# Reconstructing QCD Spectral Functions with Gaussian Processes

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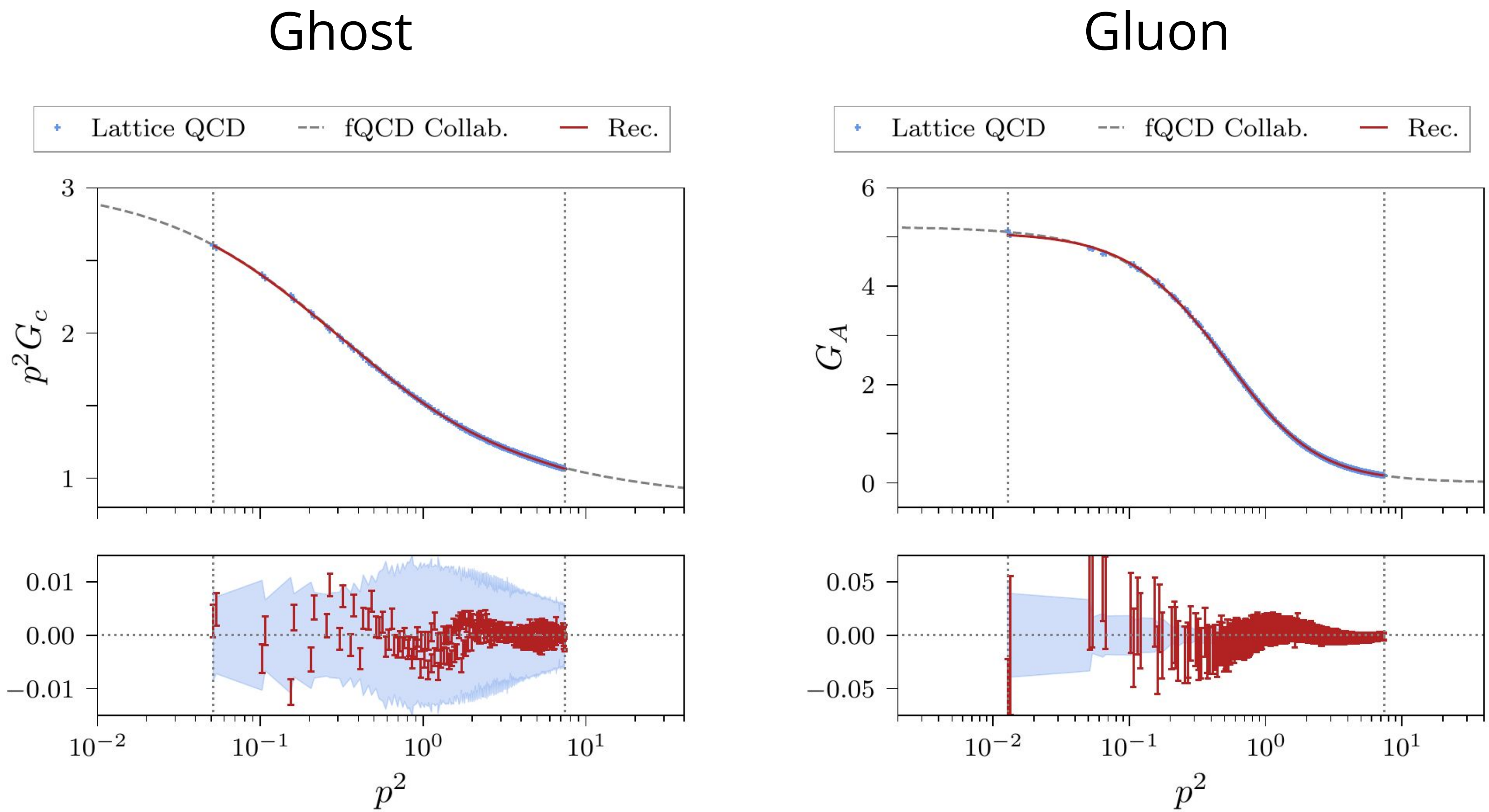
# Results Teaser



# Motivation

- Imaginary-time accessible via lattice and functional methods
- Real-time properties still notoriously difficult
- Applications
  - Hadronic resonance spectrum
  - Scattering processes
  - Transport & non-equilibrium phenomena in heavy-ion collisions

