

# Inclusive processes and spectral reconstruction in lattice QCD

John Bulava

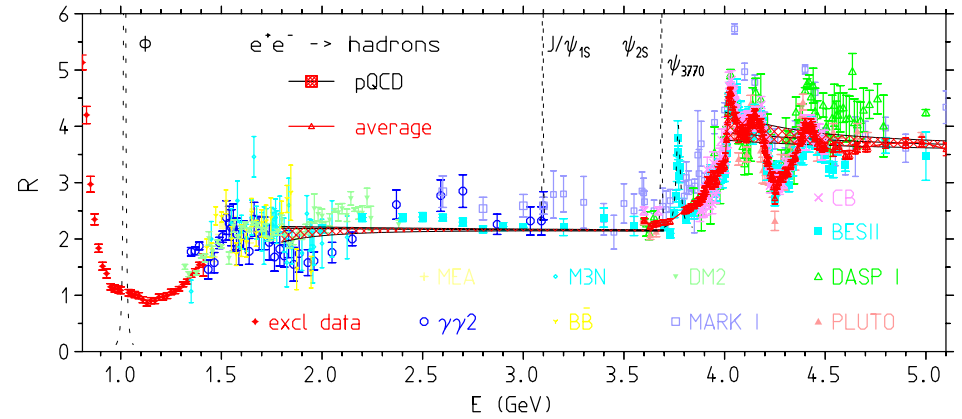
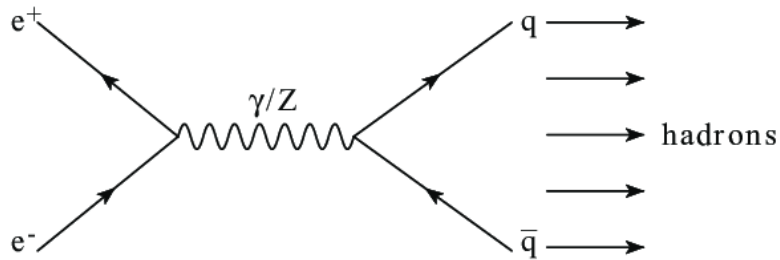
DESY-Zeuthen



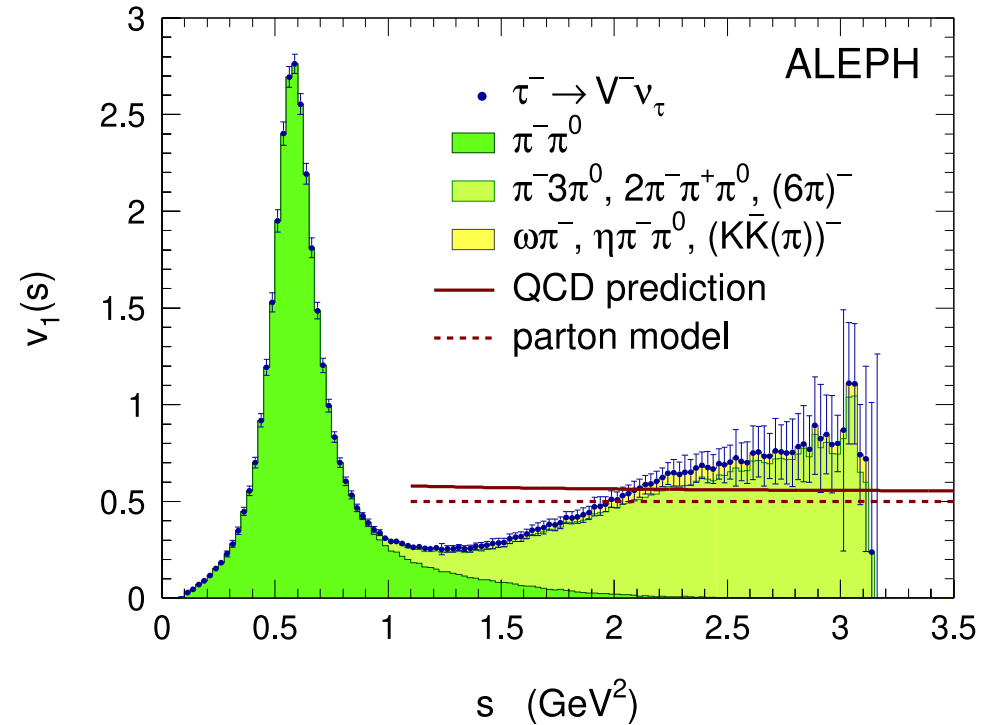
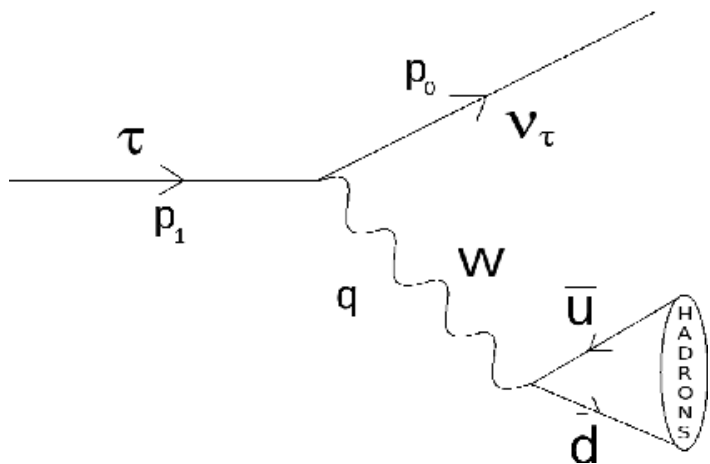
Theory Seminar, IJCLab  
Orsay, FR  
Mar. 2<sup>nd</sup>, 2023

# Inclusive processes in QCD

R-ratio:

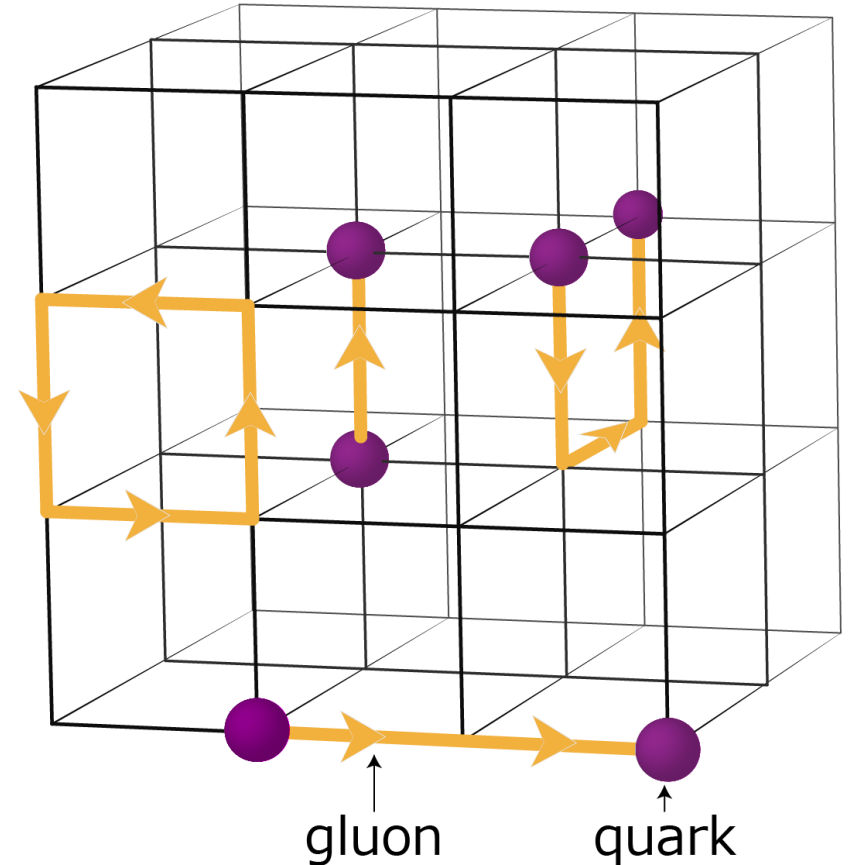


Hadronic Tau decays:



# Lattice QCD: (without electroweak interactions)

- First-principles computer simulation of quarks and gluons
- Euclidean time:  $\tau = -it$
- Sources of error:
  - Finite lattice spacing ( $a$ )
  - Finite spatial extent ( $L$ )
  - Monte Carlo  $\Rightarrow$  statistical errors
- Current state of the art:  $L/a \approx 100$   
 $\Rightarrow m_\pi L \sim 4$  and  $a \gtrsim 0.05$  fm
- Complements experiment:
  - Predictions for the real world
  - Can vary quark masses, number of colors, number of flavors



# Observables from lattice QCD: Euclidean correlation functions

- Large time separation: ground state saturation

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

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

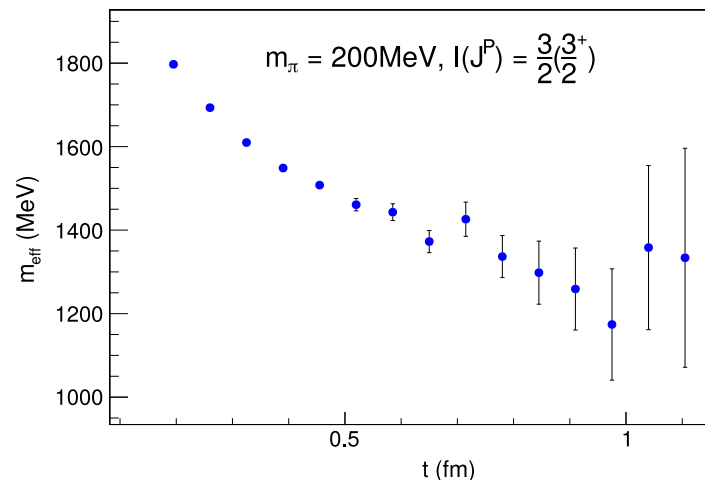
- Generalized Eigenvalue methods provide a few excited states:

C. Michael, I Teasdale '83; M. Luescher, U. Wolff '90; B. Blossier *et al.* '09

$$C(t)v_n(t) = \lambda_n(t)C(t_0)v_n(t) \quad \lim_{t \rightarrow \infty} \lambda_n(t) = e^{-E_n t}$$

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

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



=>



# Real-time scattering in Euclidean lattice QCD

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

L. Maiani, M. Testa, *Phys. Lett.* **B245** (1990) 585  
M. Bruno, M. T. Hansen, *JHEP* **06** (2021) 043

Consider  $\gamma^* \rightarrow \pi(\mathbf{p}) + \pi(-\mathbf{p})$

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

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

In general: 'wrong' form factor and 'off-shell' scattering amplitude.

