

Neural network applications to spectral reconstruction

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In collaboration with

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- ▶ Motivations
- ▶ Spectral reconstruction as an inverse problem
- ▶ Case study: the light vector resonance
- ▶ Summary & perspectives

Motivations

Motivations

- ▶ Traditional lattice analysis: extract energies and matrix elements through fitting the exponential behaviour of correlators.
- ▶ **Density of state increases quickly with the volume.**
Standard analysis increasingly challenging.
- ▶ Non-gapped correlators (QED, scattering, ...)
Even ground state challenging at large volume.
- ▶ Reconstruction of **long-distance effects.**
- ▶ **How to go beyond exponential fits?**

Spectral reconstruction as an inverse problem

Spectral integral equation

- ▶ In the case of 2-point functions
Källén-Lehmann spectral representation

$$D(q^2) = \int d^4x \langle \phi(x) \phi(0)^\dagger \rangle e^{-iq \cdot x} = \int_0^{+\infty} ds \frac{\rho(s)}{q^2 + s}$$

- ▶ Spectral reconstruction from lattice data:
Find ρ given D .

- ▶ Integral operator $(S\rho)(q^2) = \int ds \frac{\rho(s)}{q^2 + s}$.
Solution " $\rho = S^{-1}D$ ".

Linear problem

Naive approach

- ▶ Arbitrary discretisation q_j^2 and s_k

$$S_{jk} = \frac{1}{q_j^2 + s_k}$$

- ▶ Distinct points: unique solution

$$\det(S) = \frac{\prod_{k>j} (q_j^2 - q_k^2)(s_j - s_k)}{\prod_{j,k} (q_j^2 + s_k)}$$

- ▶ In practice: extremely ill-conditioned matrix (typically $\kappa \simeq \mathcal{O}(10^{100})$)

Appropriateness of machine learning

- ▶ Machine-learning approach: **fit a parametrisation of the inverse transform** on a relevant functional space.
- ▶ Advantage here:
trivial to construct random problem-solution pairs.
- ▶ Neural networks are just a specific parametrisation.
- ▶ Existing work: [Kades *et al.*, arXiv:1905.04305]

Challenges

- ▶ Determine an appropriate neural architecture.
- ▶ Establish a strategy for generating training and validation datasets.
- ▶ Design a Monte-Carlo strategy to validate predictions on synthetic lattice data.
- ▶ *Investigate generalisation of trained models.*
- ▶ *Compare against existing methods.*

Case study: the light vector resonance

Generalities

- ▶ Vector-vector spectral representation

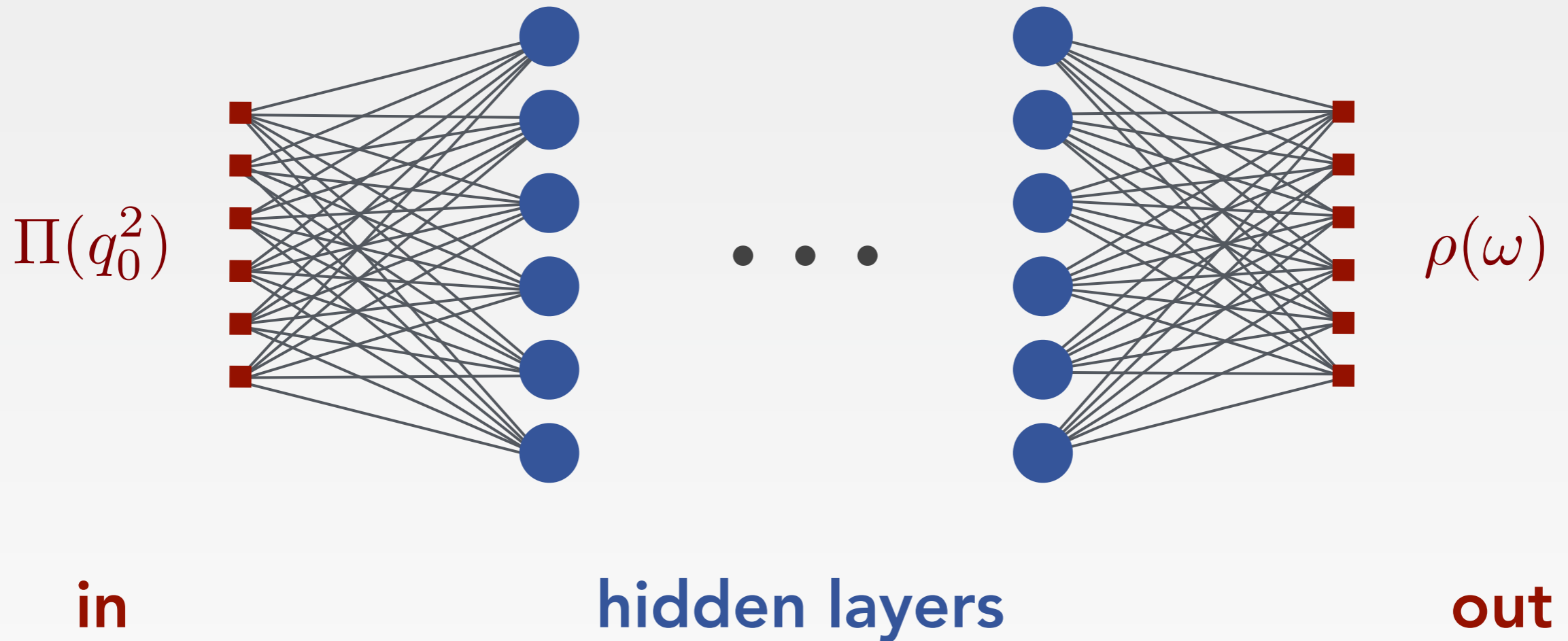
$$C_{\mu\nu}(t) = \int d^3\mathbf{x} \langle 0 | \mathsf{T}[J_\mu(t, \mathbf{x}) J_\nu(0)] | 0 \rangle$$

$$\Pi_{\mu\nu}(q_0) = \int dt C_{\mu\nu}(t) e^{-iq_0 t} = \delta_{\mu\nu} q_0^2 \Pi(q_0^2)$$

$$\Pi(q_0^2) = \int_0^{+\infty} ds \frac{\rho(s)}{q_0^2 + s}$$

$$\rho(s) = \frac{1}{3s} \int d\alpha \sum_\mu |\langle 0 | J_\mu(0) | \alpha \rangle|^2 \delta(\omega_\alpha^2 - s)$$

Neural network architecture



Size	$\frac{N_T}{2} - 1$	N_h	N_ω
Step	$\frac{2\pi}{T}$		$\delta\omega$

● : $\tanh(x)$ ■ : x

Data preconditioning

- ▶ **Momentum space input layer**

Reduce the hierarchy of weights, accelerate training.
Just a change of basis on the input layer.

- ▶ **Linear scaling enforcement**

Always normalise in and out by the input average.
Quality of prediction insensitive to overall scale.

Training

- ▶ Loss function: 2-norm difference

$$L(\Pi, \rho) = \frac{1}{N} \sum_j \|F(\Pi_j) - \rho_j\|_2^2$$

F : neural net

- ▶ Training: stochastically minimise L on a training set
Monitor loss through an independent validation set.
- ▶ Mini-batch size 4
- ▶ ADAM minimiser with “reduce-on-plateau” adaptive learning rate.

Training/Validation set

- ▶ Training set: 5000 random Breit-Wigner examples

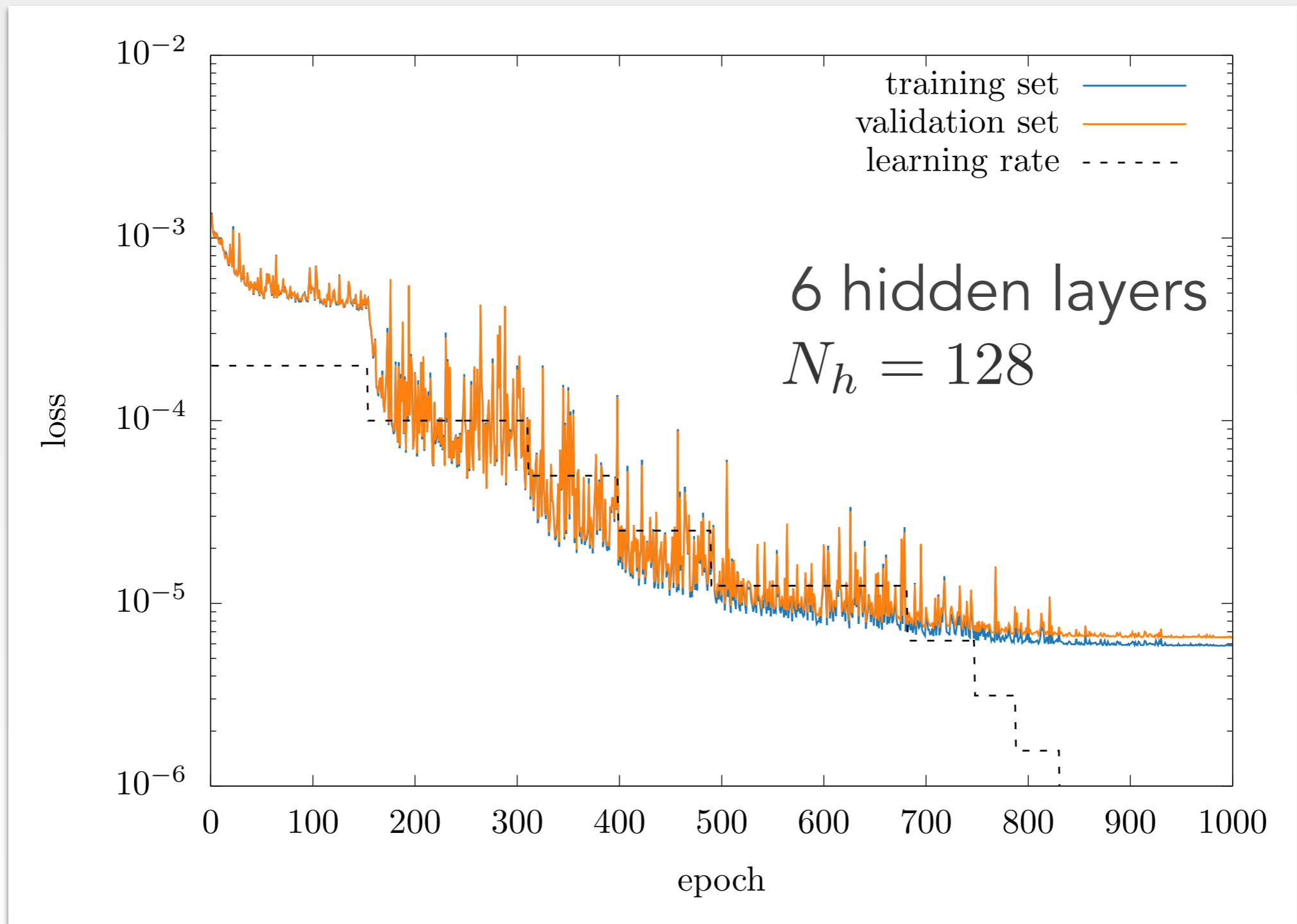
$$300 \text{ MeV} \leq M \leq 1000 \text{ MeV}$$