➔ From Euclidean to Minkowski
via spectral reconstruction

# Spectral Functions

- Spectral representation of two-point correlators

$$G(p_0) = \int_0^\infty \frac{\mathrm{d}\omega}{\pi} \frac{\omega \rho(\omega)}{\omega^2 + p_0^2} = \int_0^\infty \mathrm{d}\omega\, K(p_0, \omega)\, \rho(\omega)$$

$$\rho(\omega) = 2\,\mathrm{Im}\, G(-\mathrm{i}(\omega + \mathrm{i}0^+))$$

- Properties of the spectral function
  - Vanishing spectral weight: $\int_0^\infty \frac{\mathrm{d}\omega}{\pi} \omega \rho_{A/c}(\omega) = 0$
  - Decomposition into resonance peaks and continuous part:

$$\rho_c(\omega) = \frac{\pi}{Z_c} \frac{\delta(\omega)}{\omega} + \tilde{\rho}_c(\omega)\ , \quad \int_0^\infty \frac{\mathrm{d}\omega}{\pi}\, \omega\, \tilde{\rho}_c(\omega) = -\frac{1}{Z_c}$$

# Gaussian Process Regression

- GP describes distribution over functions

$$\rho(\omega) \sim \mathcal{GP}(\mu(\omega), C(\omega, \omega'))$$

- Multivariate Gaussian distribution for evaluation at specific nodes

$$\begin{pmatrix} \rho(\omega_1) \\ \vdots \\ \rho(\omega_N) \end{pmatrix} \sim \mathcal{N}\left( \begin{pmatrix} \mu(\omega_1) \\ \vdots \\ \mu(\omega_N) \end{pmatrix}, \begin{pmatrix} C(\omega_1,\omega_1) & \dots & C(\omega_1,\omega_N) \\ \vdots & \ddots & \vdots \\ C(\omega_N,\omega_1) & \dots & C(\omega_N,\omega_N) \end{pmatrix} \right)$$

- Joint distribution of observations and predictions

$$\begin{pmatrix} \rho(\omega) \\ \hat{\boldsymbol{\rho}} \end{pmatrix} \sim \mathcal{N}\left( \begin{pmatrix} \mu(\omega) \\ \hat{\boldsymbol{\mu}} \end{pmatrix}, \begin{pmatrix} C(\omega,\omega) & \hat{\mathbf{C}}^T(\omega) \\ \hat{\mathbf{C}}(\omega) & \hat{\mathbf{C}} + \sigma_n^2 \cdot \mathbf{1} \end{pmatrix} \right)$$

$$\hat{\mu} \equiv \mu(\hat{\omega}_i),\ \hat{\mathbf{C}}_i(\omega) \equiv C(\hat{\omega}_i, \omega),\ \hat{\mathbf{C}}_{ij} \equiv C(\hat{\omega}_i, \hat{\omega}_j)$$

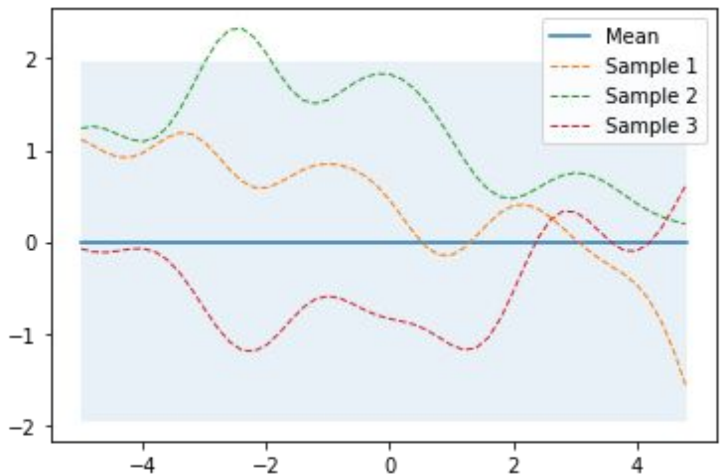
- Conditional distribution of predictions given observations