# 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)

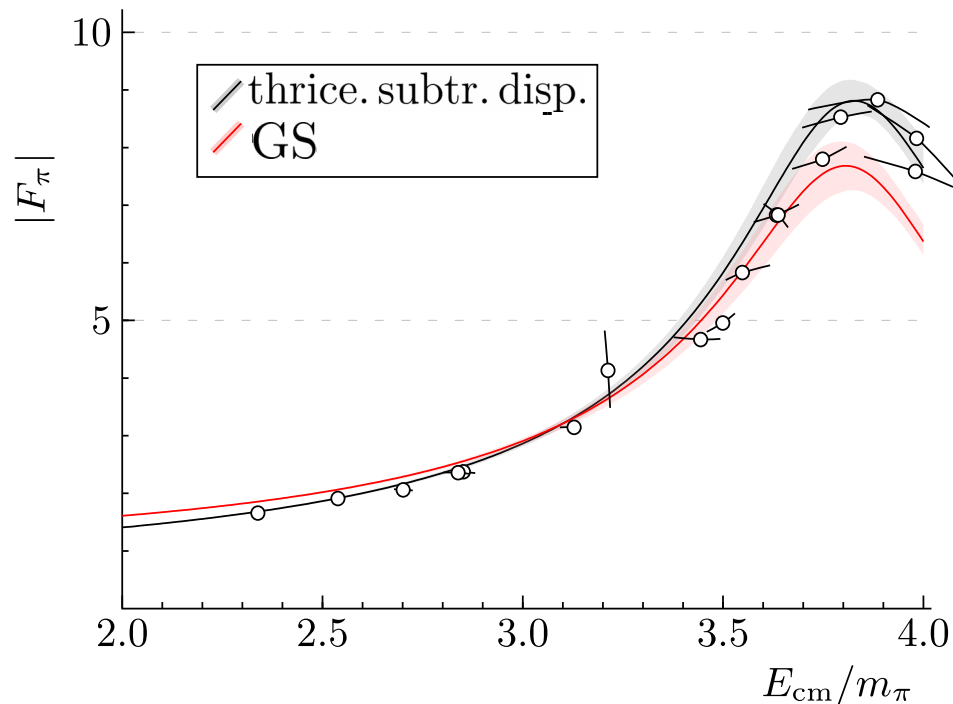
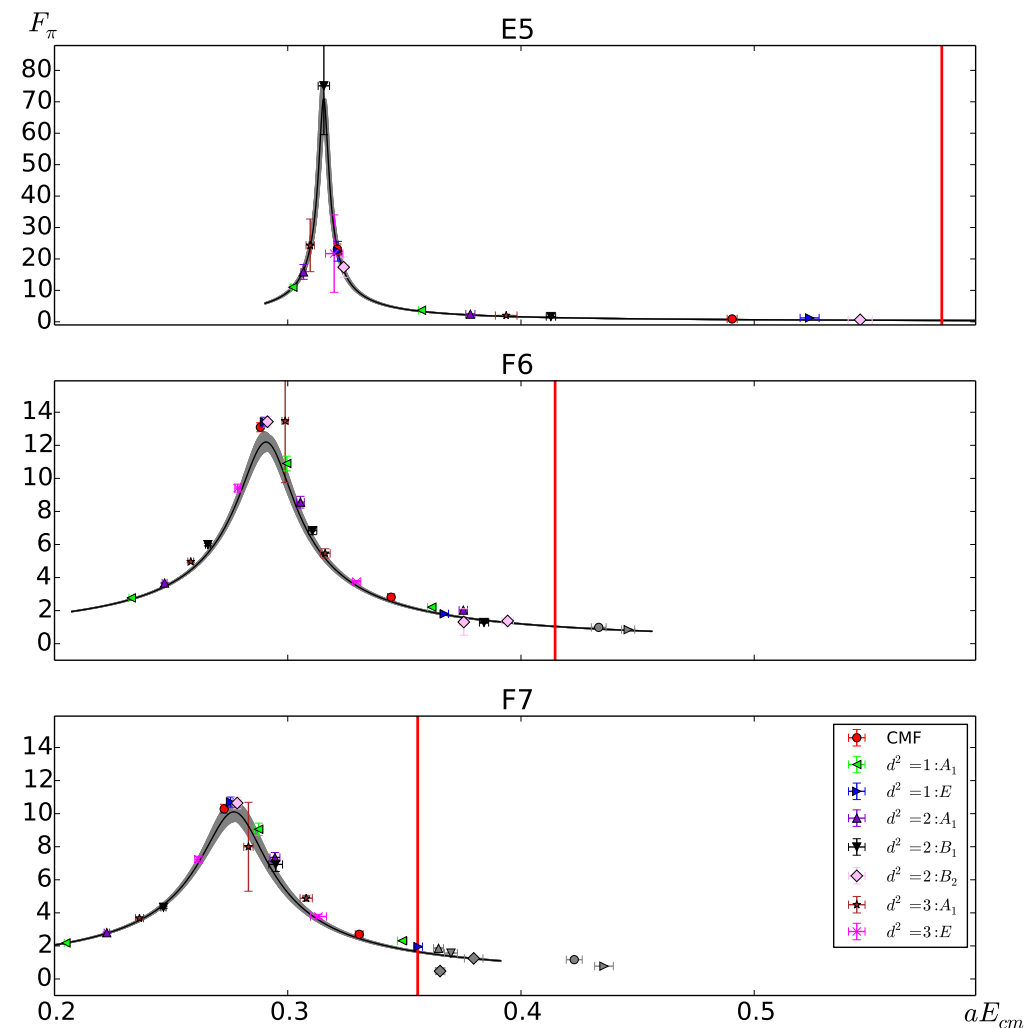
For  $E_{\text{cm}} < 4m_\pi$  :

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

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

- The matrix  $R_{L, \ell\ell'}(\Lambda)$  mixes partial waves
  - Formalism requires explicit treatment of *all* open scattering channels
  - All individual finite-volume energies/matrix elements must be extracted
- Not applicable to inclusive processes (at arbitrary energies)!

# Recent finite-volume results



Left:  $N_f = 2$ ,  $m_\pi = 265 - 437$  MeV

F. Erben, J. Green, D. Mohler, H. Wittig,  
Phys. Rev. D101 (2020)

Right:  $N_f = 2 + 1$ ,  $m_\pi = 200$  MeV

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

# Smearred spectral densities

Euclidean  $n$ -point correlation functions:

$$C_n(\tau_1, \dots, \tau_{n-1}) = \langle \mathcal{O}_1(\tau_1) \dots \mathcal{O}_n(0) \rangle$$

Alternative approach: Spectral reconstruction

$$C_2(\tau) = \int d\omega \rho(\omega) e^{-\omega \tau} \rightarrow$$
$$\rho_\epsilon(E) = \int d\omega \rho(\omega) \delta_\epsilon(E - \omega)$$

Notoriously ill-posed Inverse problem!