$$120 \text{ MeV} \leq \Gamma \leq 300 \text{ MeV}$$

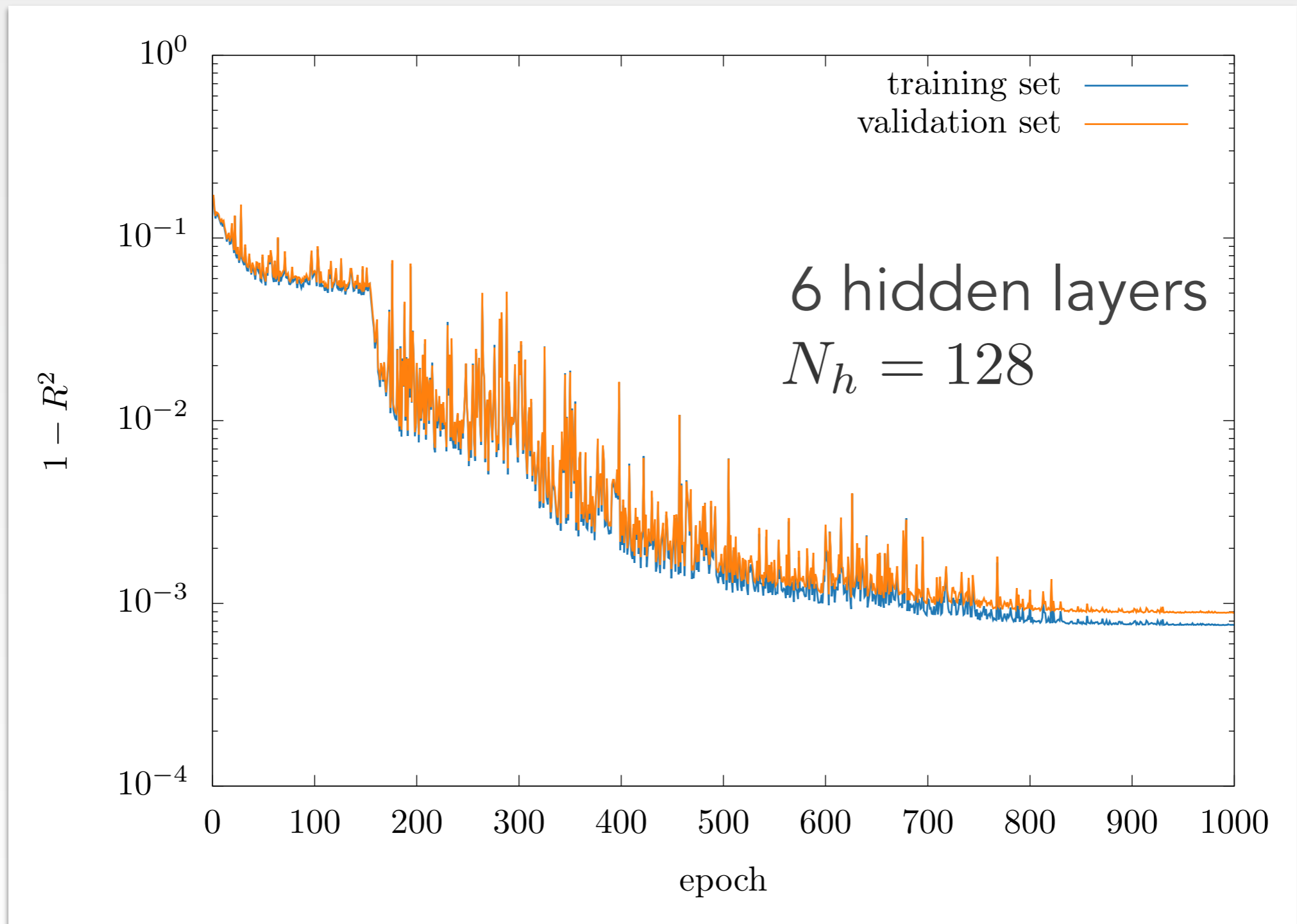
- ▶ Validation set: same, with 1000 examples.
- ▶ Loss function value not very meaningful.
- ▶ R^2 -score more useful

