

Real-time dynamics via spectral reconstruction: Introducing a general framework based on Gaussian process regression

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Why Spectral Reconstruction?

- Real-time calculations are hard
- Lattice: sign problem
- Functional methods: conceptually possible, still hard

- Källén-Lehmann spectral representation

$$G_E(p^2) = \int_0^\infty \frac{d\omega}{\pi} \frac{\omega}{\omega^2 + p^2} \rho(\omega)$$

- Extracting $\rho(\omega)$ by inversion is ill-conditioned for discrete and noisy data
⇒ need of regularization, preferably motivated by physics
- Desirable: incorporation of additional prior information in the form of constraints and biases

Gaussian Process Regression

- Describe the spectral function $\rho(\omega)$ by a Gaussian process \mathcal{GP} prior

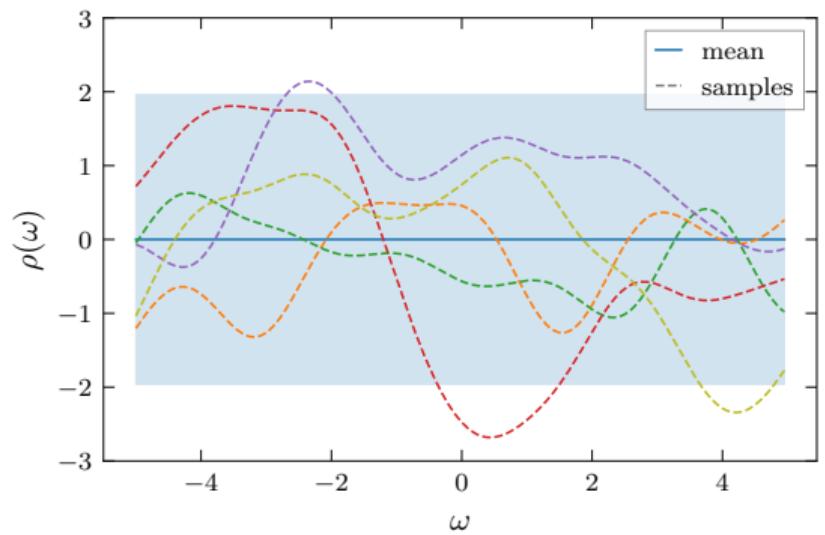
$$\rho(\omega) \sim \mathcal{GP}(\mu(\omega), C(\omega, \omega'))$$

- GPs are normal distributions in *function* space
- GPs are the infinite dimensional extension of multivariate Gaussian distributions
- Finite dimensional subset of the GP at distinct points $\omega_1, \dots, \omega_N$

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

$$\mu(\omega) = 0,$$

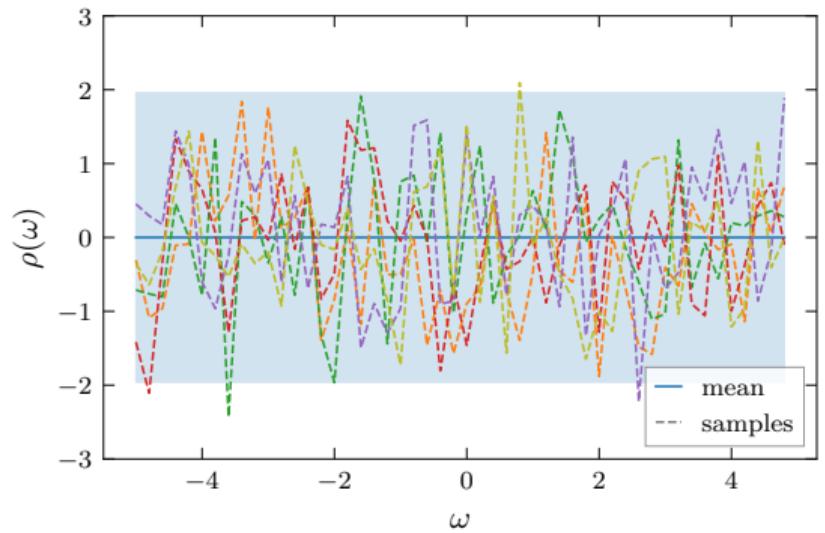
$$C(\omega, \omega') = \sigma^2 \exp\left(-\frac{(\omega - \omega')^2}{2\ell^2}\right)$$