→ partially regulated by the smearing



# Smearred spectral densities

- Approximation of Dirac-delta:

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

- Implement  $i\epsilon$ -prescription

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

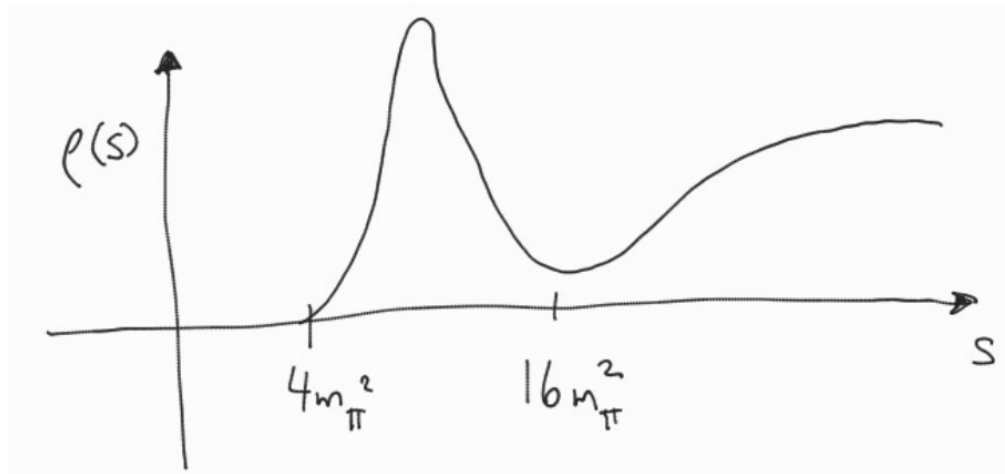
- Cut off high energies (Heaviside approx.):

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

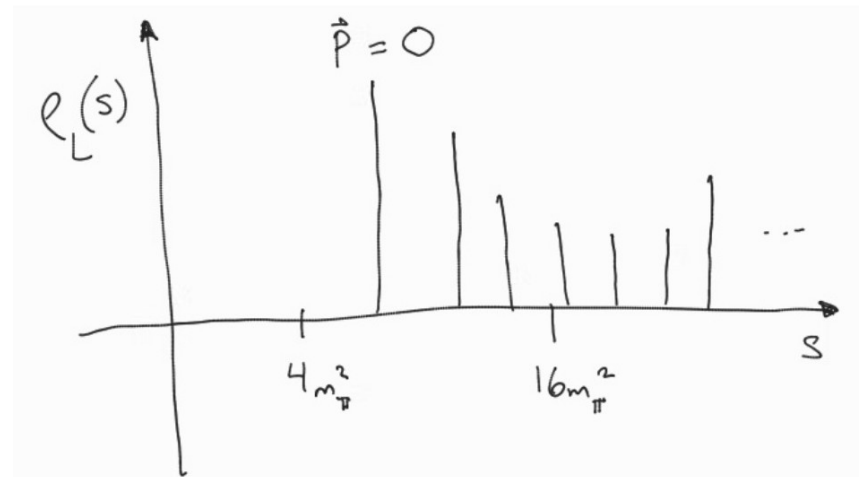
- Dispersion relations, sum rules, ....

# Finite vs. infinite volume

Infinite volume: continuous



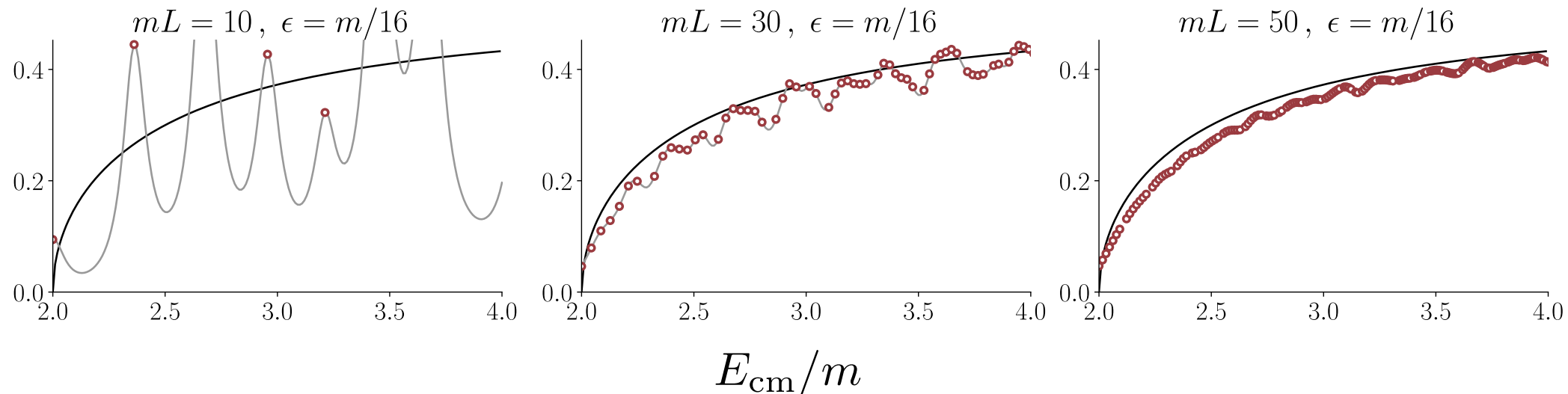
Finite volume: sum of Dirac-delta peaks.



Not 'close' to infinite volume at finite  $L$ !

# Finite vs. infinite volume

Smearred spectral densities: a bridge between finite- and infinite-volume:



→ Infinite-volume limit well-defined at finite smearing width

→ 'Small enough' smearing width => close to unsmeared spectral density

Smearing regulates inverse problem AND provide infinite volume limit!

# Spectral Reconstruction

Backus, Gilbert '68, '70

F. Pijpers, M. Thompson '92

M. R. Hansen, A. Lupo, N. Tantalo, PRD99 (2019)

Linear ansatz:

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

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

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

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),...

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

Conserved (global) current:

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

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

$$\begin{aligned} \rho(E) &= \sum_{\alpha} \delta(\mathbf{P}_{\alpha}) \delta(E - E_{\alpha}) |_{\text{out}} \langle \alpha | \hat{j}(0) | 0 \rangle|^2 \\ &= \sum_{n=2,4,6,\dots} \rho^{(n)}(E) \end{aligned}$$

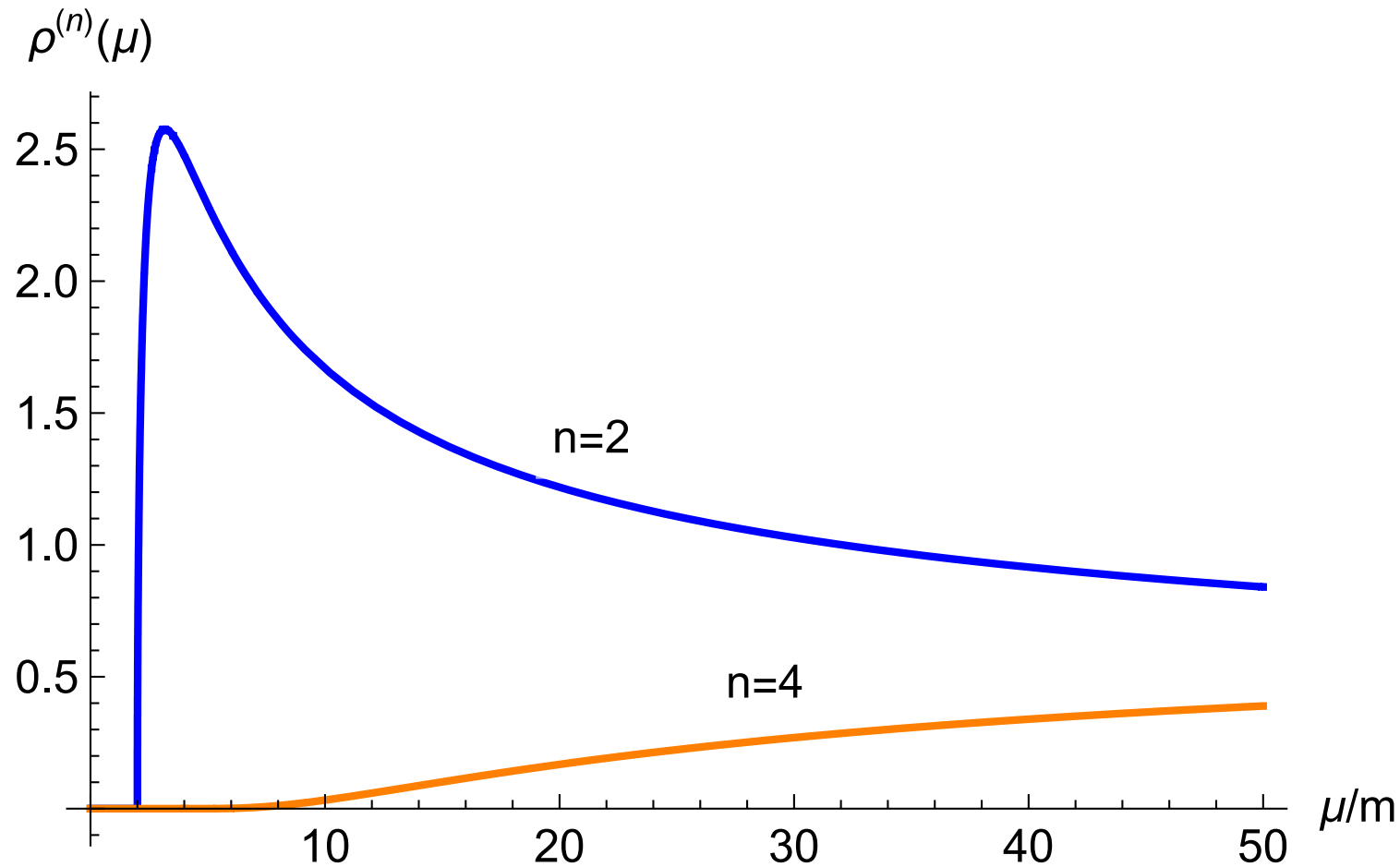
# Controlled Test

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  $\delta_\epsilon^x(E - \omega)$ :