$$R^2 = 1 - \frac{\|F(\Pi) - \rho\|_2^2}{\text{Var}(\rho)}$$

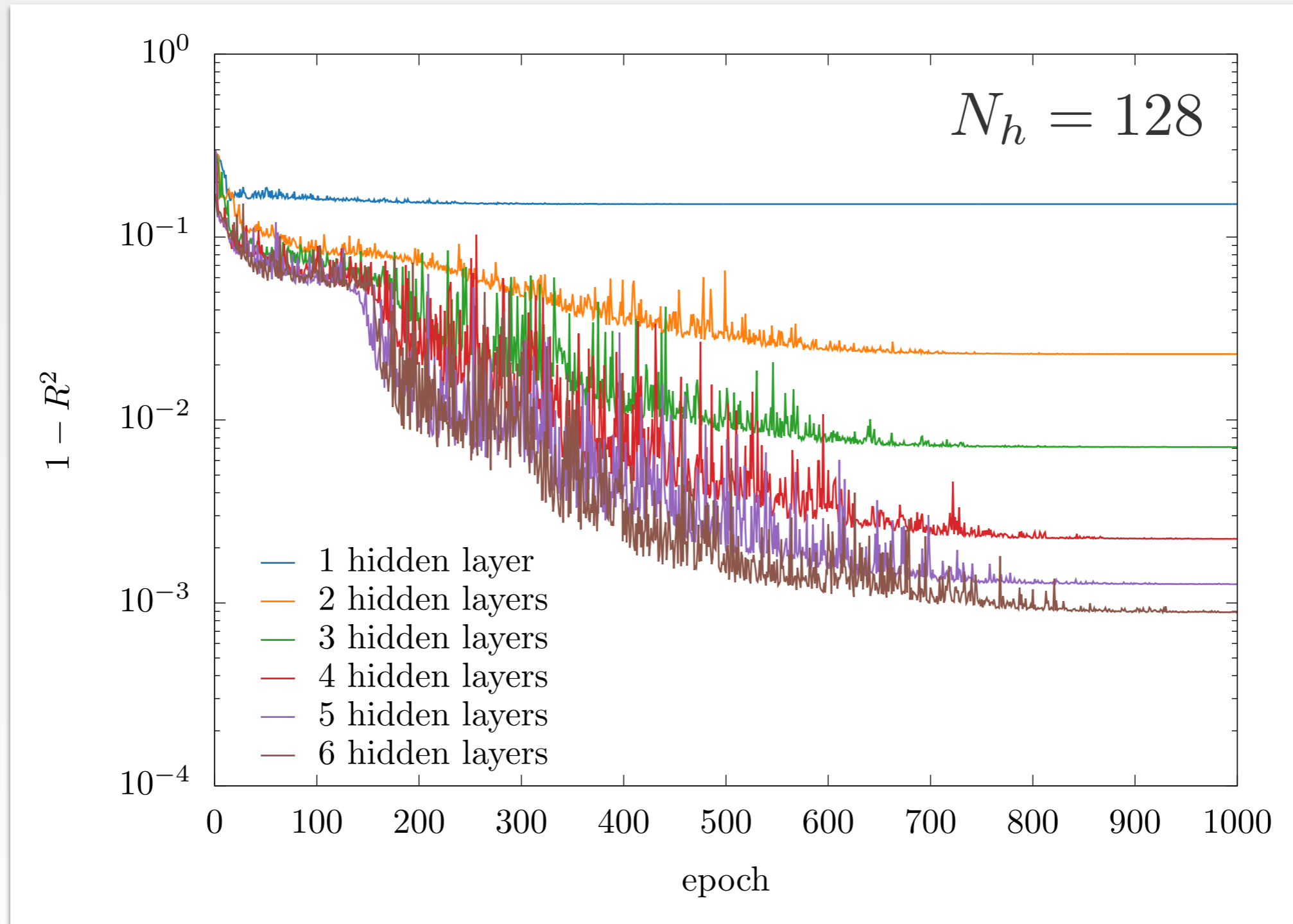
Learning curve example



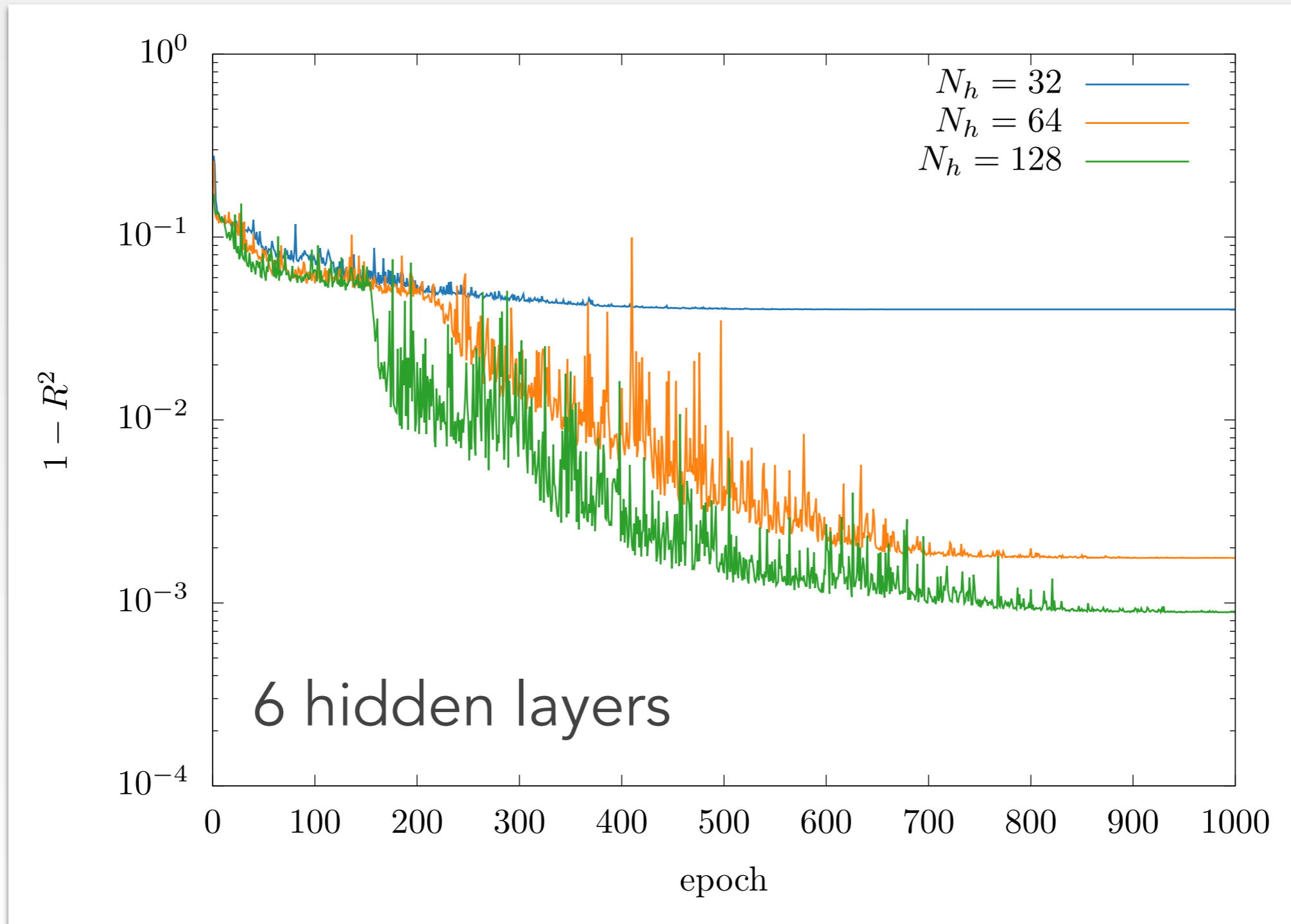
Learning curve example



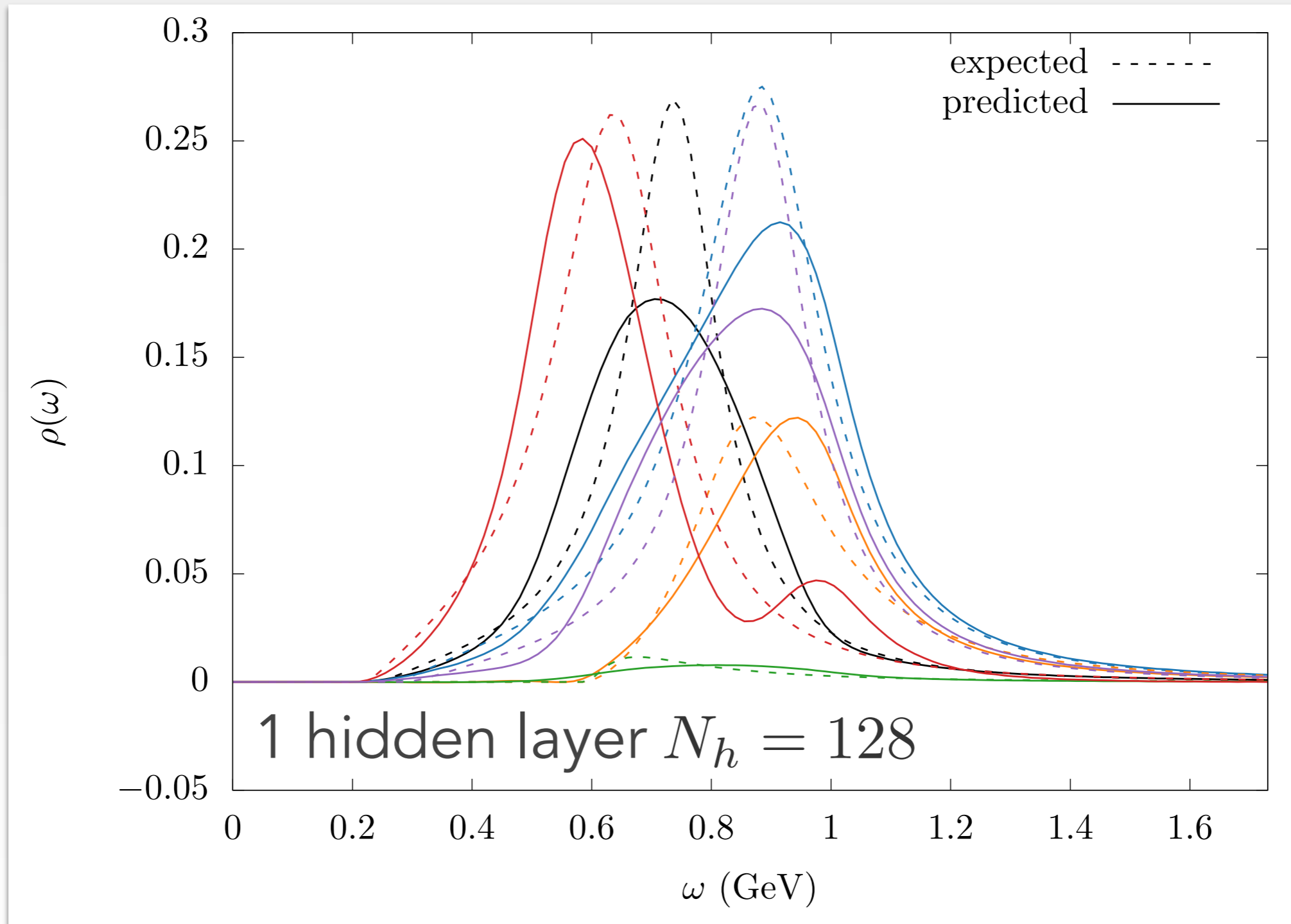
Learning curves vs. hidden layers



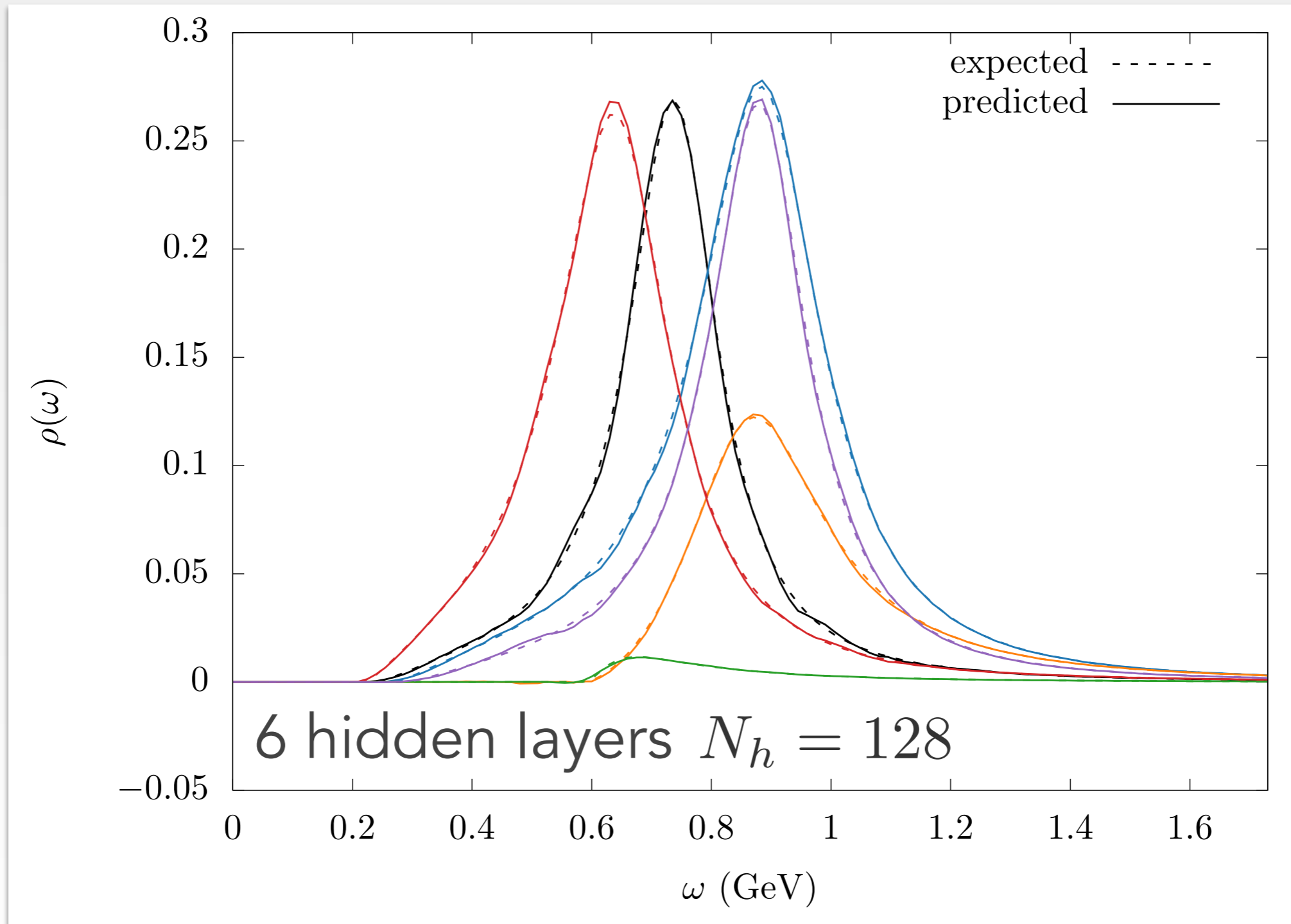
Learning curves vs. hidden layer size



Validation set sample



Validation set sample



Synthetic lattice data

- ▶ Correlator based on Gunaris-Sakurai parametrisation with physical parameters.
- ▶ Phenomenological variance model (work in progress)

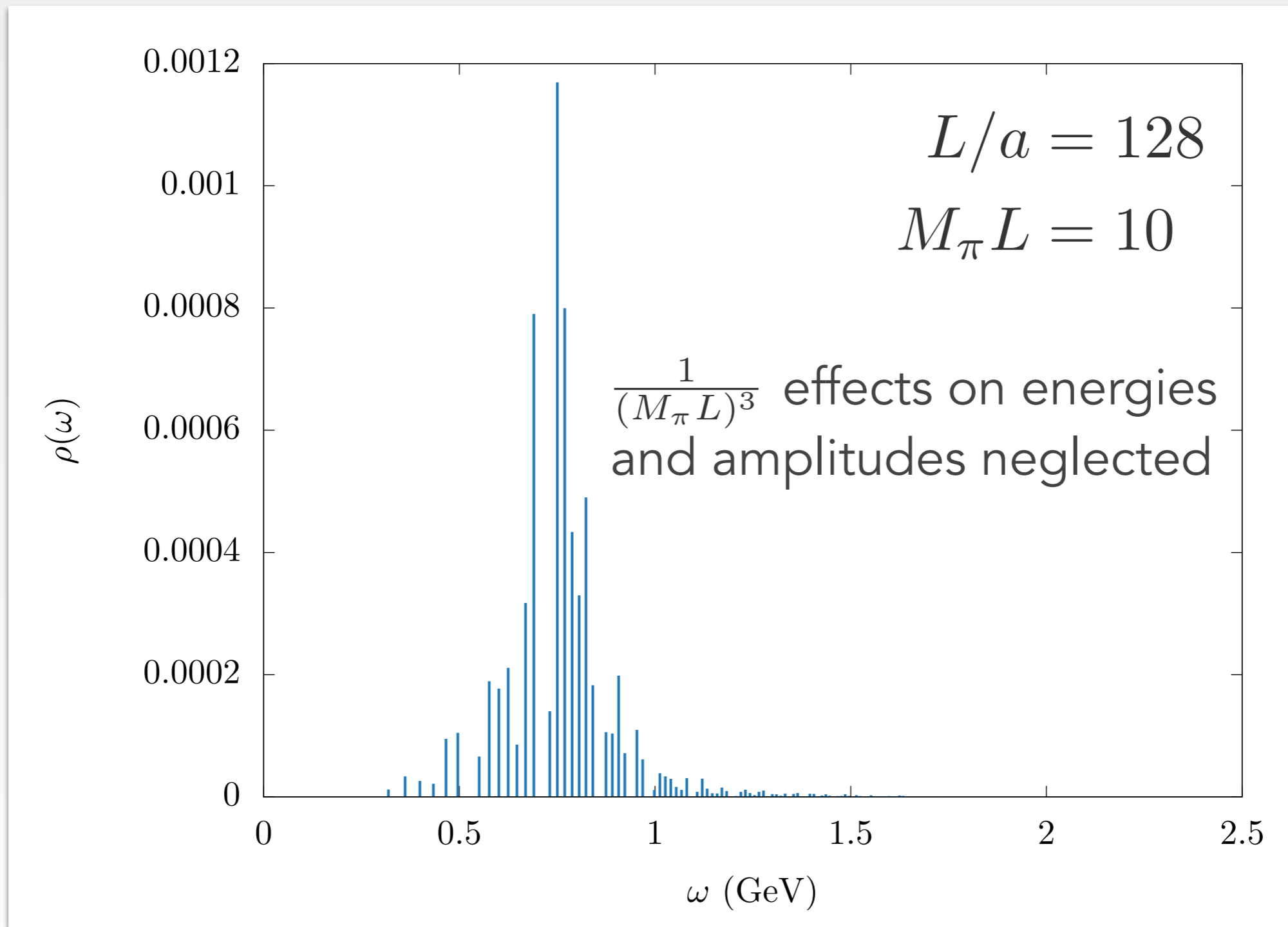
$$C_{jk} = \frac{1}{1 + \frac{1-\alpha}{\alpha}(j-k)^2} \quad \rho_j = \frac{1}{j^2} \frac{\beta}{1 + \gamma^2(j-1)^2}$$