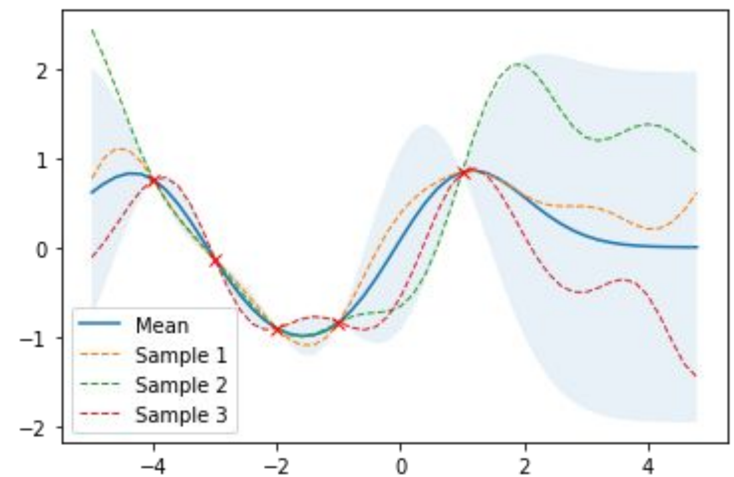
$$\rho(\omega)|\hat{\rho} \sim \mathcal{N}\left( \mu(\omega) + \hat{\mathbf{C}}^T(\omega) \left(\hat{\mathbf{C}} + \sigma_n^2 \cdot \mathbf{1}\right)^{-1} (\hat{\boldsymbol{\rho}} - \hat{\mu}) ,\right. \\ \left. C(\omega,\omega) - \hat{\mathbf{C}}^T(\omega) \left(\hat{\mathbf{C}} + \sigma_n^2 \cdot \mathbf{1}\right)^{-1} \hat{\mathbf{C}}(\omega) \right)$$

# Gaussian Process Regression

$$\rho(\omega) \sim \mathcal{GP}(\mu(\omega), C(\omega, \omega'))$$

$$\rho(\omega)|\hat{\rho} \sim \mathcal{N}\left(\mu(\omega) + \hat{\mathbf{C}}^T(\omega)\left(\hat{\mathbf{C}} + \sigma_n^2 \cdot \mathbf{1}\right)^{-1}(\hat{\boldsymbol{\rho}} - \hat{\mu})\,, \right.$$
$$\left. C(\omega,\omega) - \hat{\mathbf{C}}^T(\omega)\left(\hat{\mathbf{C}} + \sigma_n^2 \cdot \mathbf{1}\right)^{-1}\hat{\mathbf{C}}(\omega)\right)$$



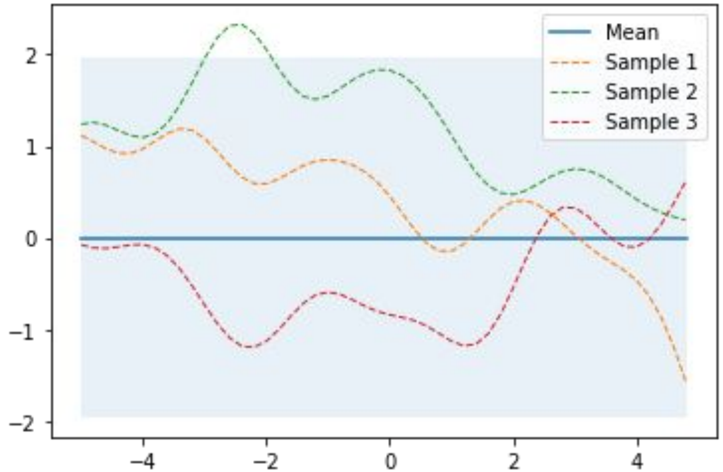

(without observational noise)

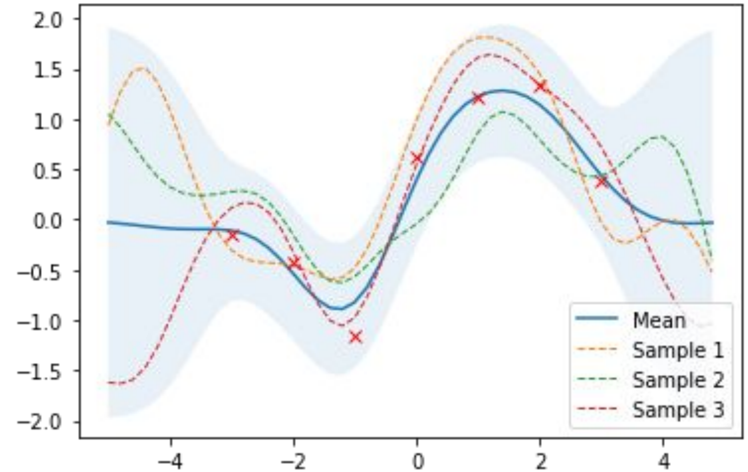
krasserm.github.io/2018/03/19/gaussian-processes/