Gaussian Process Regression

$$\mu(\omega) = 0,$$

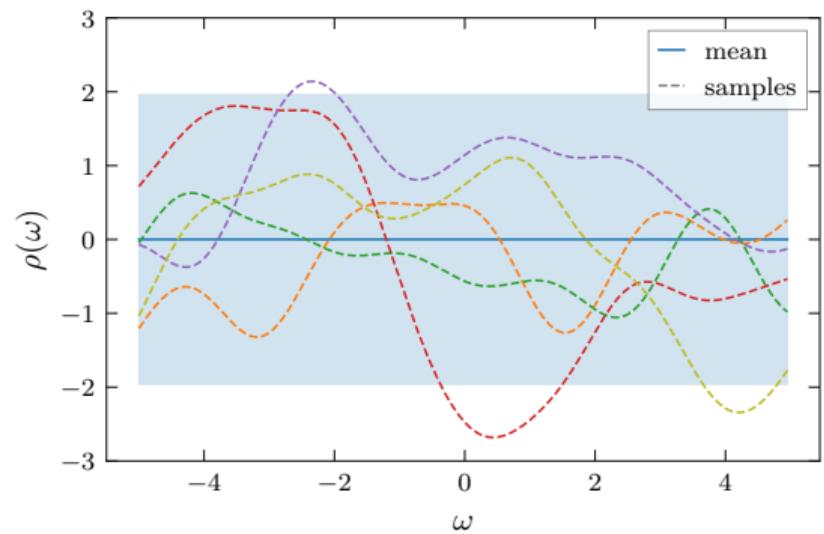
$$C(\omega, \omega') = \sigma^2 \delta(\omega - \omega')$$



$$\mu(\omega) = 0,$$

$$C(\omega, \omega') = \sigma^2 \exp\left(-\frac{(\omega - \omega')^2}{2\ell^2}\right)$$

RBF Kernel



Joint distribution of observations $\hat{\rho}(\hat{\omega})$ and predictions $\rho(\omega)$

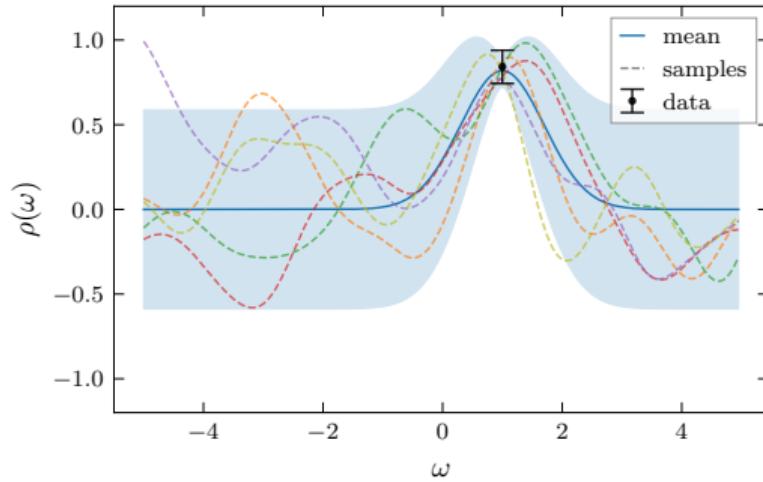
$$\begin{pmatrix} \rho(\omega) \\ \hat{\rho} \end{pmatrix} \sim \mathcal{N} \left(\begin{pmatrix} \mu(\omega) \\ \hat{\mu} \end{pmatrix}, \begin{pmatrix} C(\omega, \omega) & \hat{C}^\top(\omega) \\ \hat{C}(\omega) & \hat{C} + \sigma_n^2 \mathbb{1} \end{pmatrix} \right)$$

with $\hat{C}_i(\omega) = C(\hat{\omega}_i, \omega)$, $\hat{C}_{ij} = C(\hat{\omega}_i, \hat{\omega}_j)$.