C_{jk} : correlation between $\Pi(q_j^2)$ and $\Pi(q_k^2)$

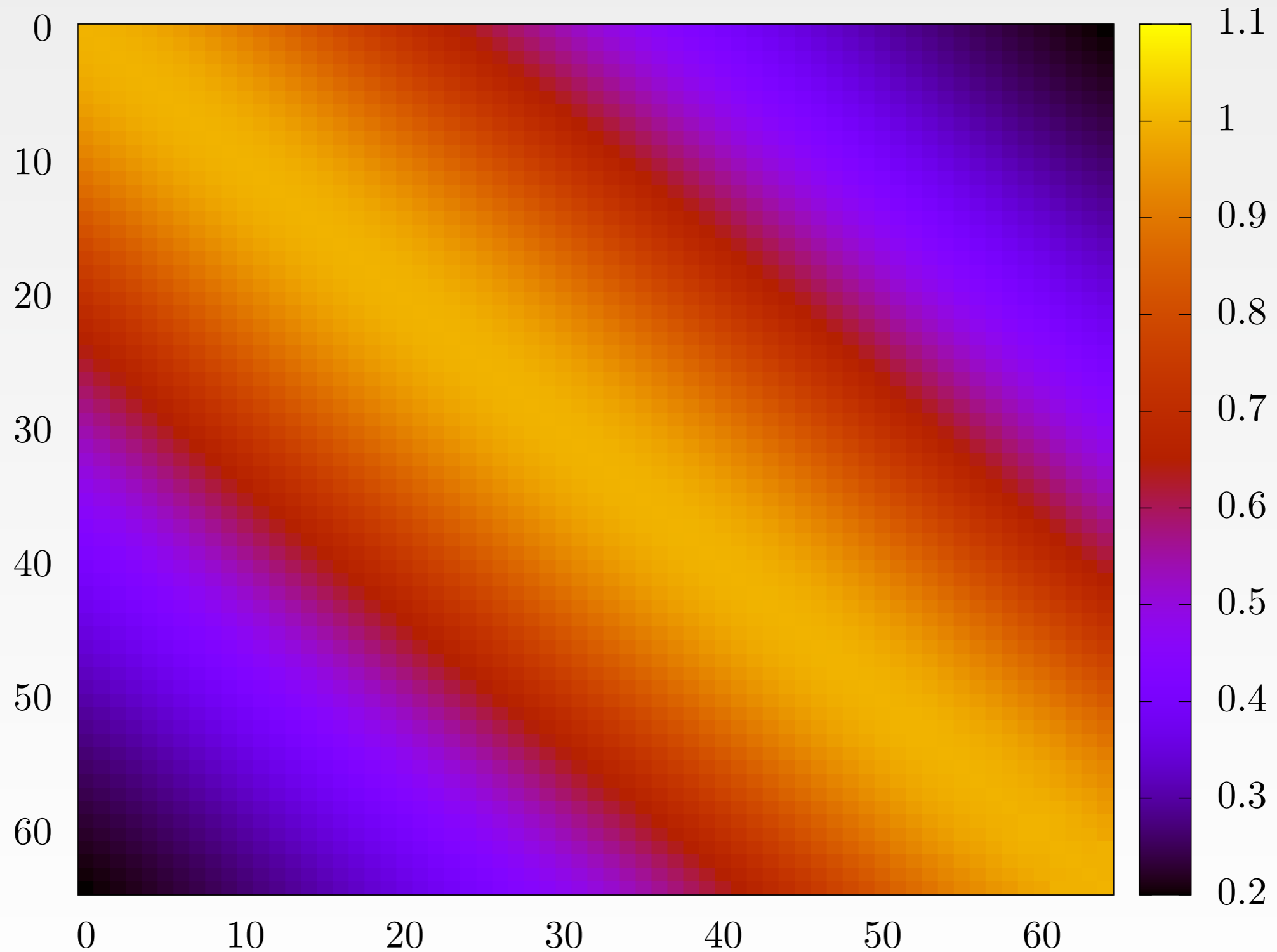
ρ_j : relative error on $\Pi(q_j^2)$

- ▶ Realistic for $\alpha = 99.9\%$ $\beta = \mathcal{O}(1\%)$ $\gamma = 0.0039$

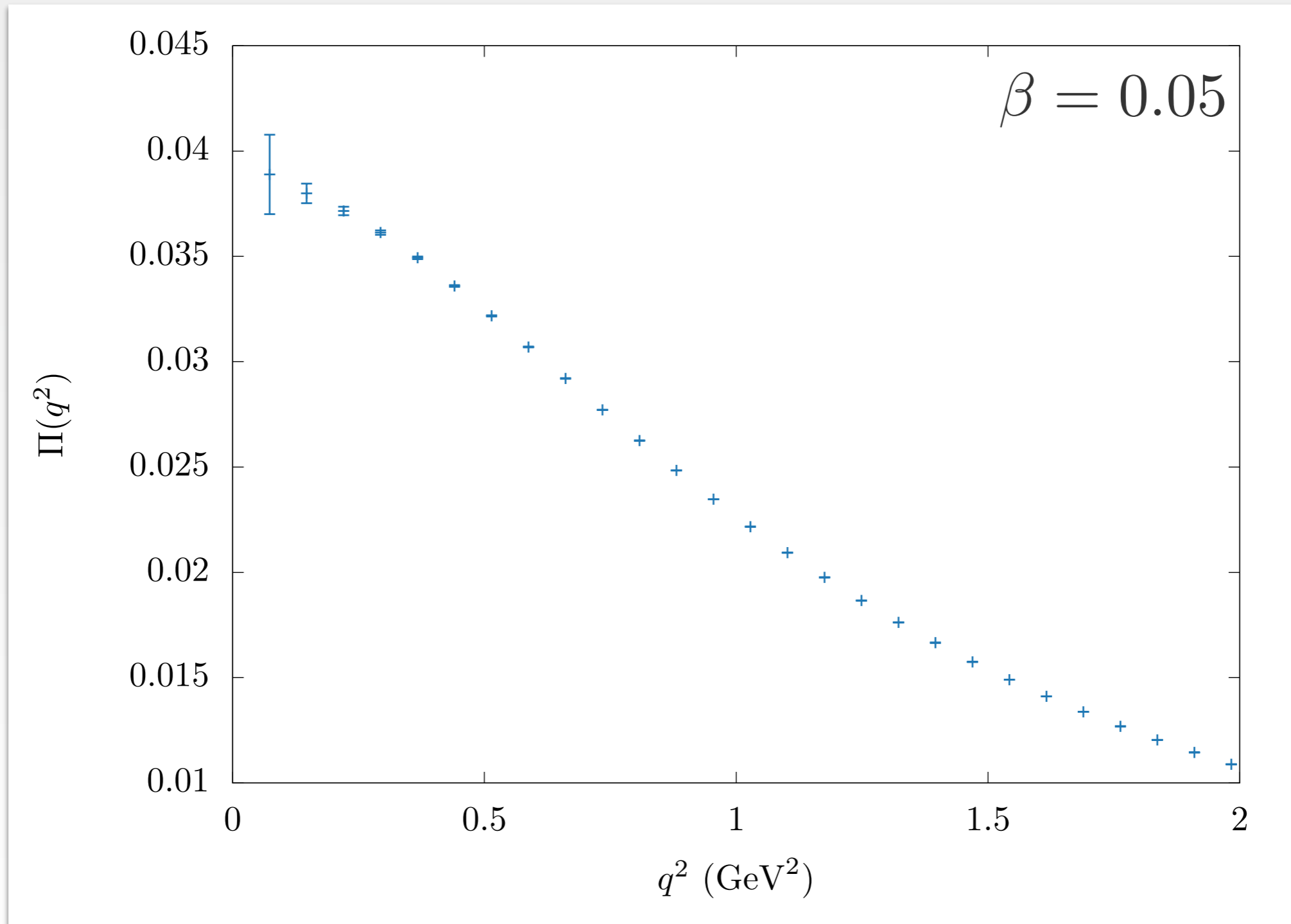
Finite-volume spectrum



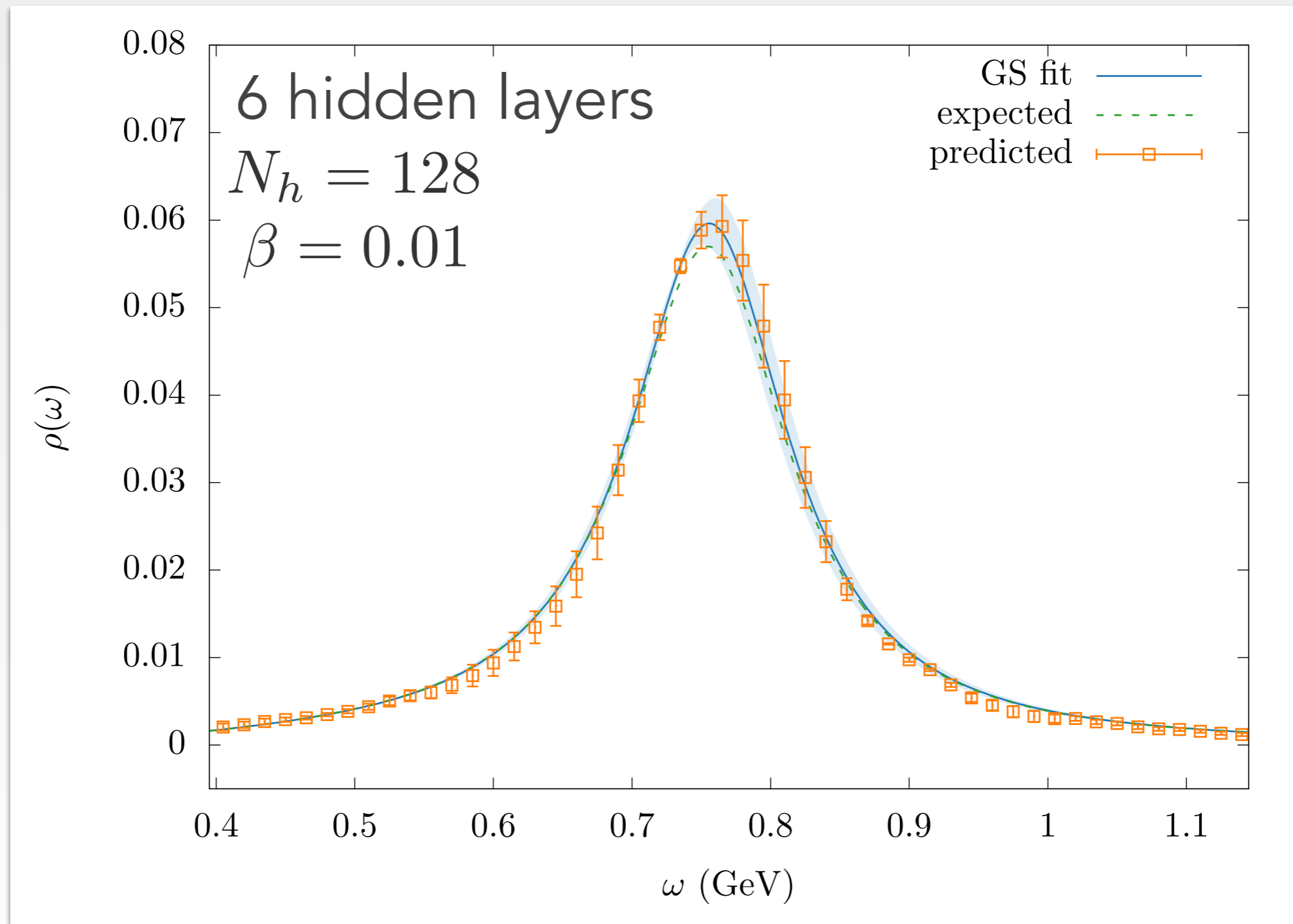
Synthetic lattice data



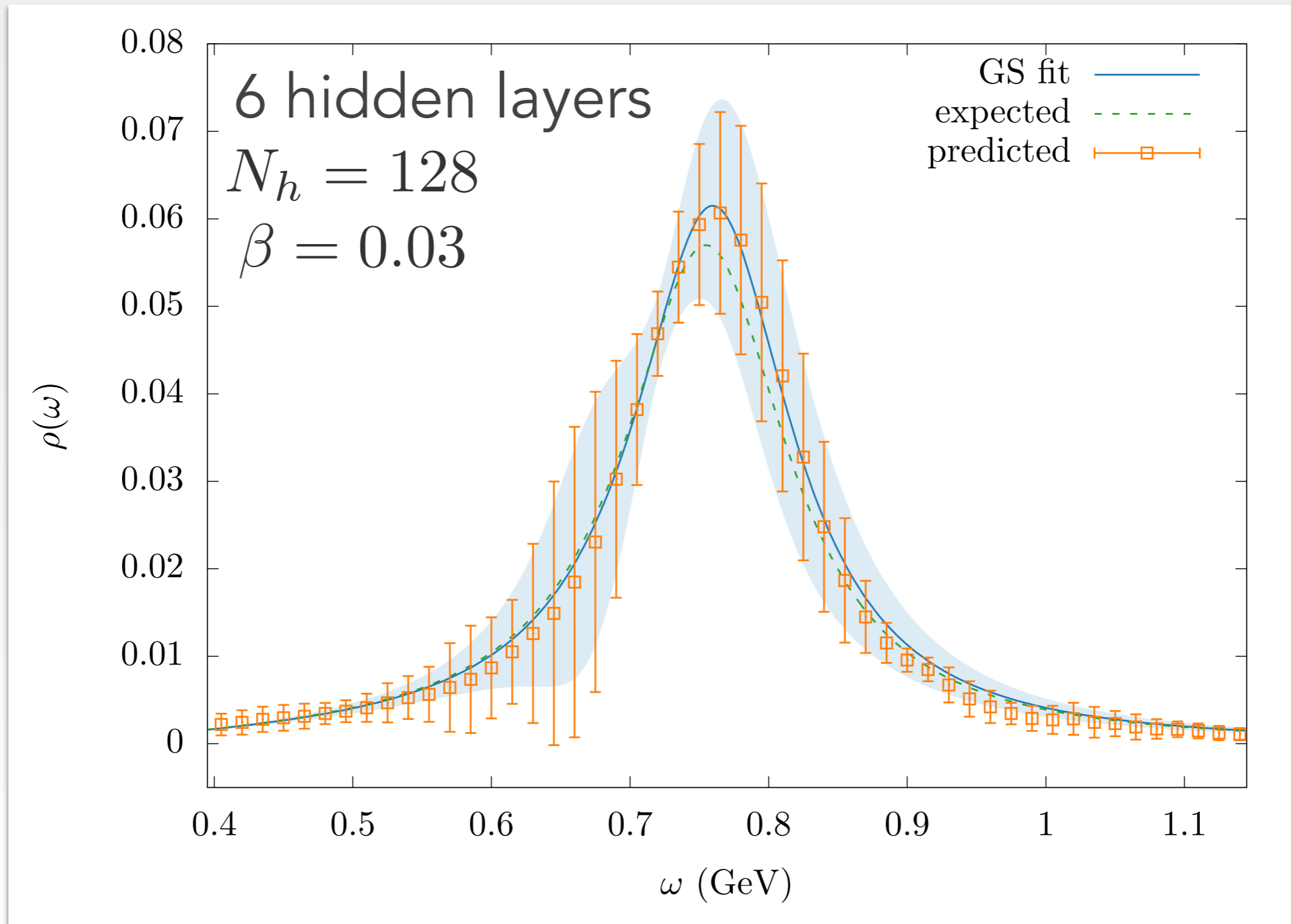
Synthetic lattice data



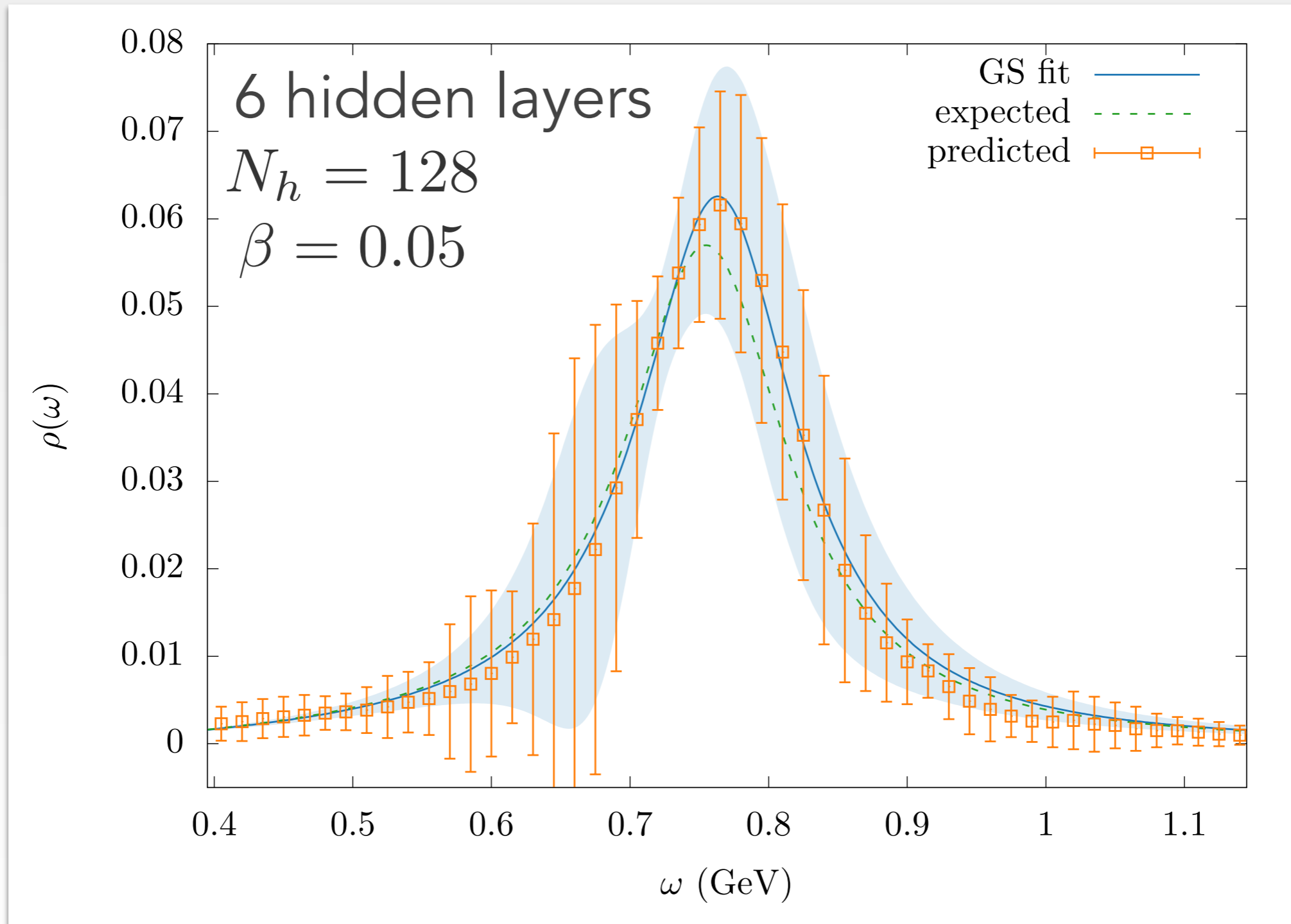
Prediction validation



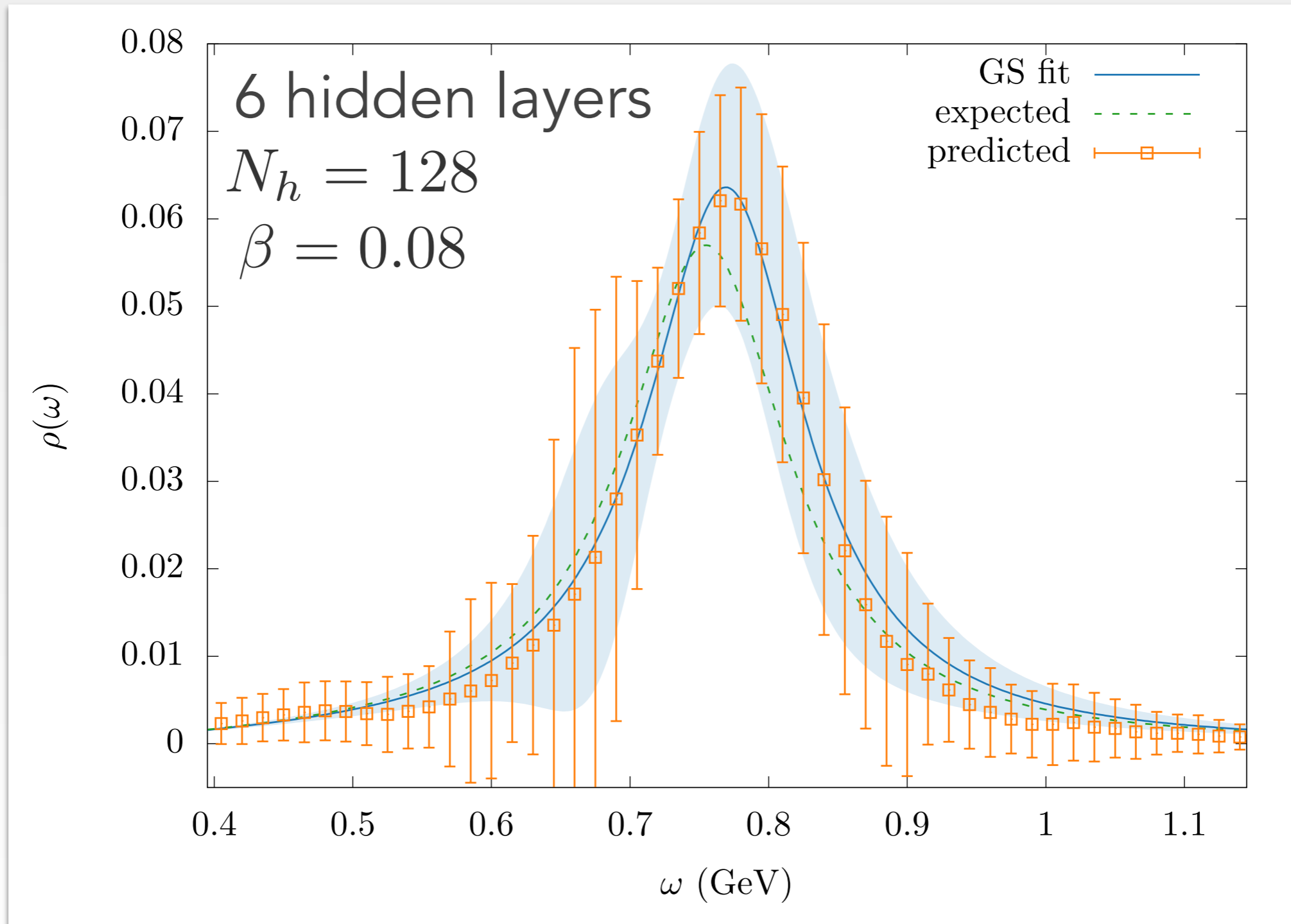
Prediction validation



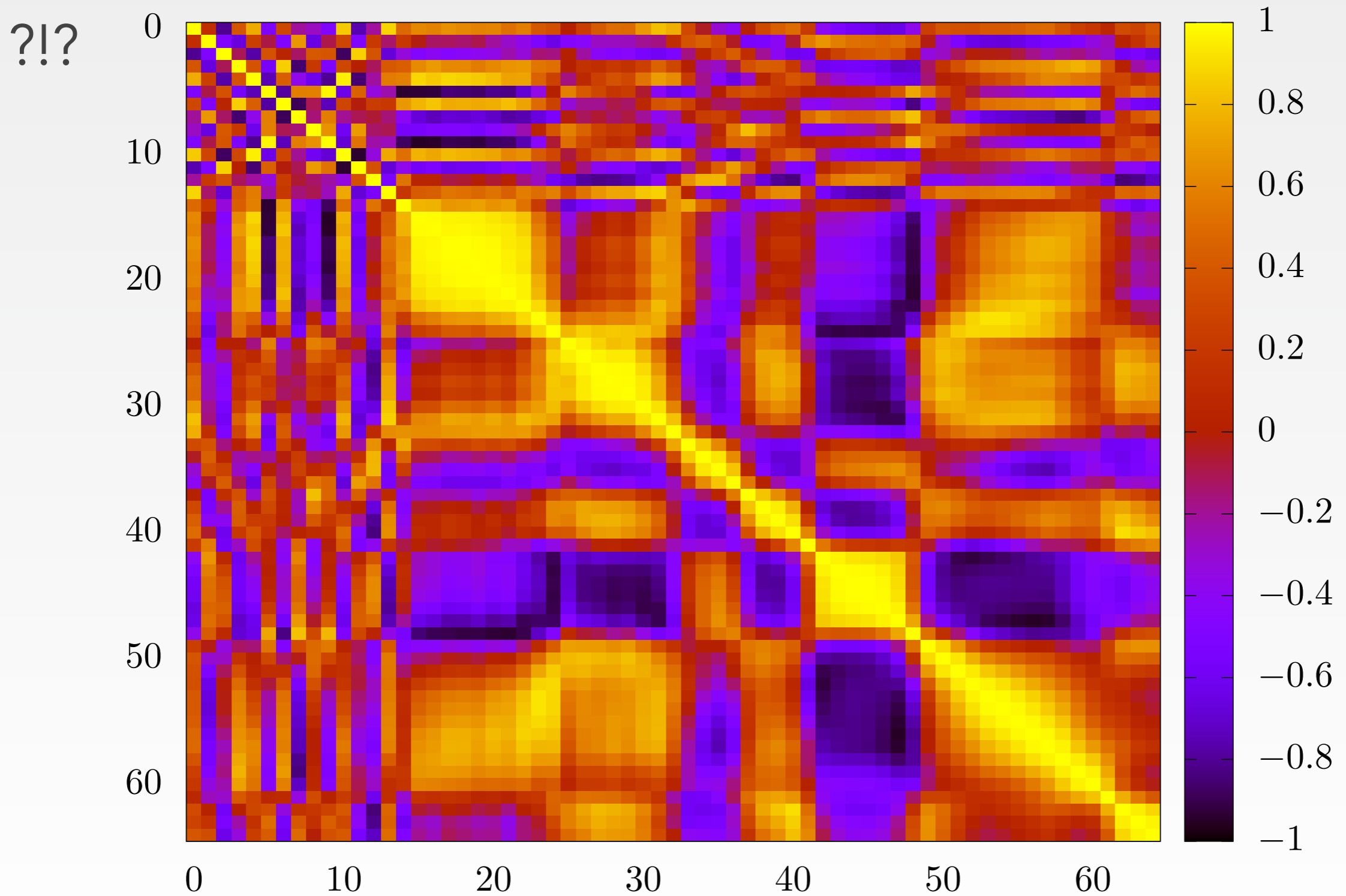
Prediction validation



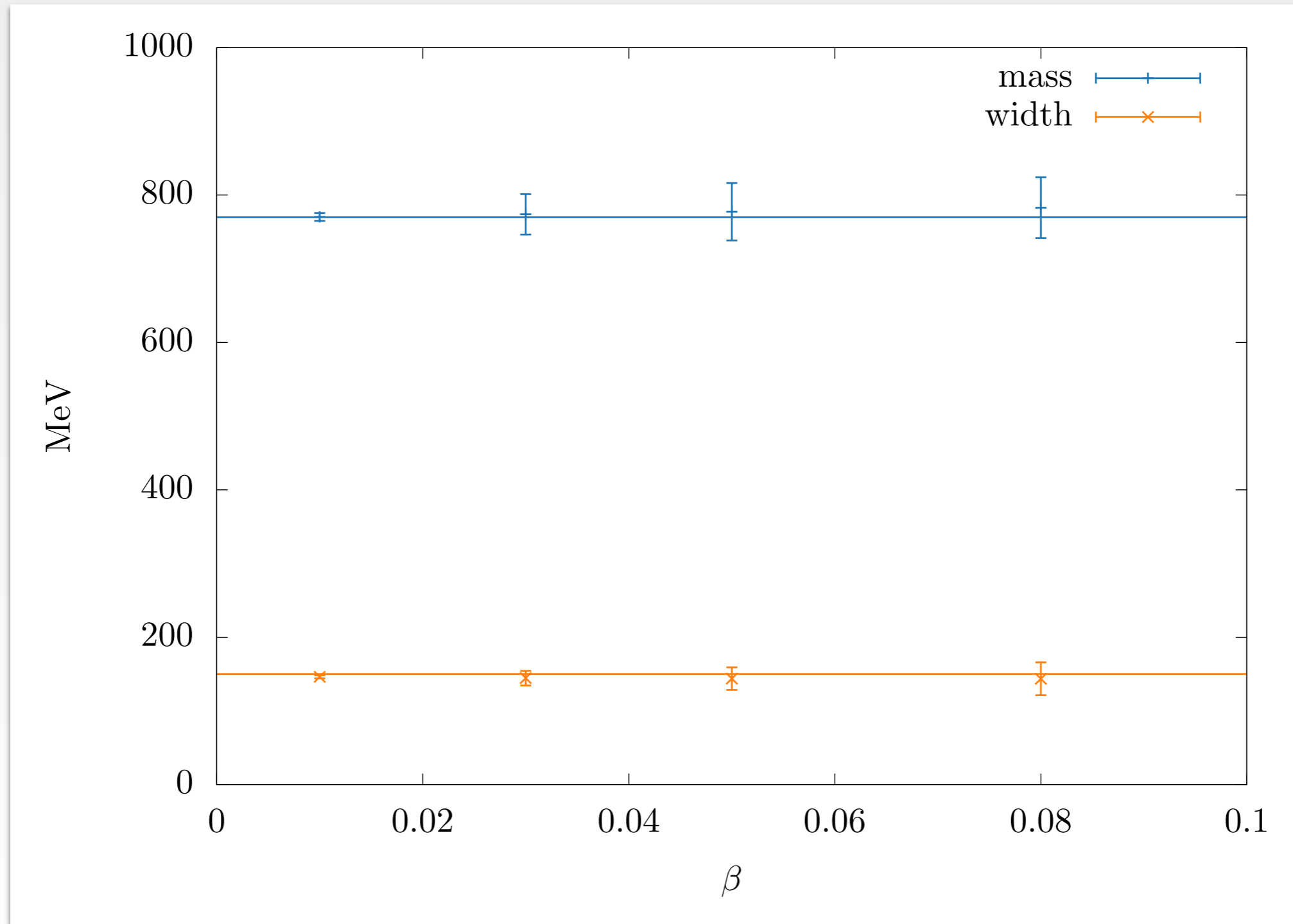
Prediction validation



Prediction correlations



Summary of prediction validations



Summary & perspectives

Summary

- ▶ Neural networks are an **attractive approach to inverse problems** for data analysis.