# Gaussian Process Regression

$$\rho(\omega) \sim \mathcal{GP}(\mu(\omega), C(\omega, \omega'))$$

$$\rho(\omega)|\hat{\rho} \sim \mathcal{N}\left(\mu(\omega) + \hat{\mathbf{C}}^T(\omega)\left(\hat{\mathbf{C}} + \sigma_n^2 \cdot \mathbf{1}\right)^{-1}(\hat{\boldsymbol{\rho}} - \hat{\mu}) \;, \right.$$
$$\left. C(\omega, \omega) - \hat{\mathbf{C}}^T(\omega)\left(\hat{\mathbf{C}} + \sigma_n^2 \cdot \mathbf{1}\right)^{-1}\hat{\mathbf{C}}(\omega)\right)$$




(with observational noise)

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# Spectral Reconstruction with GPR

- Gaussian process for spectral function

$$\rho(\omega) \sim \mathcal{GP}(\mu(\omega), C(\omega, \omega'))$$

- Gaussian distribution for correlator via KL integral

$$G_i \sim \mathcal{N}\Big(\int \mathrm{d}\omega \;\, K(p_i, \omega)\mu(\omega),$$
$$\int \mathrm{d}\omega\, \mathrm{d}\omega' K(p_i, \omega) C(\omega, \omega') K(p_j, \omega')\Big)$$
$$\equiv \mathcal{N}(\tilde{\mu}_i, \tilde{C}_{ij})$$

- Inverse inference step

$$\rho(\omega)\,|\,G_i \sim \mathcal{GP}\Big(\mu(\omega) +$$
$$\sum_{i,j=1}^{N_G} \int \mathrm{d}\omega' \, K(p_i, \omega') C(\omega', \omega) \left(\tilde{C} + \sigma_n^2 \cdot \mathbf{1}\right)^{-1}_{ij} (G_j - \tilde{\mu}_j)$$
$$C(\omega, \omega') - \sum_{i,j=1}^{N_G} \int \mathrm{d}\omega' \mathrm{d}\omega'' \, K(p_i, \omega') C(\omega', \omega)$$
$$\left(\tilde{C} + \sigma_n^2 \cdot \mathbf{1}\right)^{-1}_{ij} K(p_j, \omega'') C(\omega'', \omega)\Big)$$

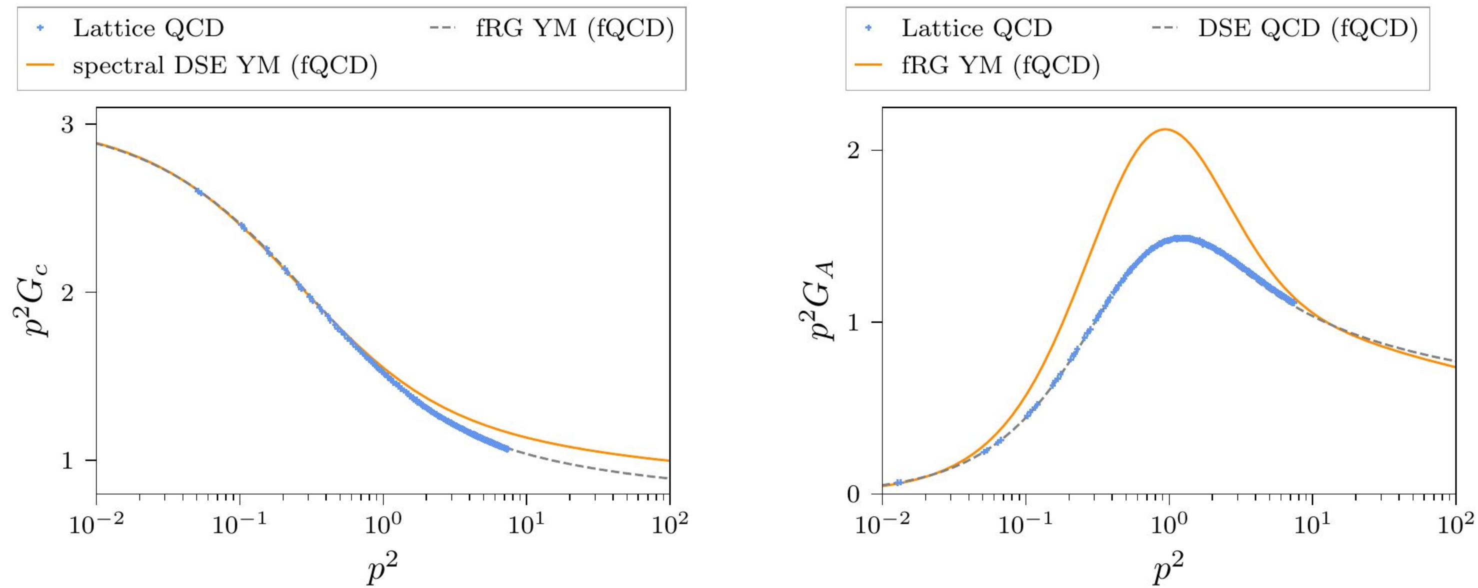
- Kernel parametrization, e.g. radial basis function