GP Posterior has closed analytic form

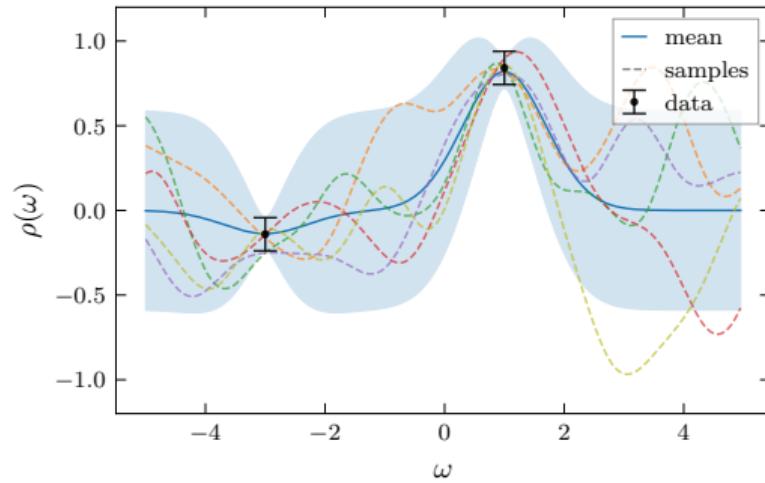
$$\begin{aligned} \rho(\omega) | \hat{\rho} &\sim \mathcal{N} \left(\hat{C}^\top(\omega) \left(\hat{C} + \sigma_n^2 \mathbb{1} \right)^{-1} \hat{\rho}, \right. \\ &\quad \left. C(\omega, \omega) - \hat{C}^\top(\omega) \left(\hat{C} + \sigma_n^2 \mathbb{1} \right)^{-1} \hat{C}(\omega) \right) \end{aligned}$$

Gaussian Process Regression - Prediction



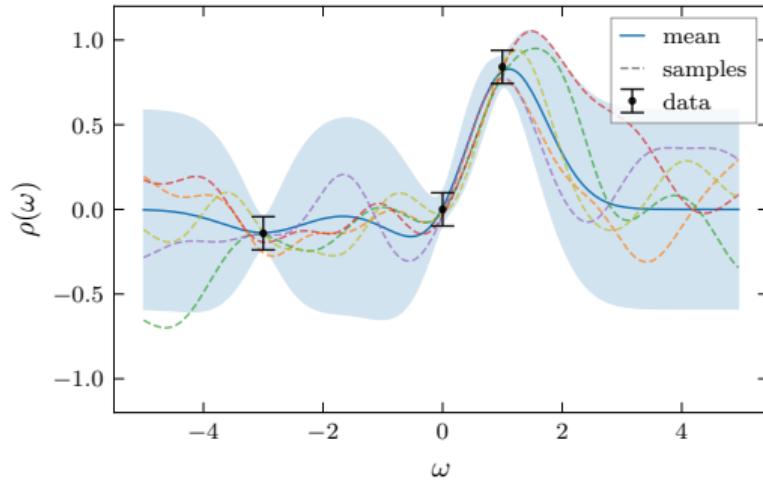
$$\rho(\omega)|\hat{\rho} \sim \mathcal{N}\left(\underbrace{\hat{C}^\top(\omega) (\hat{C} + \sigma_n^2 \mathbb{1})^{-1} \hat{\rho}}_{\text{mean}}, \underbrace{C(\omega, \omega) - \hat{C}^\top(\omega) (\hat{C} + \sigma_n^2 \mathbb{1})^{-1} \hat{C}(\omega)}_{\text{covariance}}\right)$$