- ▶ Neural networks allow to **infer non-linear generalisations** to linear algorithms.
- ▶ Spectral reconstruction: possible for unsmearred density using **deep** neural networks.
- ▶ **Seems to survive an prediction test** using realistic synthetic Monte-Carlo data.

Perspectives

- ▶ Direct comparison to Backus-Gilbert techniques.
- ▶ Study of generalisation
(multi-peaks or even more arbitrary)
- ▶ Other approaches e.g. classifiers?
- ▶ Test on real large-volume lattice data.



Thank you!

Monument Valley 25/08/2019

Infinite-volume 2-pion contribution

- ▶ Amplitude and spectral measure separation

$$A(\omega_\alpha^2) = \sum_\mu |\langle 0 | J_\mu(0) | \alpha \rangle|^2 \quad \mu(s) = \int d\alpha \delta(\omega_\alpha^2 - s)$$

$$\rho(s) = \frac{1}{3s} A(s) \mu(s)$$

- ▶ 2-pion contribution

$$A_{\pi\pi}(s) = \frac{2}{\sqrt{s}} (s - 4M_\pi^2) |F_\pi(s)|^2 \quad \mu_{\pi\pi}(s) = \frac{1}{32\pi^2} (s - 4M_\pi^2)^{\frac{1}{2}}$$

$$\rho_{\pi\pi}(s) = \frac{1}{48\pi^3} \left(1 - \frac{4M_\pi^2}{s}\right)^{\frac{3}{2}} |F_\pi(s)|^2$$

Finite-volume 2-pion contribution

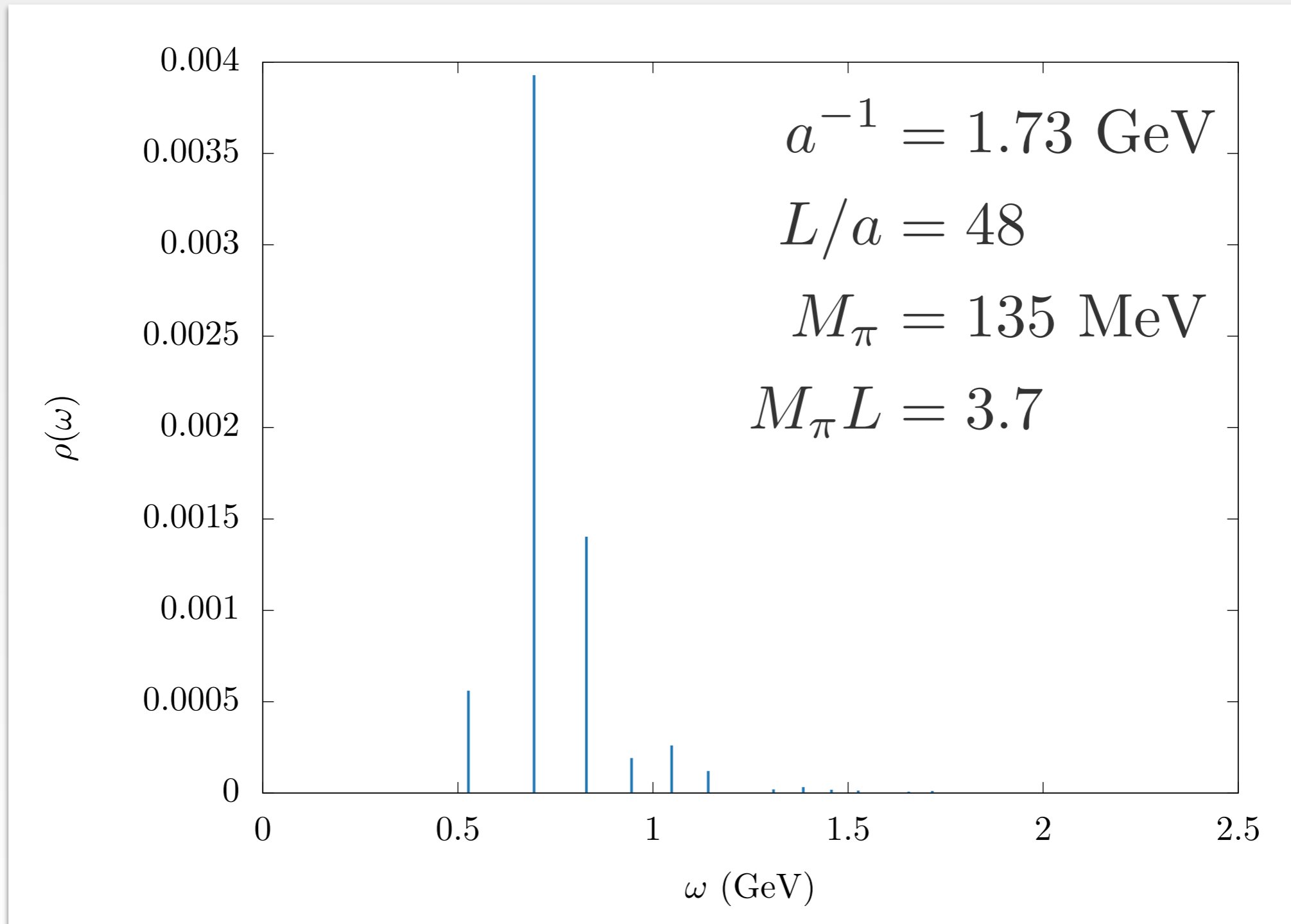
- ▶ Two assumptions:
 - 1) use free pions quantisation
 - 2) use infinite-volume amplitudes

Only accurate if $(M_\pi L)^{-3}$ can be neglected
(typically $M_\pi L \gtrsim 10$)

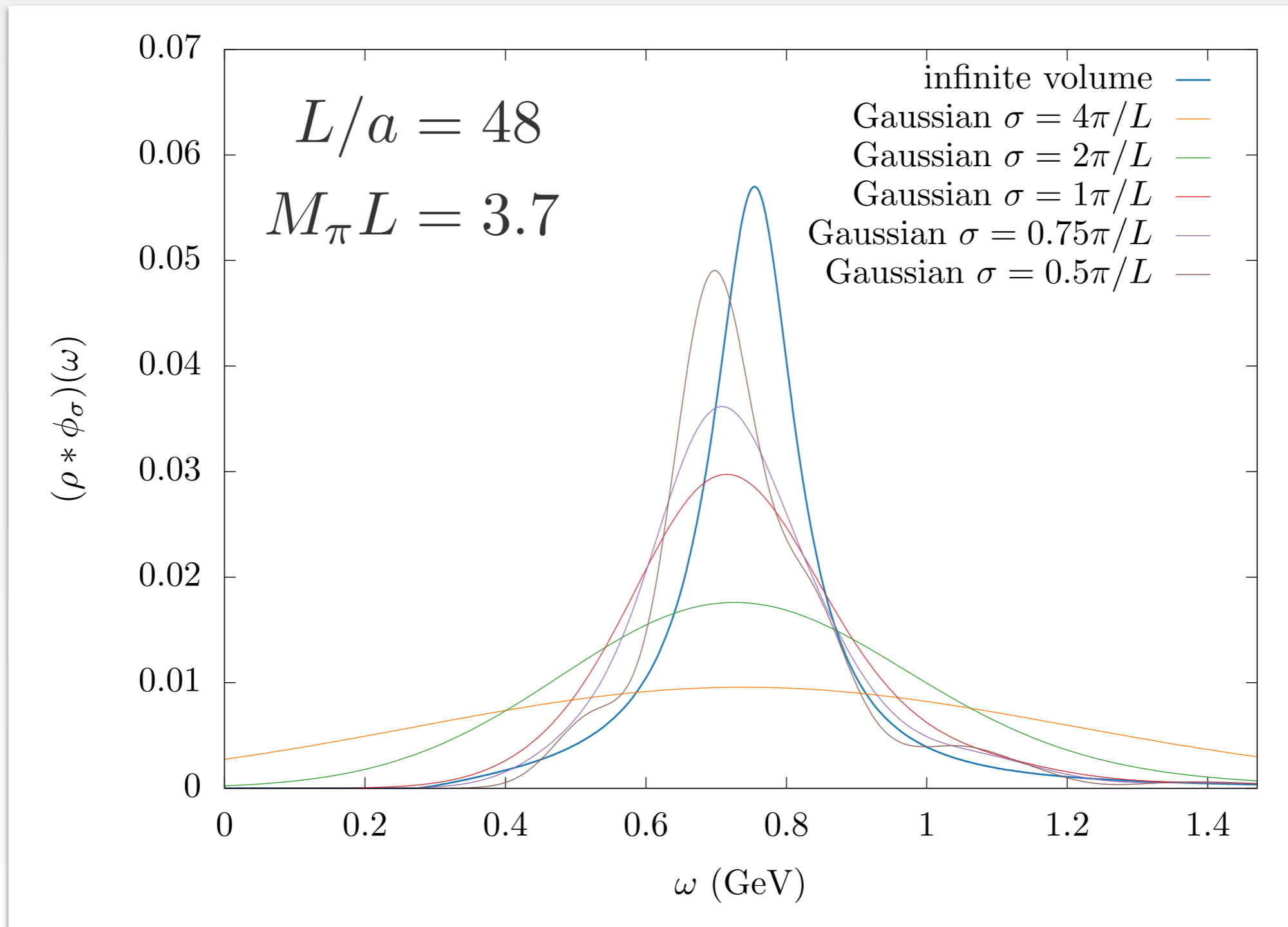
$$\mu_{\pi\pi,\text{FV}}(s) = \frac{1}{L^3} \sum_{n=0}^{+\infty} r_3(n) \delta\left[s - 4\omega_\pi\left(\frac{4\pi^2}{L^2}n\right)^2\right]$$

$$\rho_{\pi\pi,\text{FV}}(s) = \frac{2}{3L^3\sqrt{s}} \left(1 - \frac{4M_\pi^2}{s}\right) |F_\pi(s)|^2 \sum_{n=0}^{+\infty} r_3(n) \delta\left[s - 4\omega_\pi\left(\frac{4\pi^2}{L^2}n\right)^2\right]$$