$$C(\omega, \omega') = \sigma_C^2 \, \exp(-\frac{(\omega - \omega')^2}{2l^2})$$

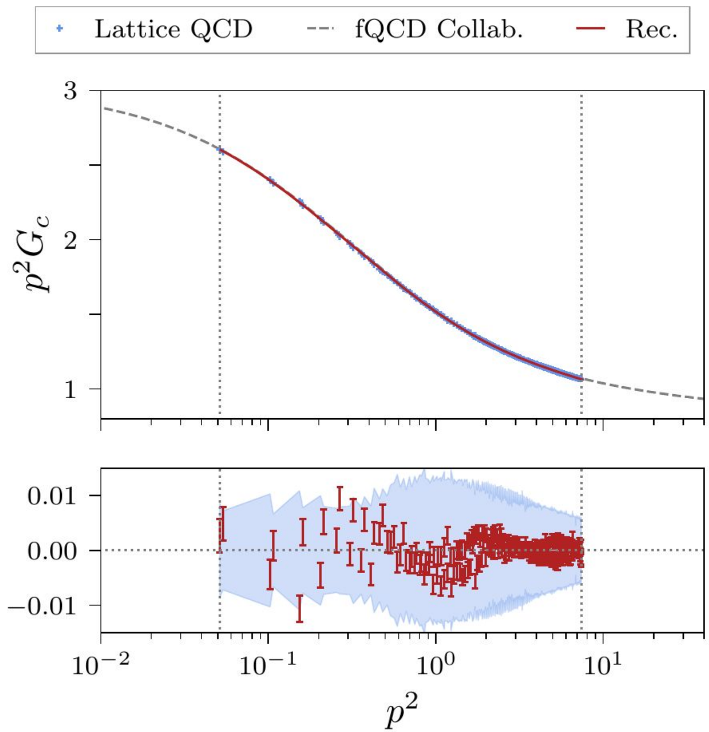
Further details: doi:10.1093/gji/ggz520

# Input Data & Benchmarks

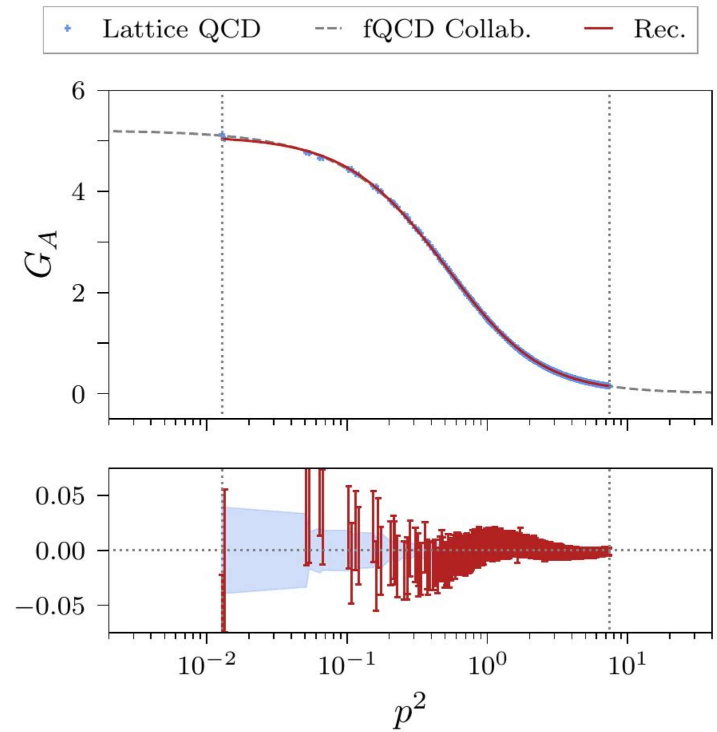
- Lattice: 2+1 flavor, Iwasaki + DWF, $m_\pi$ = 139 MeV, courtesy of RBC/UKQCD collab.
  1902.08148,1912.08232
- Functional: 2+1 flavor & Yang-Mills, DSE & fRG, courtesy of fQCD collab.
  1605.01856,1706.06326,1804.00945,1909.02991,2002.07500,2102.13053,2103.16175