Gaussian Process Regression - Prediction



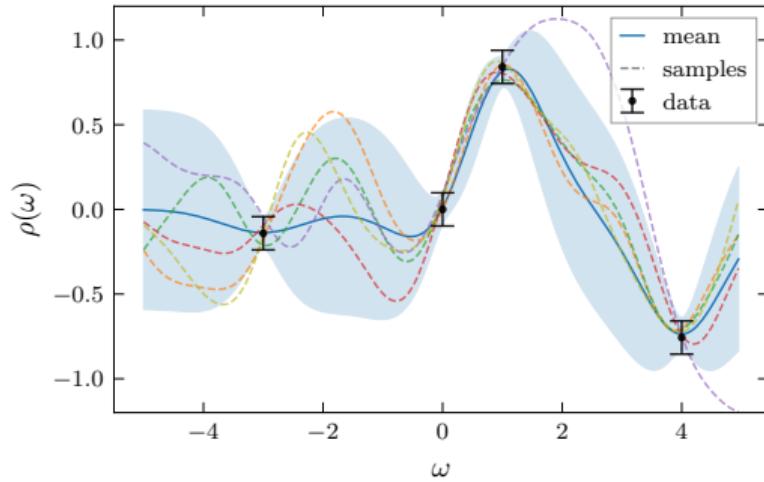
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Gaussian Process Regression - Prediction



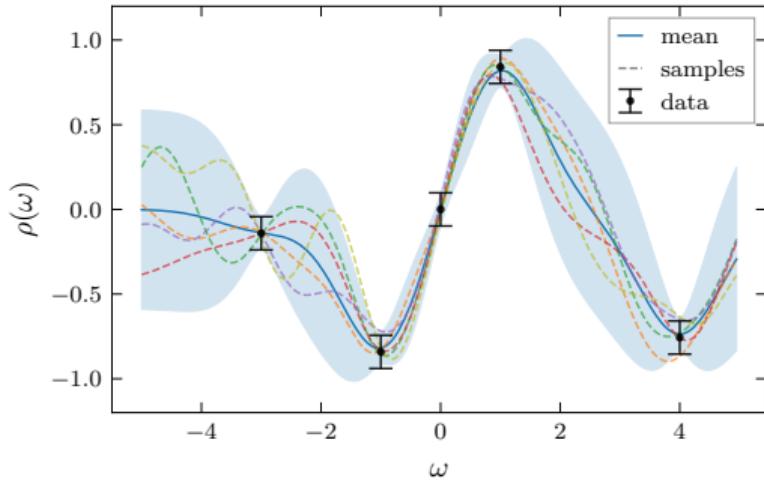
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Gaussian Process Regression - Prediction



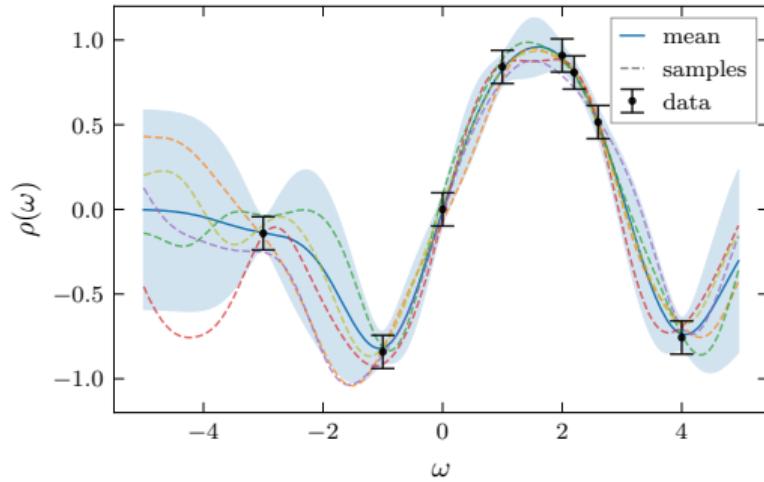
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Gaussian Process Regression - Prediction