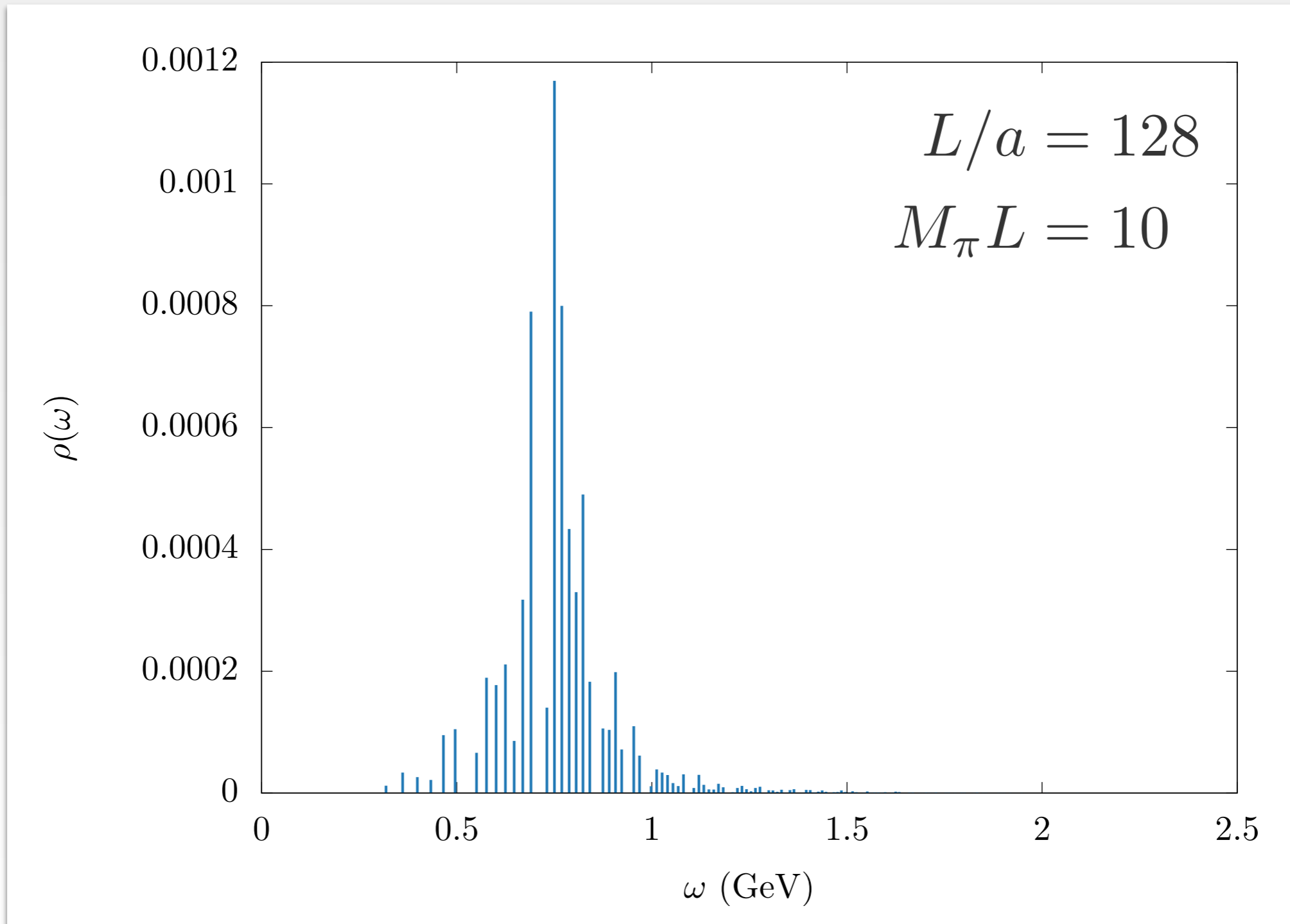
Finite-volume spectrum



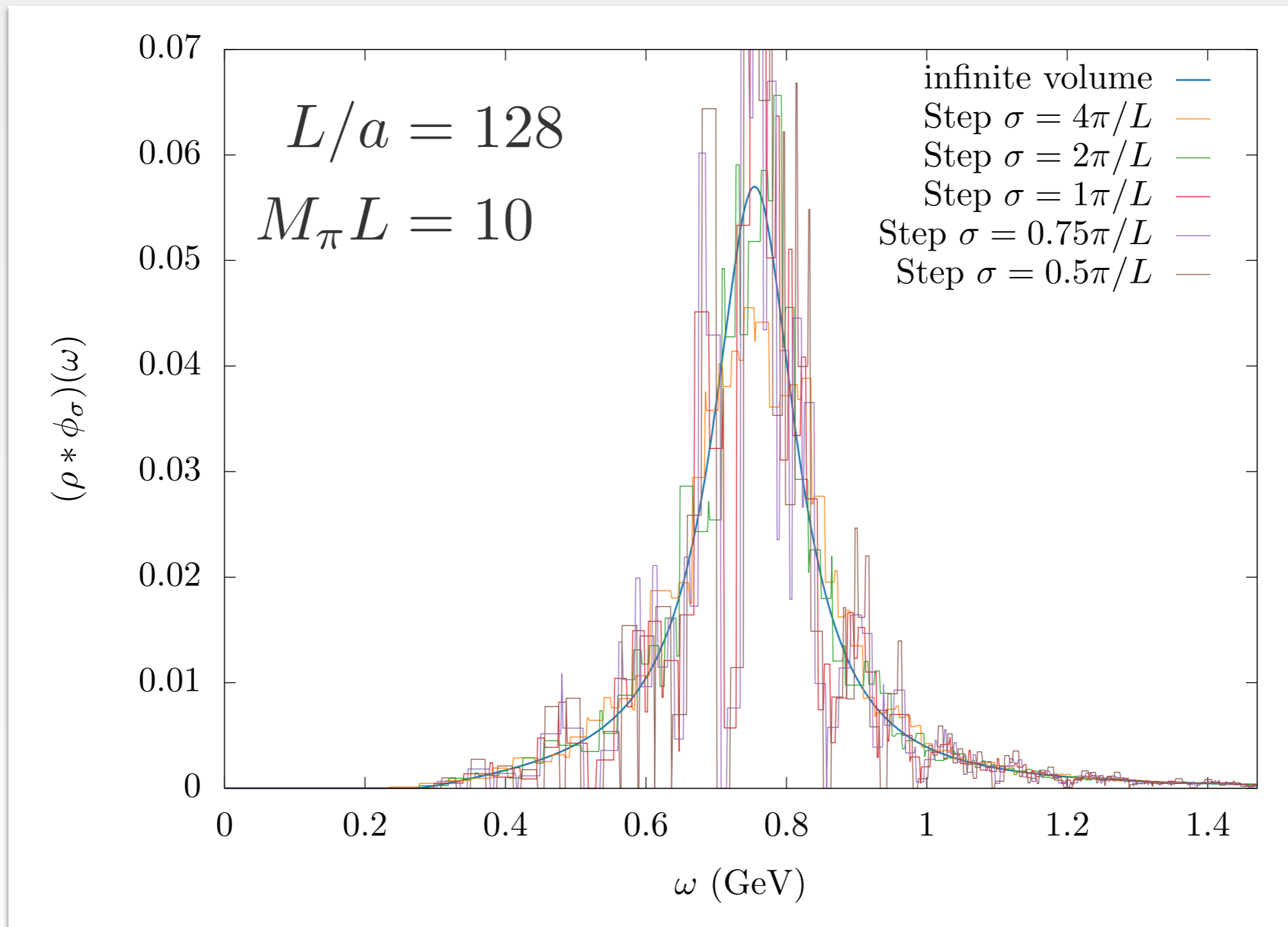
Finite-volume spectrum



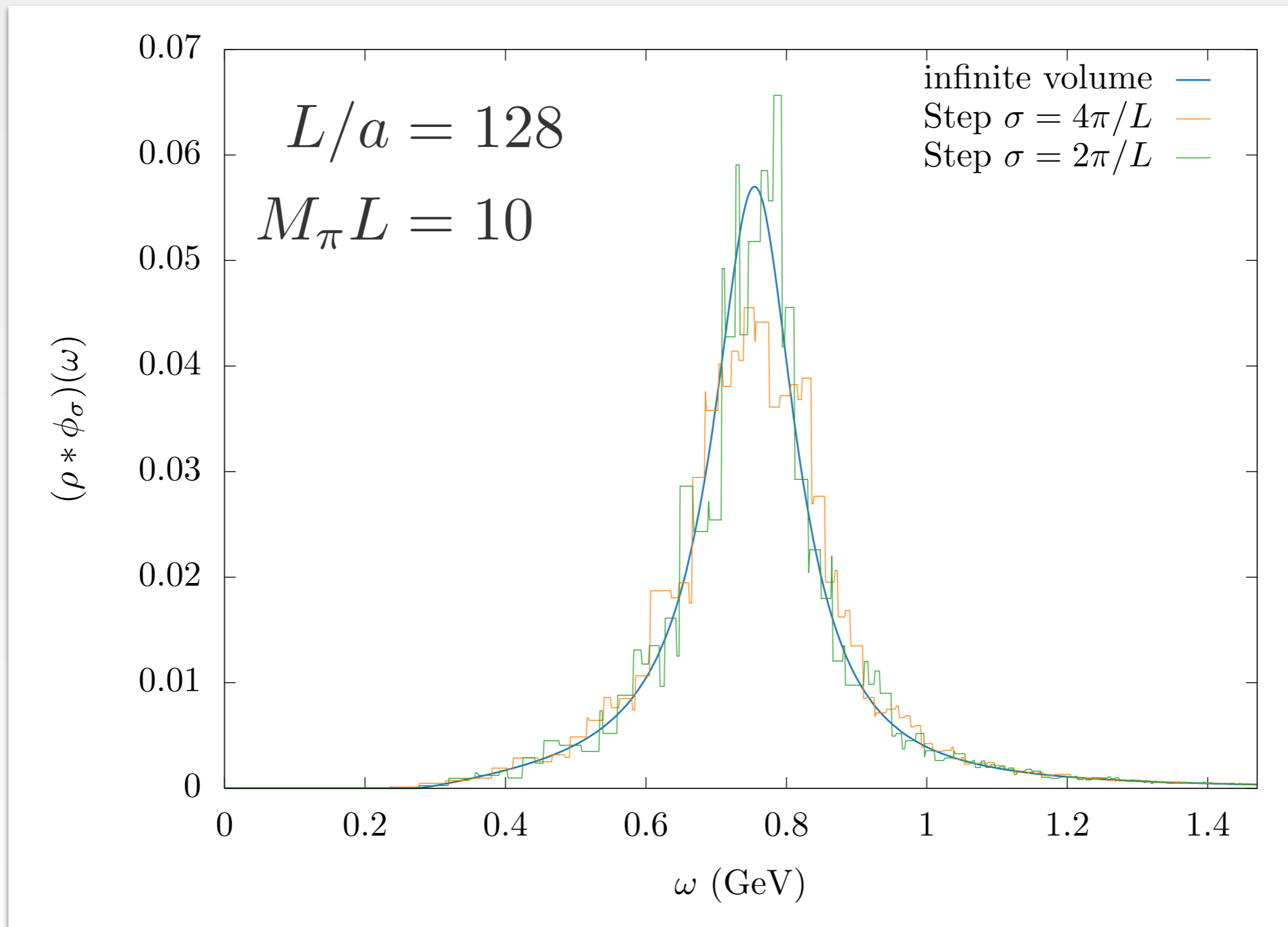
Finite-volume spectrum



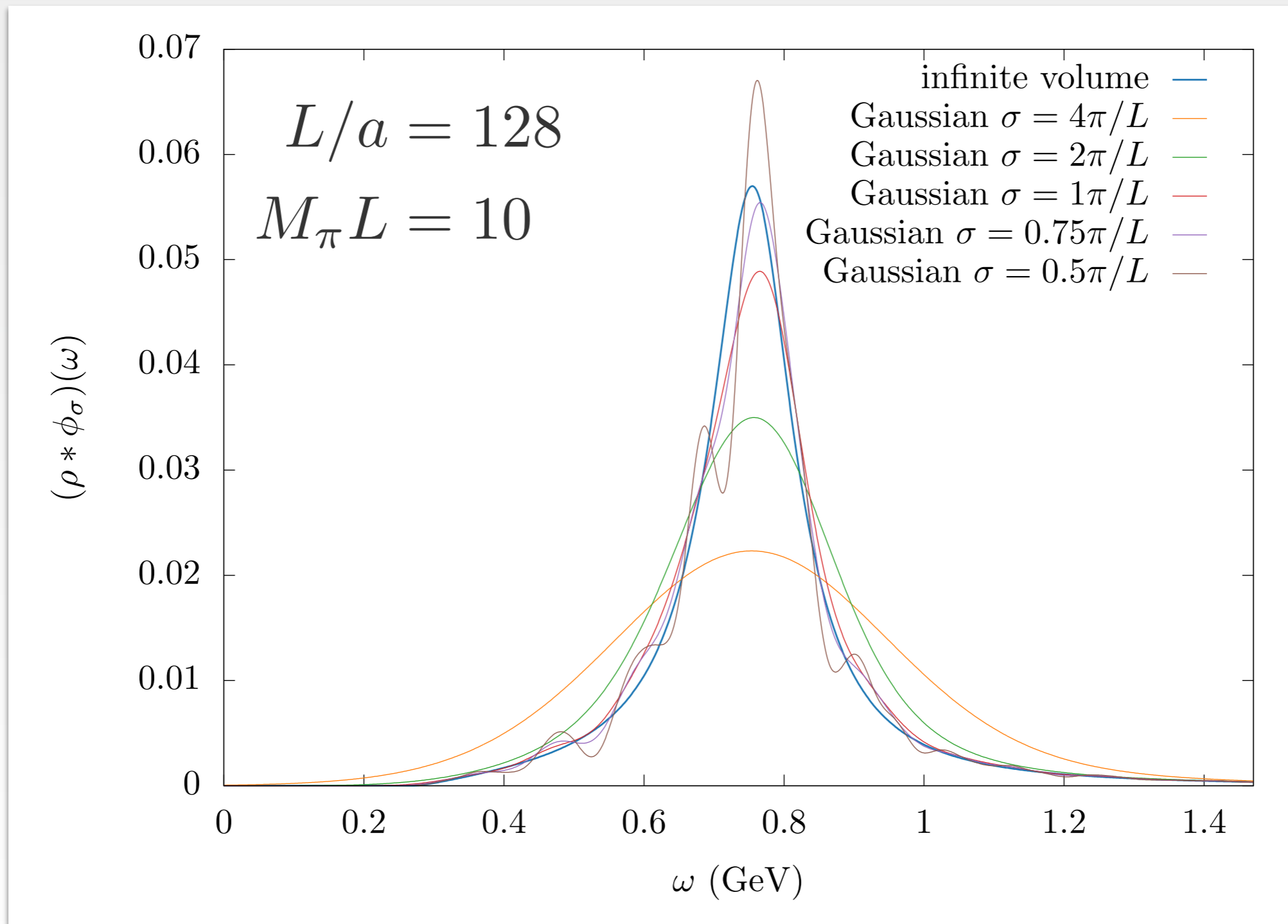
