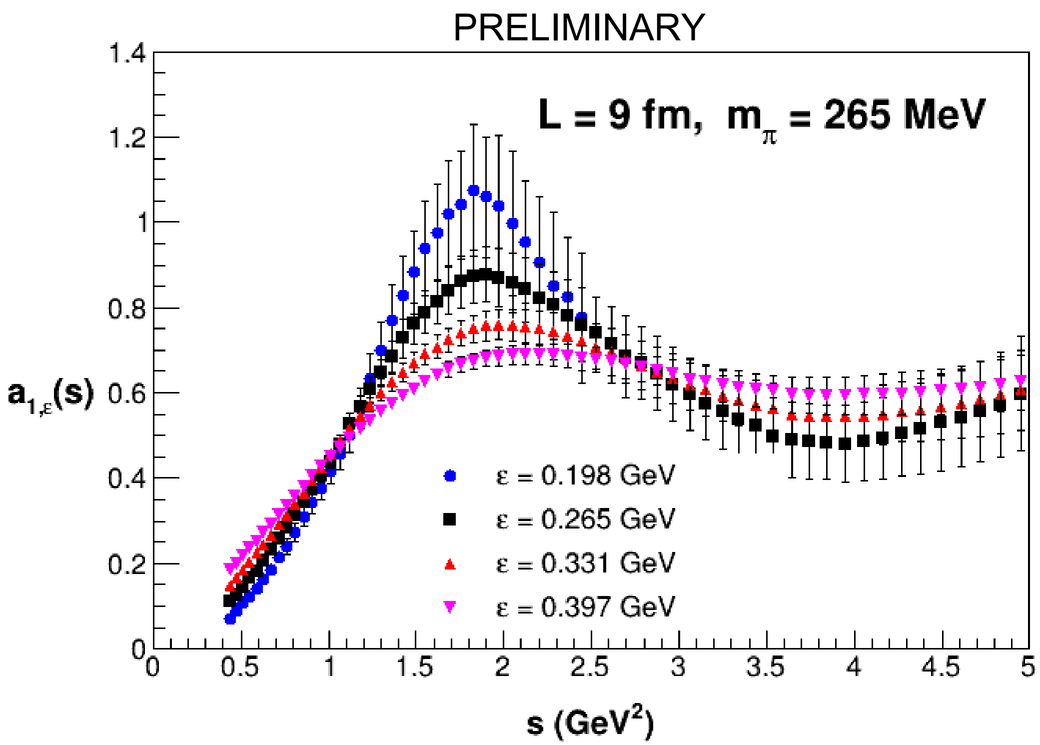
- Comparison to hadronic tau-decay (right)

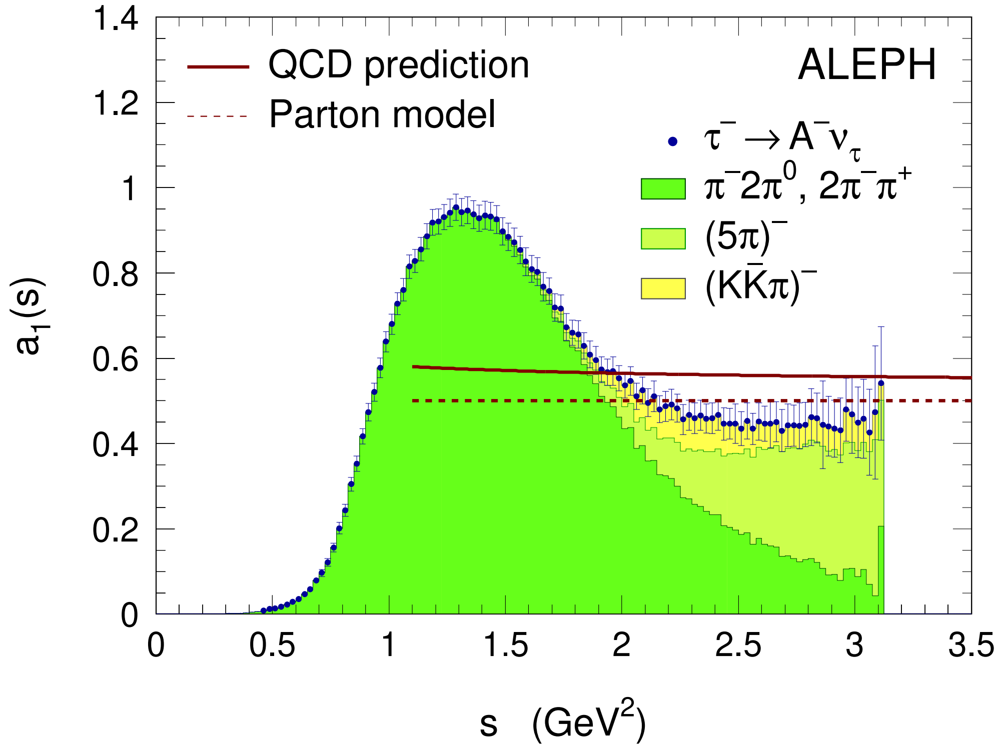
ALEPH collaboration \`05

- 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 $a_1(1260)$, 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

- Finite volume approach: successful for near-threshold amplitudes
  - ➔ Meson-meson
  - ➔ Meson-meson-meson
  - ➔ Meson-baryon
  - ➔ Baryon-baryon

- Infinite volume approach: promising, but much work to be done

- Applications to fragmentation:??