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Gaussian Process Regression - Prediction



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- Linear transformations preserve Gaussian statistics

$$G(p) = \int_0^\infty \frac{d\omega}{\pi} \frac{\omega}{\omega^2 + p^2} \rho(\omega) =: \mathcal{K} \circ \rho$$

- $\rho \sim \mathcal{GP}(\mu, C) \rightarrow G \sim \mathcal{GP}(\mathcal{K} \circ \mu, \mathcal{K} \circ C \circ \mathcal{K}^\top)$
- Joint prior over observations on G and predictions ρ

$$\begin{pmatrix} \rho \\ G \end{pmatrix} \sim \mathcal{N} \left(\begin{matrix} \mu & C & C \circ \mathcal{K}^\top \\ \mathcal{K} \circ \mu, \mathcal{K} \circ C & \mathcal{K} \circ C \circ \mathcal{K}^\top + \sigma_n^2 \mathbb{1} \end{matrix} \right)$$

- Works for **every** type of linearly connected data, e.g. derivative or normalization data
Horak, Pawłowski, Rodríguez-Quintero, JT, Urban, Wink, Zafeiropoulos, [arXiv:2107.13464](https://arxiv.org/abs/2107.13464)

- The kernel fully characterizes the GP, implicitly controls features of the interpolation
- **Mercer's theorem:** For any continuous symmetric PSD kernel $C(x, y)$, there exists an orthonormal basis of continuous eigenfunctions φ_i with positive eigenvalues λ_i

$$\int dx C(x, y)\varphi_i(x) = \lambda_i\varphi_i(y),$$

and the kernel can be represented as

$$C(x, y) = \sum_i \lambda_i \varphi_i(x) \varphi_i(y).$$

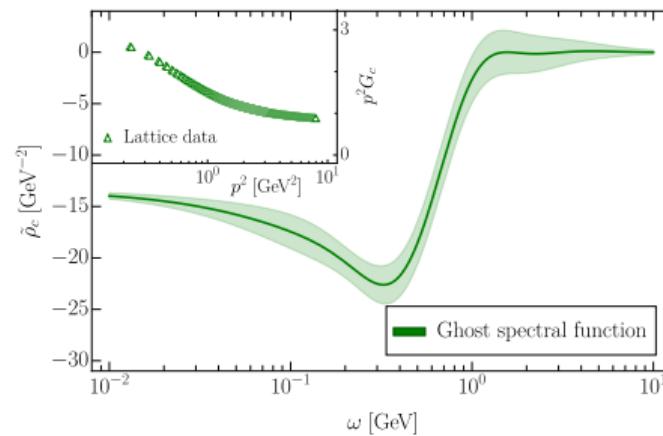
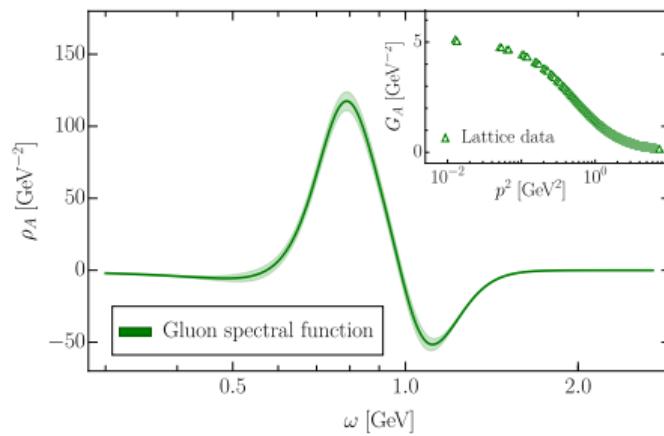
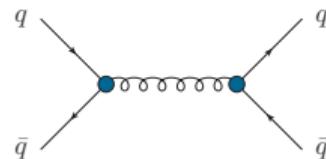
- GP posterior mean can be written as $\mu(x) = \sum_i \alpha_i \varphi_i(x)$