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

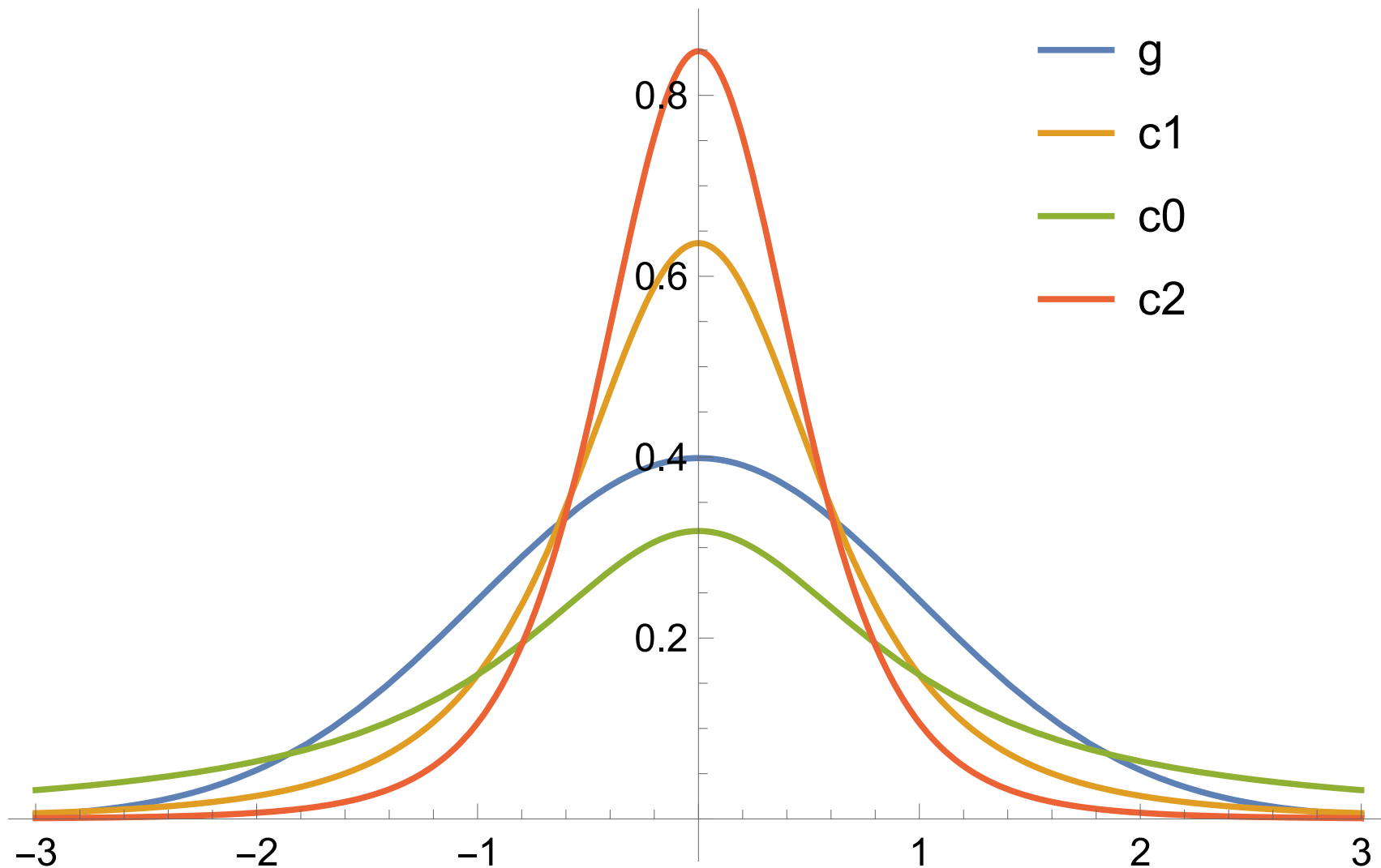
$$\delta_\epsilon^{c0}(x) = \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2},$$

$$\delta_\epsilon^{c1}(x) = \frac{2}{\pi} \frac{\epsilon^3}{(x^2 + \epsilon^2)^2},$$

$$\delta_\epsilon^{c2}(x) = \frac{8}{3\pi} \frac{\epsilon^5}{(x^2 + \epsilon^2)^3}$$

# Controlled Test

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

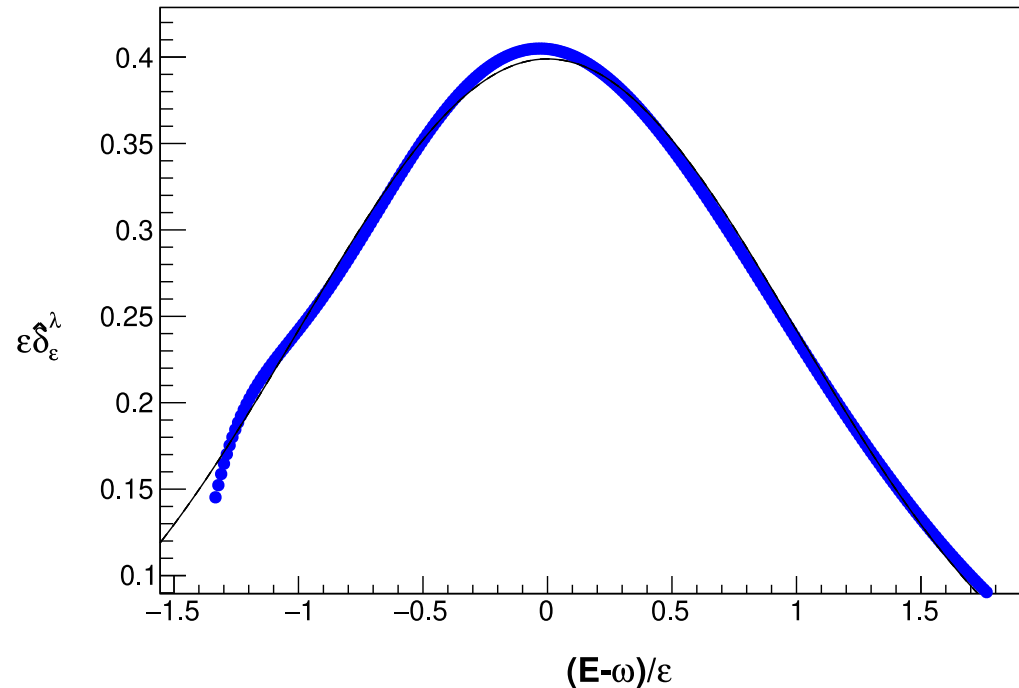
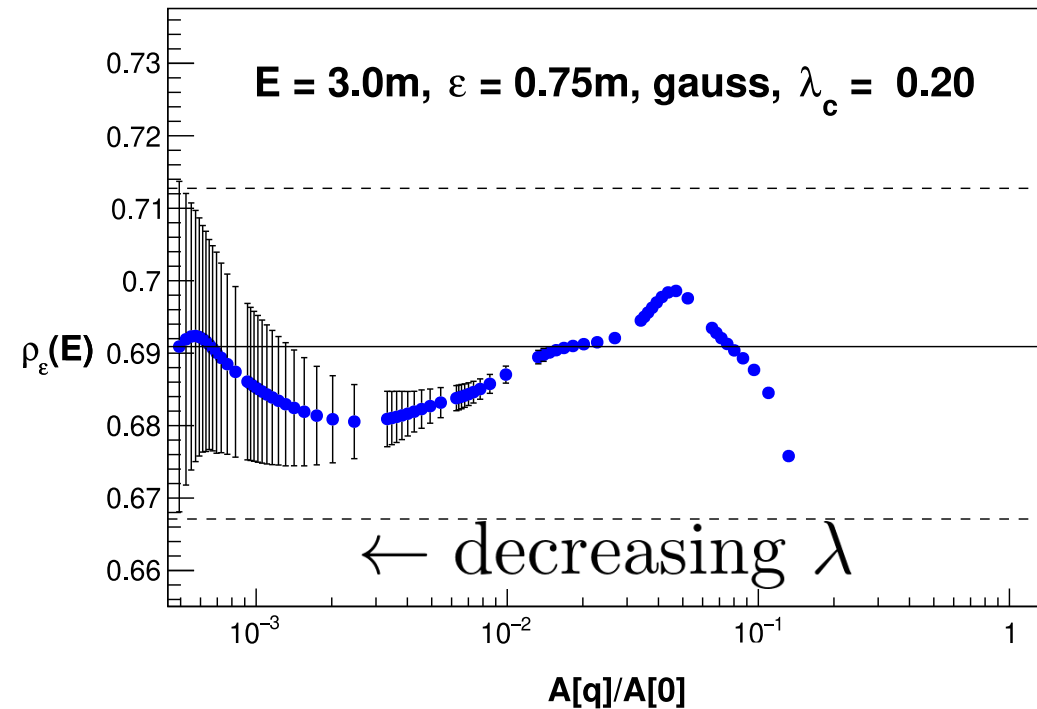