# Results

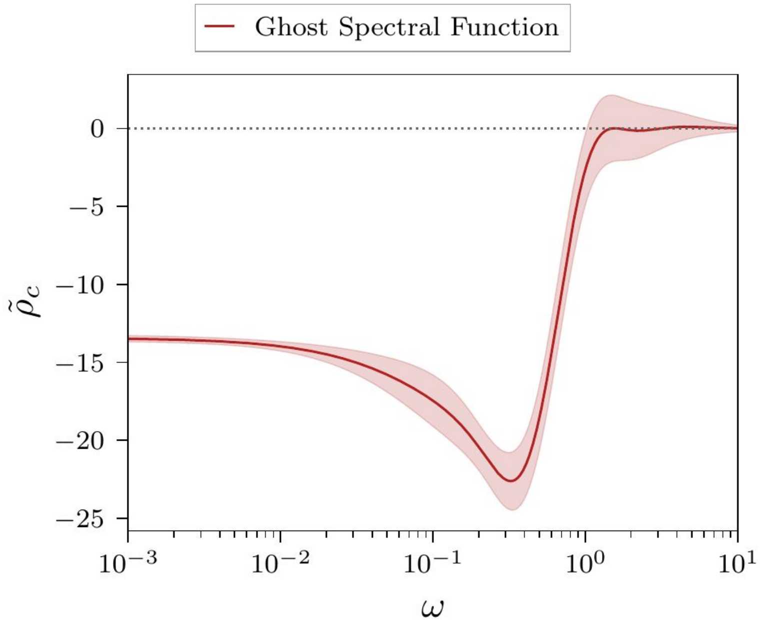


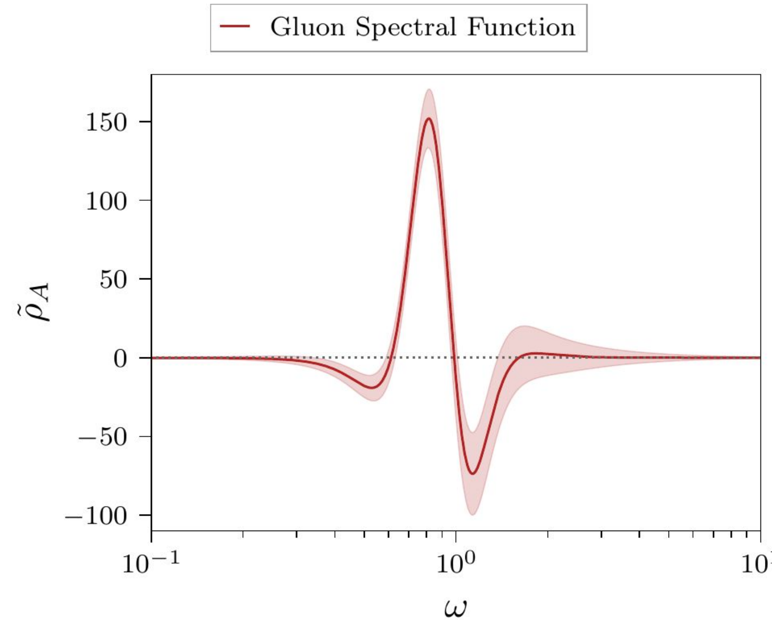

MSE: ~5e-6



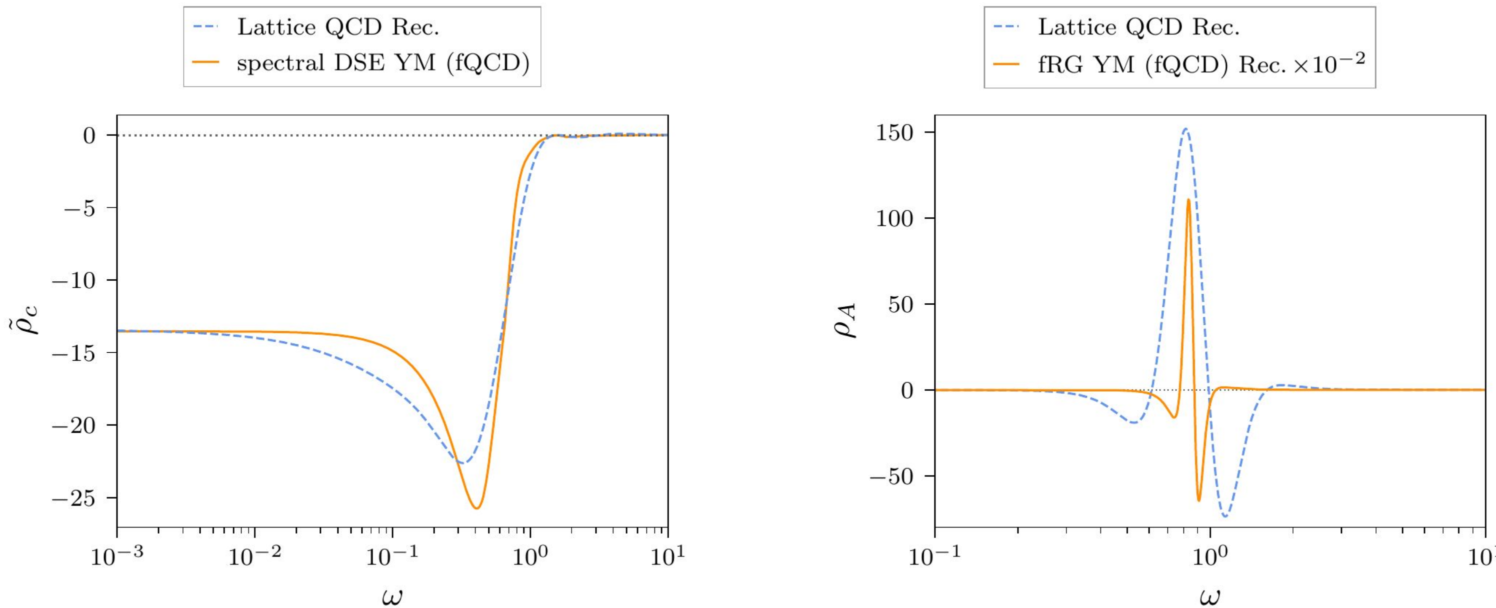

MSE: ~4e-5

# Results


Ghost Spectral Function
$\tilde{\rho}_c$
0
−5
−10
−15
−20
−25
$10^{-3}$
$10^{-2}$
$10^{-1}$
$10^{0}$
$10^{1}$
$\omega$


Gluon Spectral Function
$\tilde{\rho}_A$
150
100
50
0
−50
−100
$10^{-1}$
$10^{0}$
$10^{1}$
$\omega$