Horak, Pawłowski, JT, Urban, Wink, Zafeiropoulos, [arXiv:2301.07785](https://arxiv.org/abs/2301.07785)

- Kernels with infinite number of eigenfunctions are called *universal*, e.g. RBF kernel
- We can also restrict the functional basis
 - include asymptotics
- Control regions of asymptotics by smooth step function θ^\pm and optimize parameters

$$C(x, y) = \theta^+(x; \mu_{uv}, \ell_{uv}) \theta^+(y; \mu_{uv}, \ell_{uv}) \rho_{uv}(x) \rho_{uv}(y) \\ + \theta^-(x; \mu_{uv}, \ell_{uv}) \theta^-(y; \mu_{uv}, \ell_{uv}) C_{\text{universal}}(x, y)$$

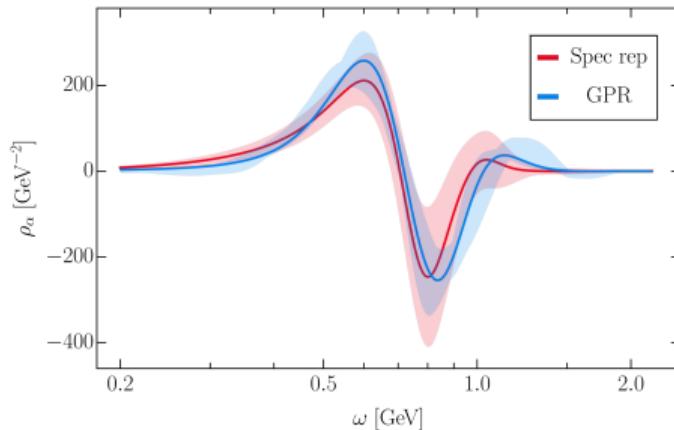
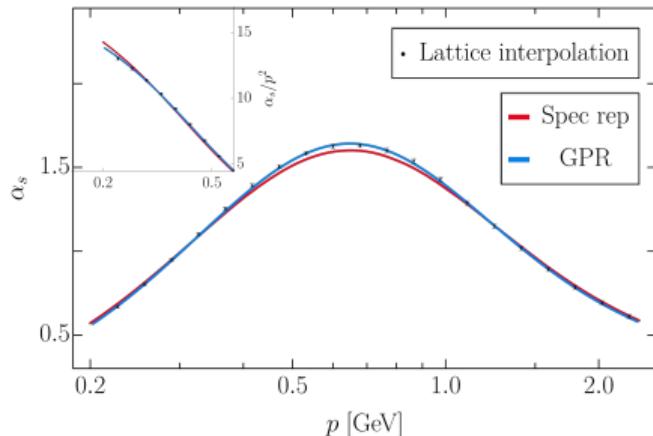
Application 1: Strong coupling at time-like momenta