# Spectral Reconstruction

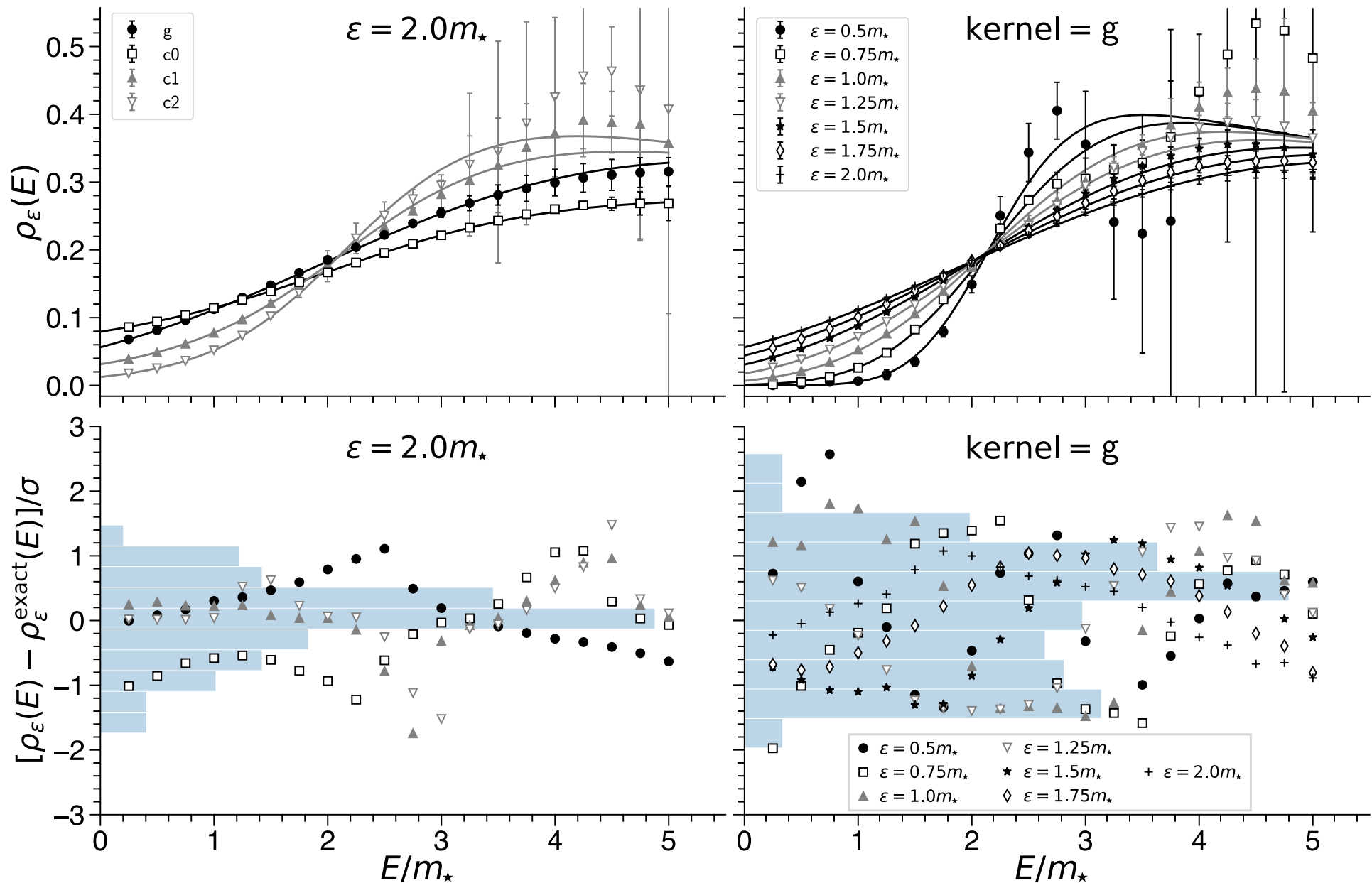
$$G_\lambda[q] = (1 - \lambda)A[q] + \lambda B[q]$$

Trade off parameter (  $\lambda$  ) 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.

# Results: extrapolation to zero width

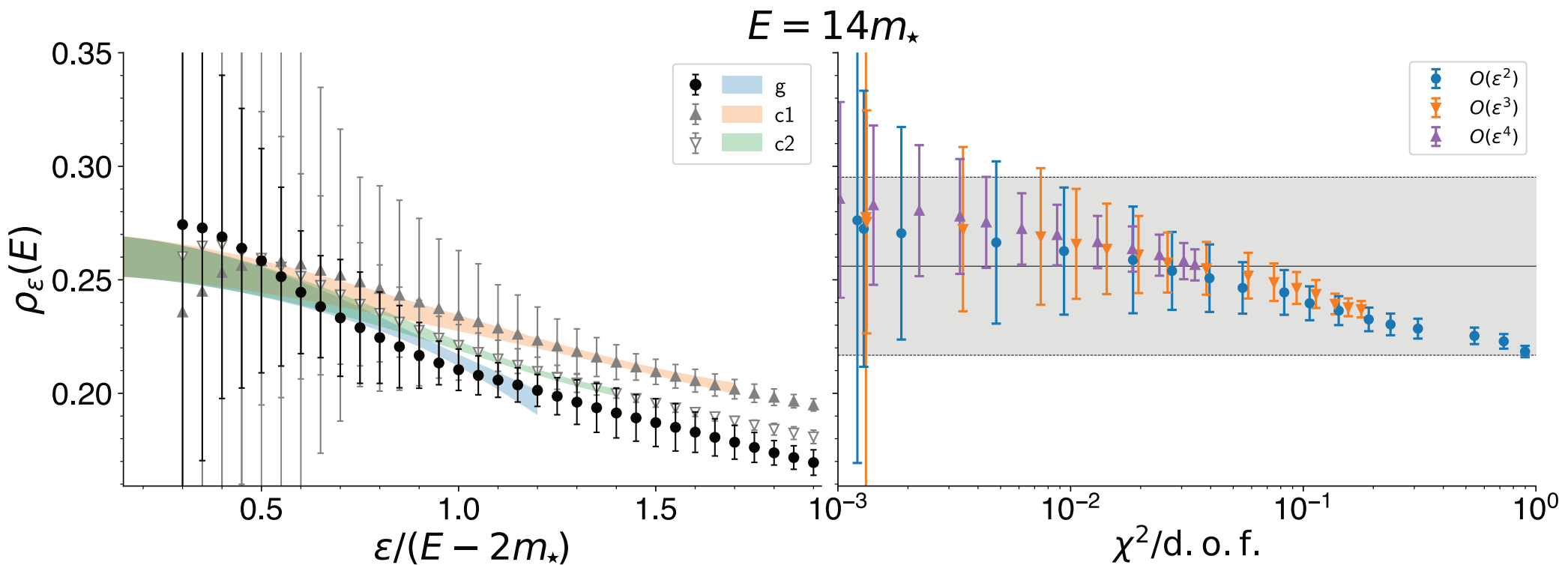
All kernels have the same  $O(\epsilon^2)$  coefficient (up to a sign):

$$\rho_\epsilon^x(E) = \rho(E) + \sum_{k=1}^{\infty} w_k^{(x)} a_k(E) \epsilon^k,$$

$x$	$w_k^x$ , even $k$	$w_k^x$ , odd $k$	$w_1^x$	$w_2^x$	$w_3^x$	$w_4^x$
g	$\frac{k!}{(-2)^{k/2}(k/2)!}$	0	0	-1	0	3
c0	1	1	1	1	1	1
c1	$(1 - k)$	$(1 - k)$	0	-1	-2	-3
c2	$\frac{1}{3}(k - 3)(k - 1)$	$\frac{1}{3}(k - 3)(k - 1)$	0	-1/3	0	1

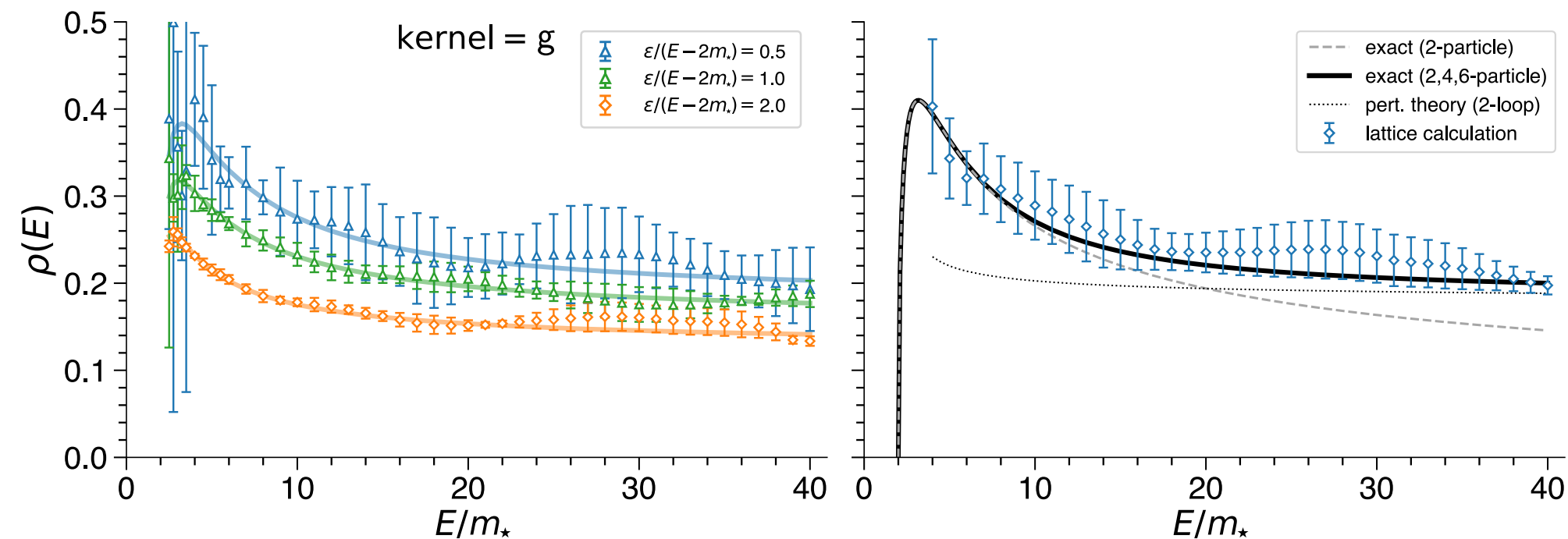
Known coefficients enable constrained extrapolation of all kernels