Finite-volume spectrum



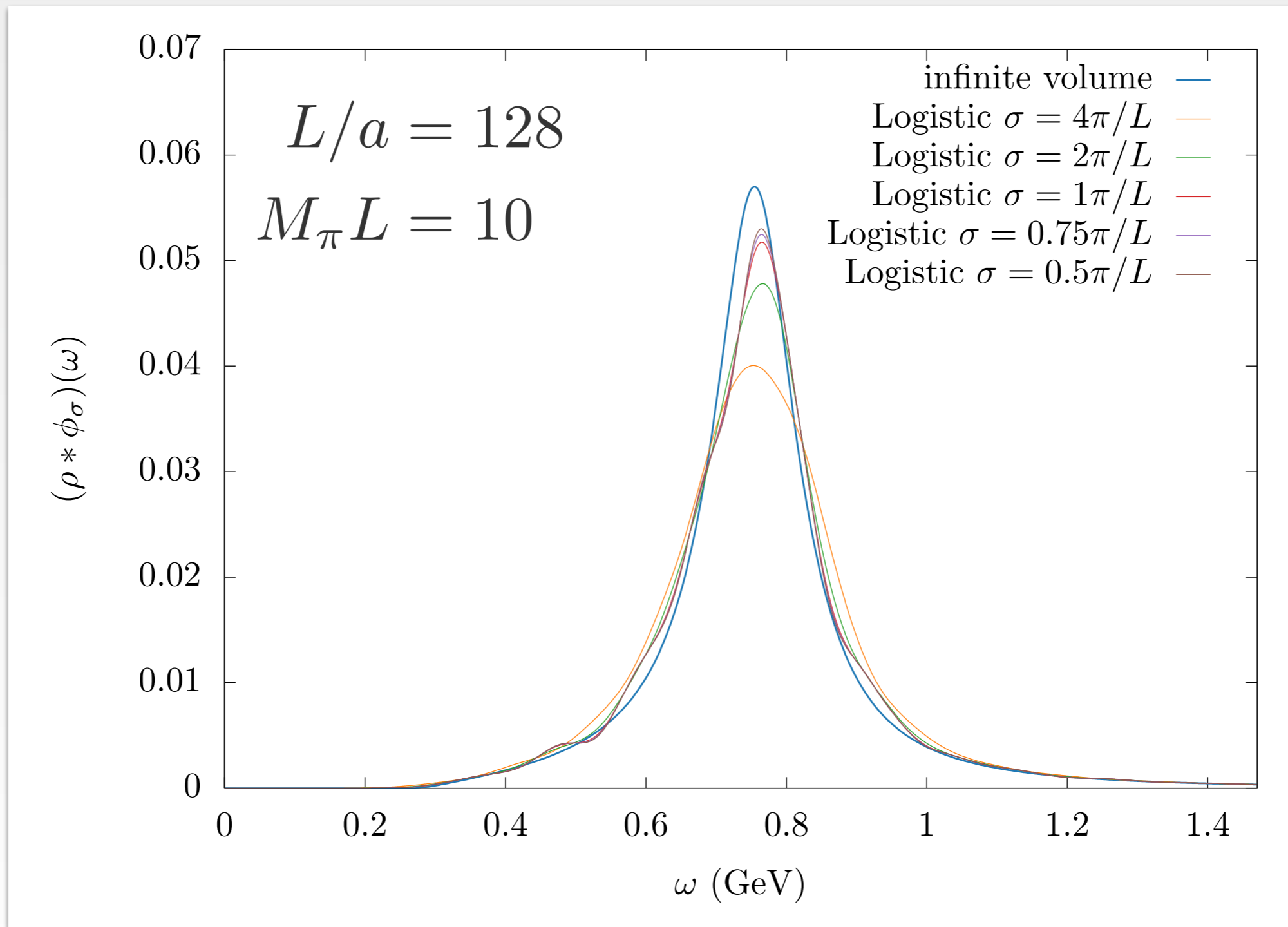
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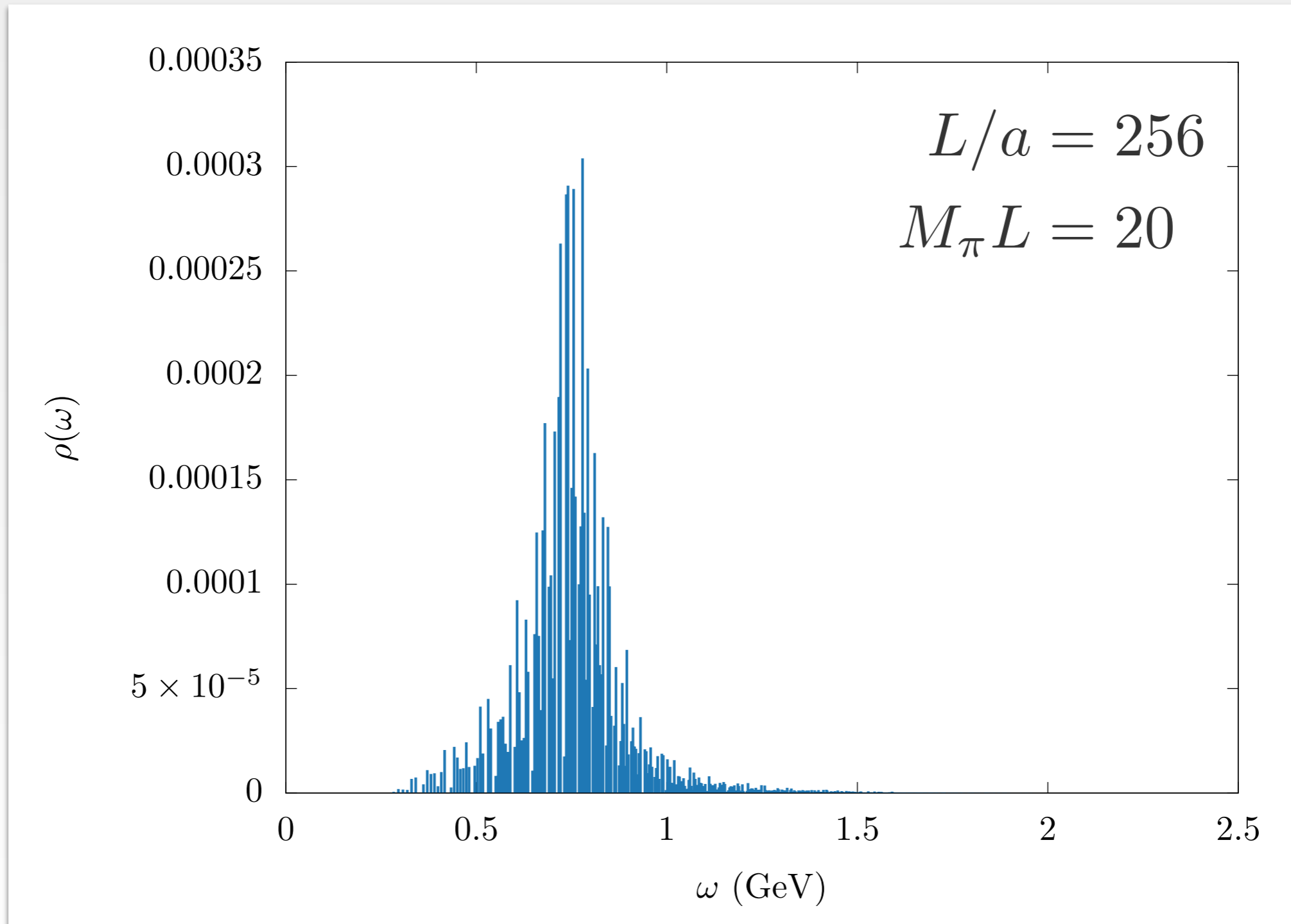
Finite-volume spectrum



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Finite-volume spectrum