Horak, Pawłowski, JT, Urban, Wink, Zafeiropoulos, arXiv:2301.07785

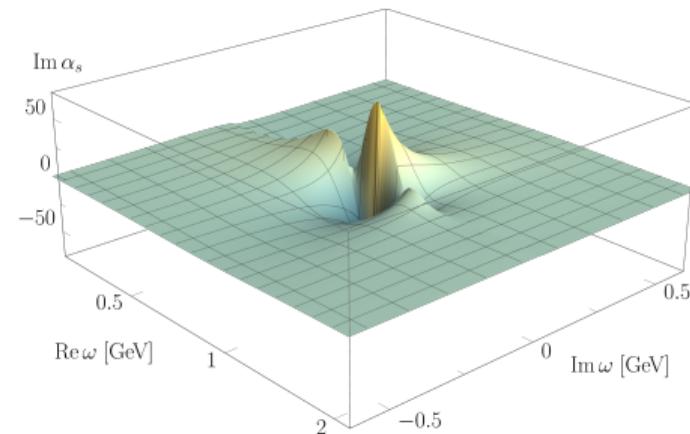
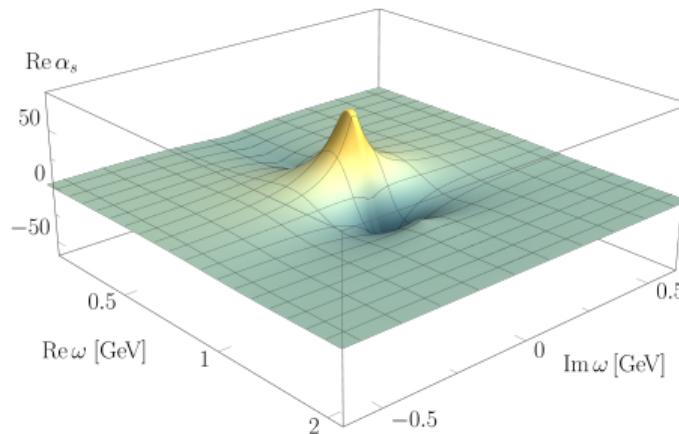
Application 1: Strong coupling at time-like momenta

$$\alpha_s(p) = \frac{g_s^2}{4\pi} \frac{1}{Z_A(p)Z_c^2(p)}, \quad \rho_\alpha(\omega) = -2 \operatorname{Im} \left[\left(\int_0^\infty \frac{d\lambda}{\pi} \frac{\lambda \rho_A(\lambda)}{\lambda^2 - \omega^2 + i0^+} \right) \times \left(\frac{1}{Z_c^0} - \omega^2 \int_0^\infty \frac{d\lambda}{\pi} \frac{\lambda \tilde{\rho}_c(\lambda)}{\lambda^2 - \omega^2 + i0^+} \right)^2 \right]$$



Horak, Pawłowski, JT, Urban, Wink, Zafeiropoulos, arXiv:2301.07785

Application 1: Strong coupling at time-like momenta



Horak, Pawłowski, JT, Urban, Wink, Zafeiropoulos, arXiv:2301.07785

Thermal photons are produced at high T from the QGP

$$\frac{d\Gamma_\gamma}{d^3\vec{k}} = \frac{\alpha_{em} n_b(\omega, T)}{2\pi^2 k} g^{\mu\nu} \rho_{\mu\nu}(\omega = |\vec{k}|, \vec{k}, T)$$