# Results: extrapolation to zero width



Key insight: larger smearing width sufficient at larger energy

# Results: extrapolation to zero width



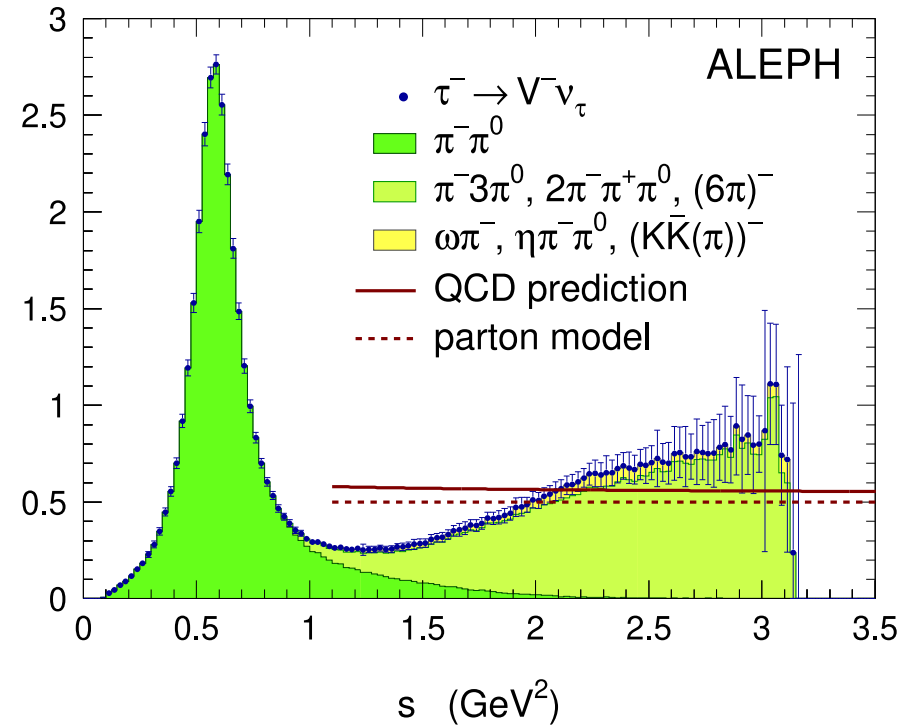
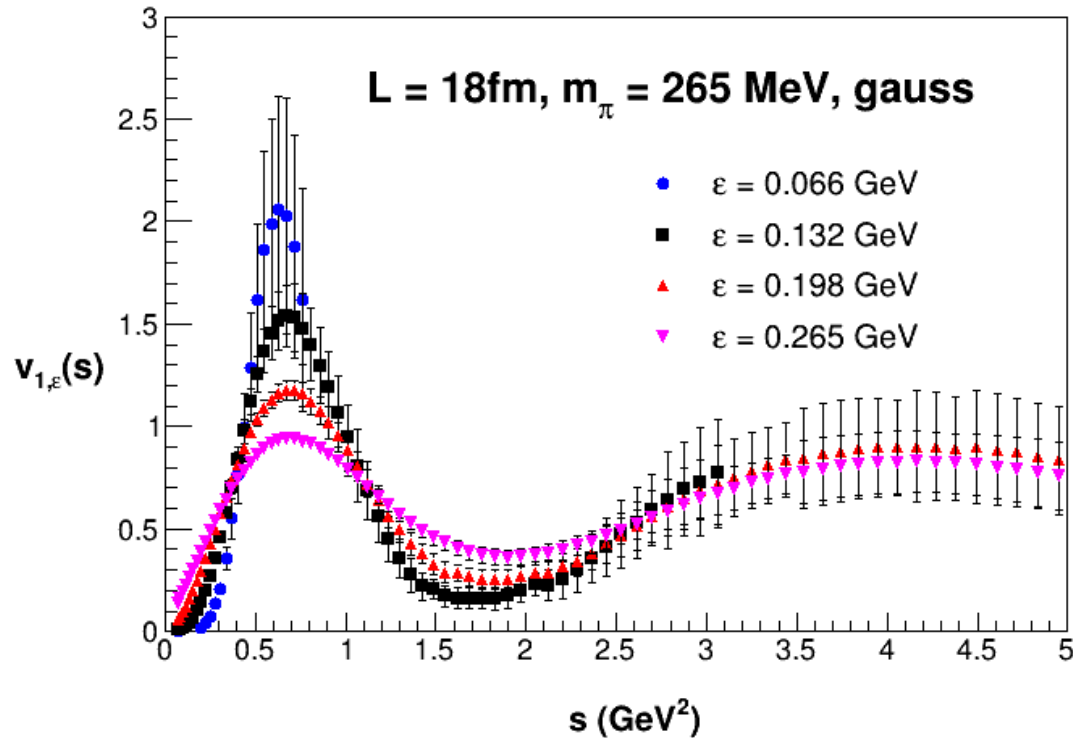
Some sensitivity to four-particle contribution at higher energies

# What about QCD?

- Large volumes needed: in O(3)-model  $mL \approx 30$
- 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  $m_\pi L \approx 3$
- Preliminary application: isovector (axial)vector correlators at
$$N_f = 2 + 1, \quad L = 6\text{fm}, 9\text{fm}, \text{ and } 18\text{fm},$$
$$a = 0.09\text{fm}, \quad m_\pi = 265\text{MeV}$$

# What about QCD?

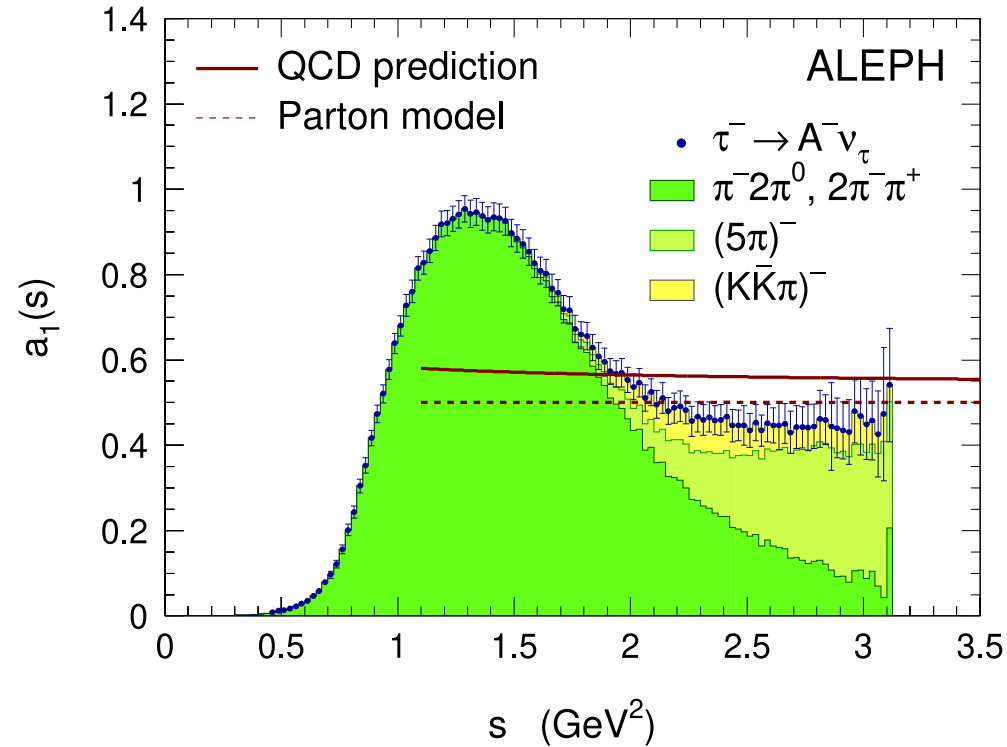
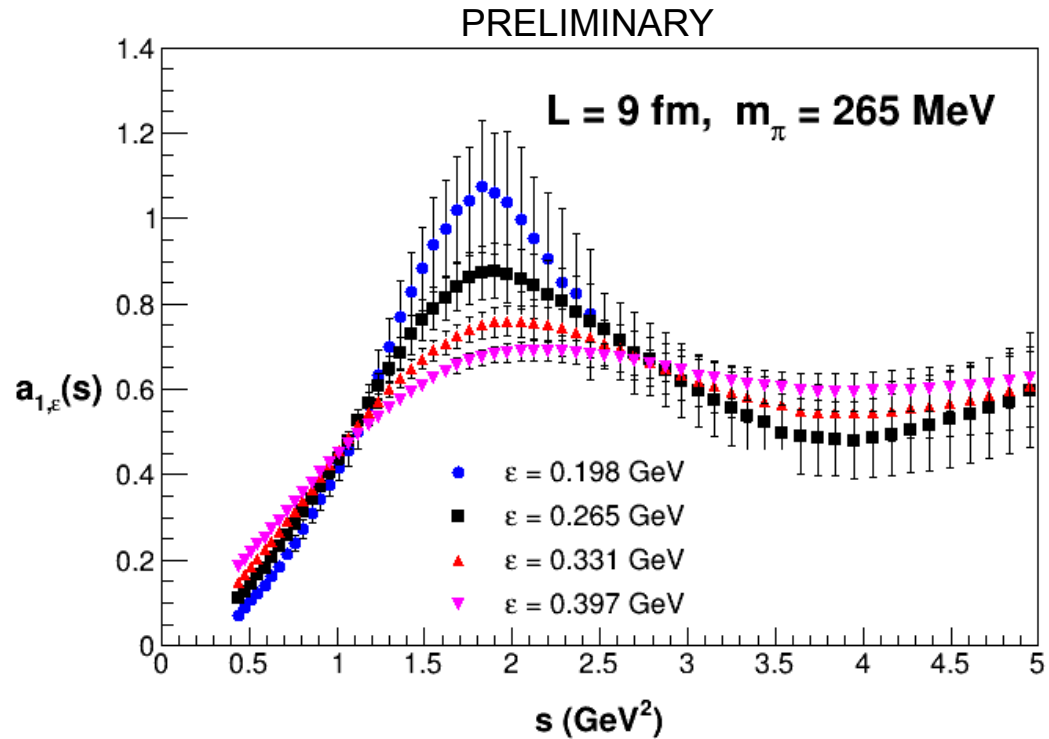
PRELIMINARY



ALEPH collaboration '05

- Comparison to hadronic tau-decay (right)
- No extrapolation to zero-width yet
- Mild indication of four-particle effects.