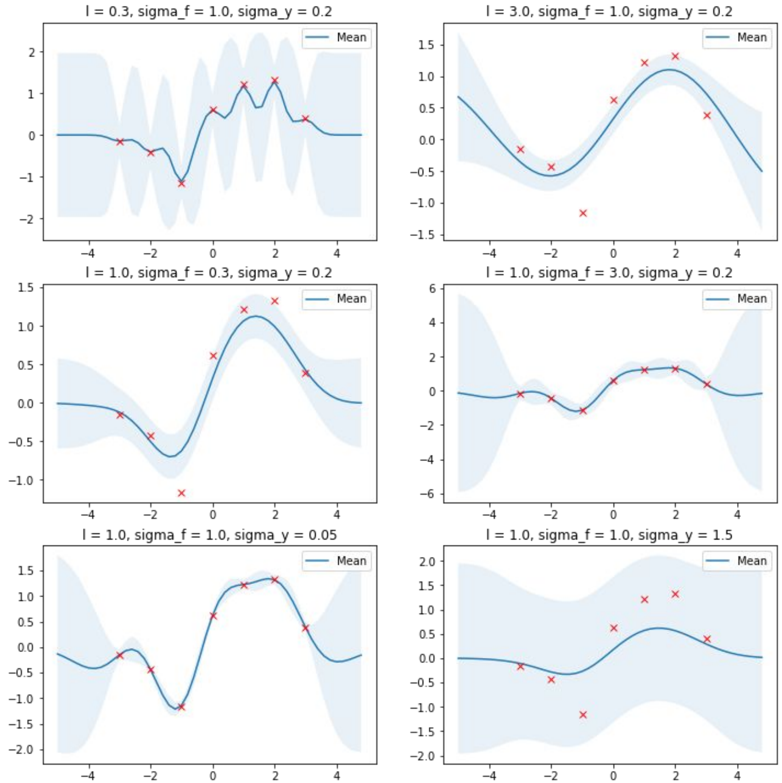
# Comparison to Yang-Mills Results



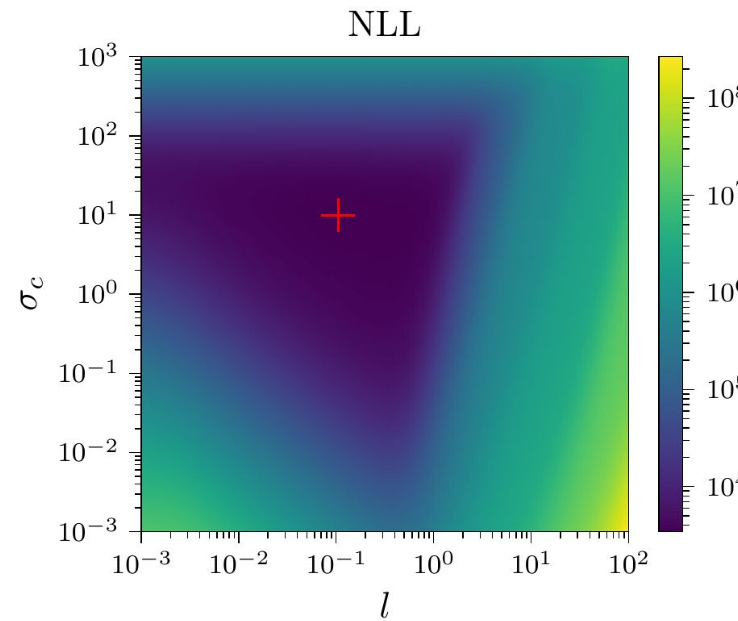

- Leading peak positions of the gluon spectral function:

  QCD: ω ~ 0.818, Yang-Mills: ω ~ 0.835

# Hyperparameter Optimization




$$p(\hat{\boldsymbol{\rho}}|\boldsymbol{\alpha}) = \left((2\pi)^N \det\left(\hat{\mathbf{C}}_\alpha + \sigma_n^2 \cdot \mathbf{1}\right)\right)^{-\frac{1}{2}} \cdot \exp\left(-\frac{1}{2}(\hat{\boldsymbol{\rho}} - \hat{\boldsymbol{\mu}})^T \left(\hat{\mathbf{C}}_{\boldsymbol{\alpha}} + \sigma_n^2 \cdot \mathbf{1}\right)^{-1} (\hat{\boldsymbol{\rho}} - \hat{\boldsymbol{\mu}})\right)$$



# Outlook

- Building blocks of diagrammatic representations for transport coefficients, bound state equations (Bethe-Salpeter, Faddeev)
- First-principle QCD inputs for phenomenological approaches to transport processes
- Improvements to reconstruction approach: custom kernels, hyperkernels, deep kernel learning, hyperpriors, derivatives

Next steps: quark spectral functions & finite temperature

Thank you!