# What about QCD?



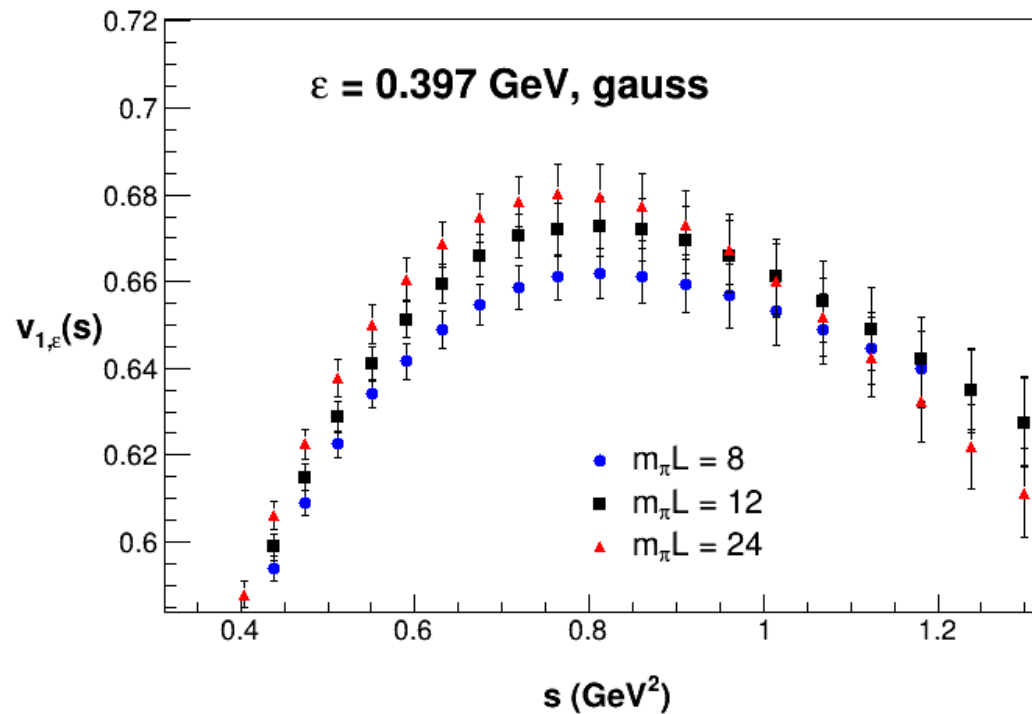
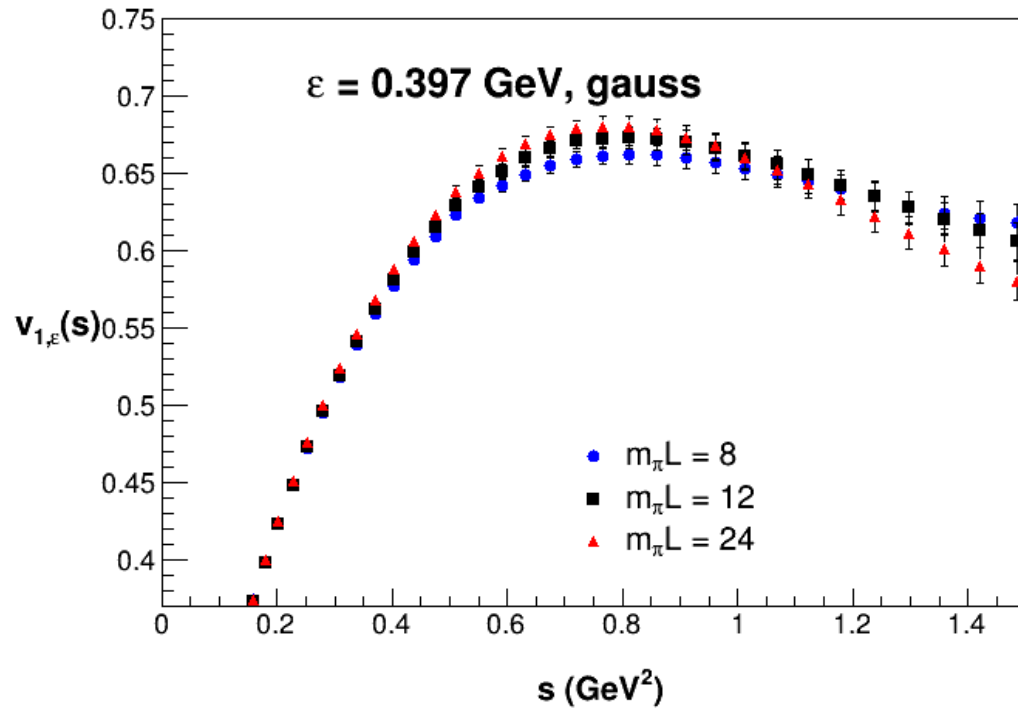
ALEPH collaboration '05

- Comparison to hadronic tau-decay (right)
- No extrapolation to zero-width yet
- Bump from  $a_1(1260)$ , indication of five pions



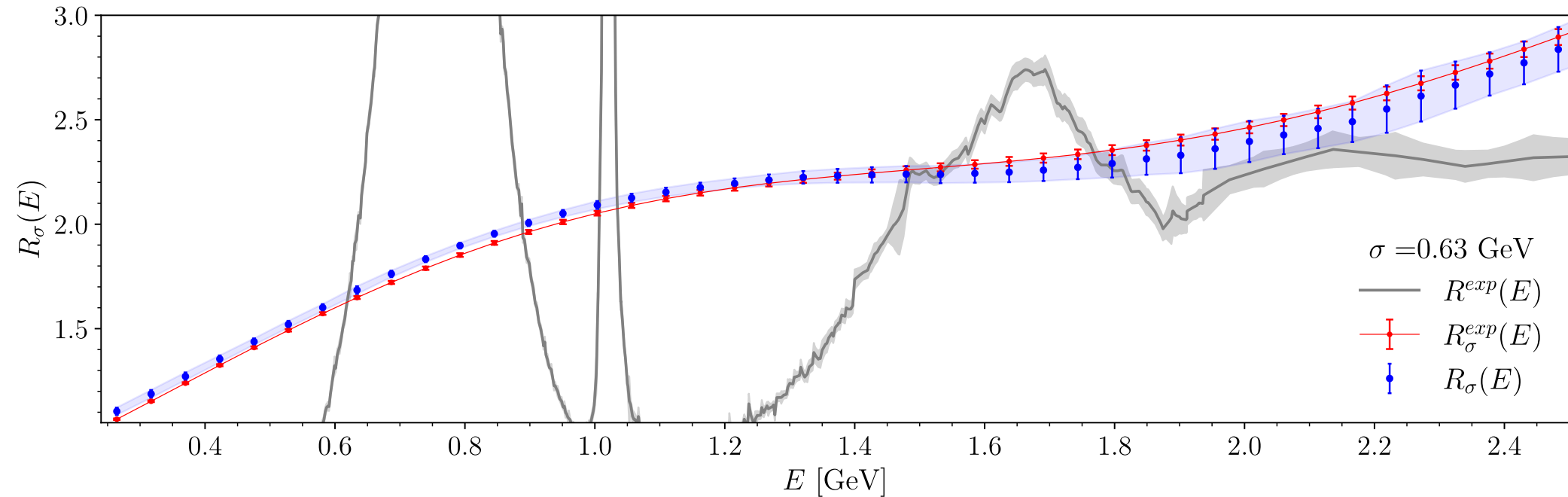
# Finite volume effects

PRELIMINARY



- Marginally significant
- Additional volumes to come, down to  $m_\pi L = 4$

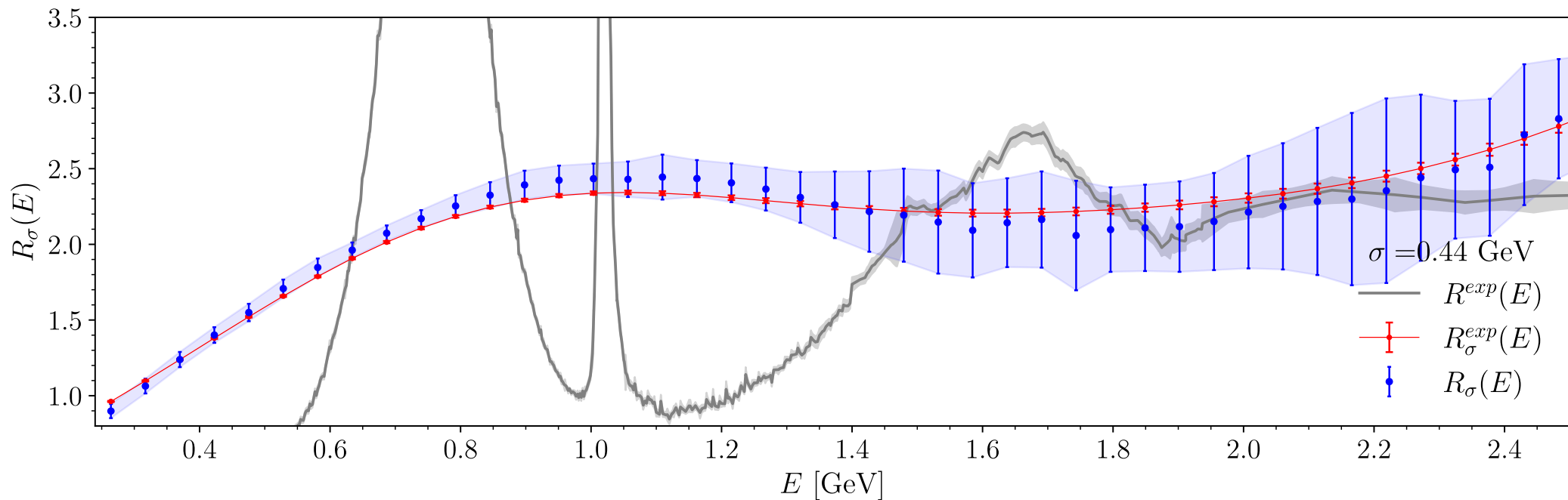
# Smeared $R$ -ratio



$$N_f = 2 + 1, \quad m_\pi = m_\pi^{\text{phys}}, \quad m_\pi L = 3.4 - 5.2$$

- Comparison between lattice and smeared pheno. data
- Smaller volumes => smaller smearing widths
- Discrepancies  $\lesssim 3\sigma$  near  $\rho(770)$

# Smeared $R$ -ratio



$$N_f = 2 + 1, \quad m_\pi = m_\pi^{\text{phys}}, \quad m_\pi L = 3.4 - 5.2$$

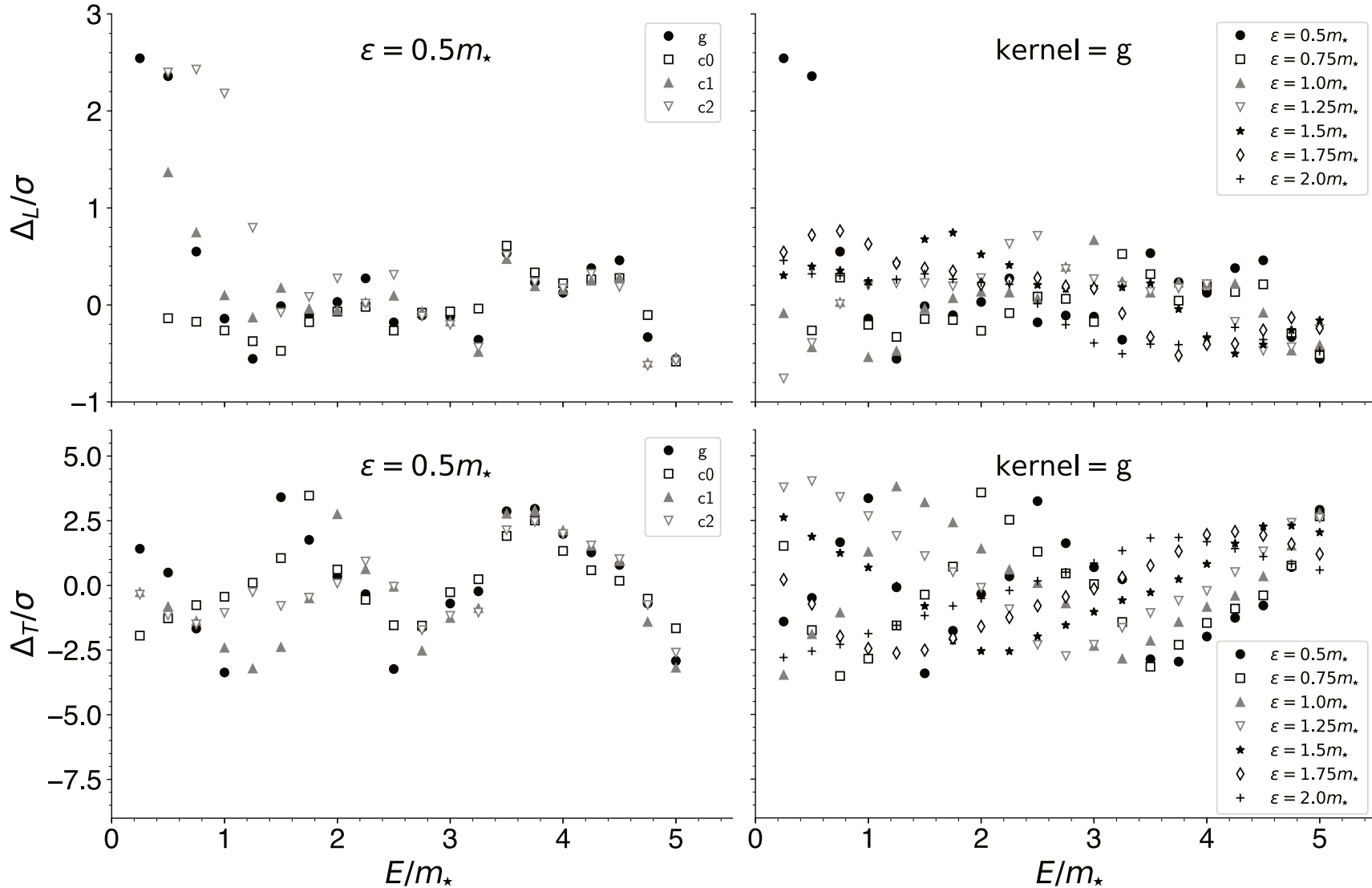
- Comparison between lattice and smeared pheno. data
- Smaller volumes => smaller smearing widths
- No significant discrepancies

# Conclusions

- The HLT approach to spectral reconstruction produces results with controlled systematic errors.
- Application to QCD: first lattice determinations of smeared (axial)vector spectral functions!
- Masterfield approach important to achieve large volume and small smearing width
- Alternative approach: Chebyshev polynomials      G. Bailas, S. Hashimoto, T. Ishikawa, PTEP '20
  - Roughly comparably effective      R. Kellermann et al., Lattice '22
- Other applications:
  - 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

# Finite-volume effects

$$\Delta_L(\epsilon, E) = \rho_{T,L,\epsilon}(E) - \rho_{T,2L,\epsilon}(E)$$

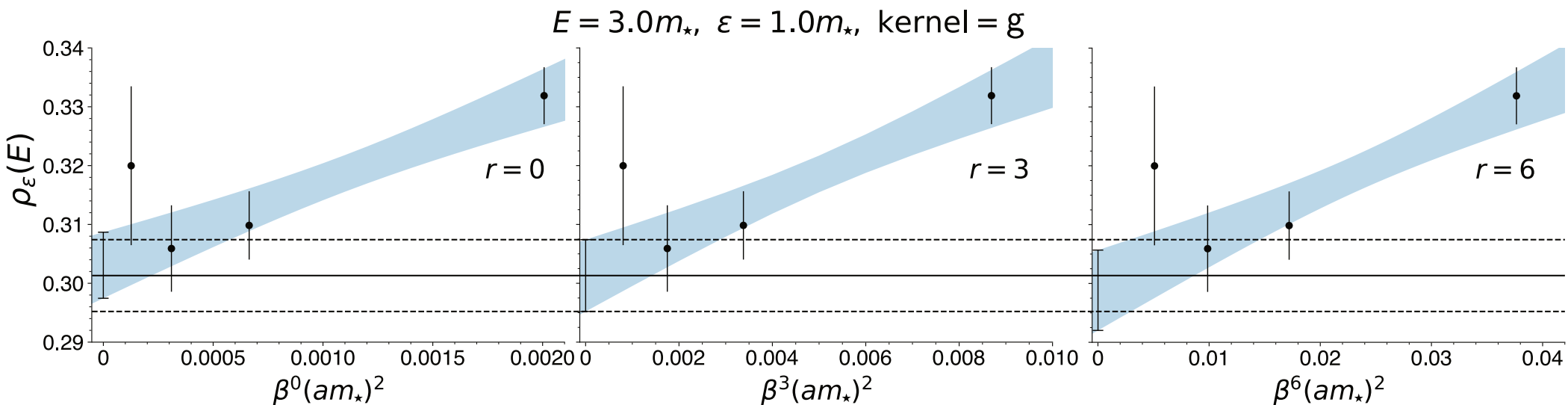


Differences taken as additional systematic error.

# Continuum Limit

Long History! For spectral quantities: ... , J. Balog, F. Niedermayer, P. Weisz, Nucl. Phys. B824 (2010)

$$\lim_{a \rightarrow 0} E(a) = E^{\text{phys}} + A\beta^3 a^2 \left( 1 + \frac{r}{\beta} + \frac{c}{\beta^2} + \dots \right)$$



Sys. error estimate from three (arbitrary) fit forms:

$$\beta^p (a/m)^2, \quad p = 0, 3, 6$$

Continuum limit possible at fixed eps and E!