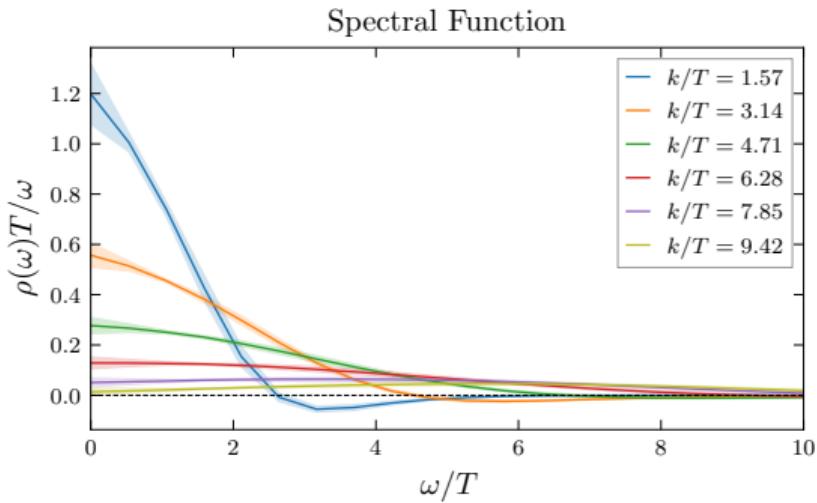
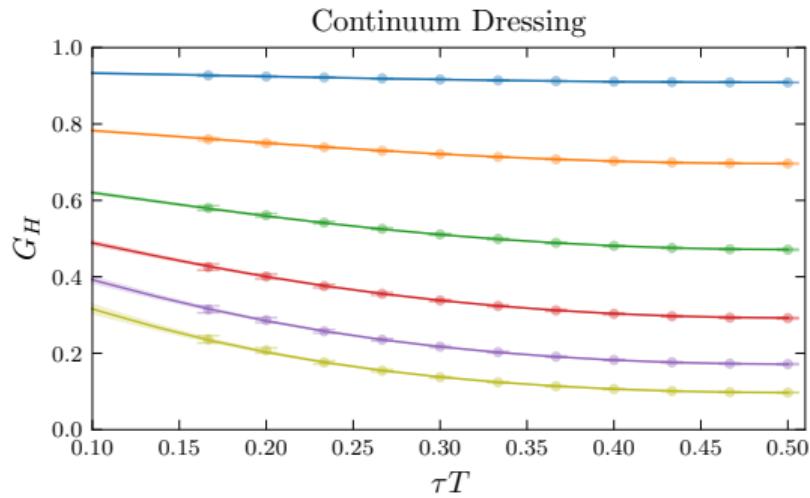
With the finite T vector current spectral function defined as

$$G_{\mu\nu}(\tau, \vec{k}) = \int_0^\infty \frac{d\omega}{\pi} \frac{\cosh(\omega(\tau - 1/(2T)))}{\sinh(\omega/(2T))} \rho_{\mu\nu}(\omega, \vec{k}, T)$$

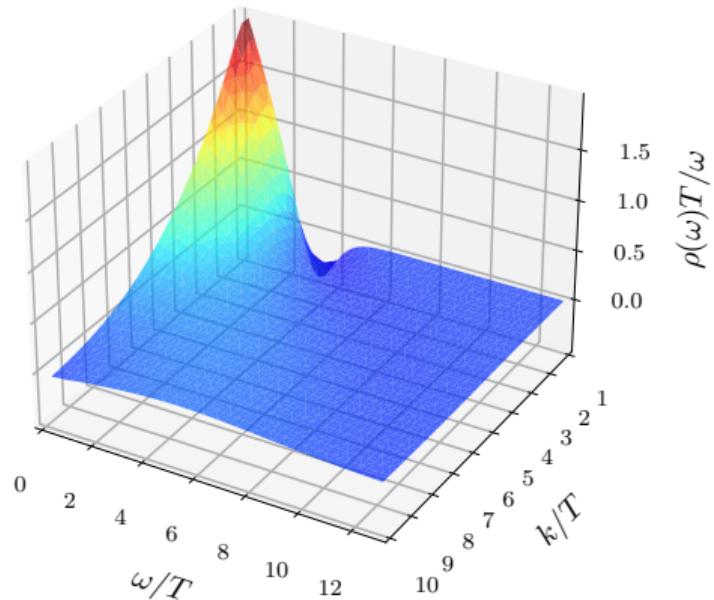
- Spectral function has a large UV tail
⇒ decompose $\rho_{\mu\nu} = P_{\mu\nu}^T \rho_T + P_{\mu\nu}^L \rho_L \Rightarrow g^{\mu\nu} \rho_{\mu\nu} = 2\rho_T + \rho_L$
- compute the T-L correlator $\rho_H = 2(\rho_T - \rho_L)$ with suppressed UV ($\sim 1/\omega^4$)
- $\rho_L(\omega = |\vec{k}|, \vec{k}) = 0 \Rightarrow$ photon rate unchanged

- Lattice data:
 - Pure Gluonic theory at $1.5T_c$, continuum extrapolated
 - $N_f = 2 + 1$ QCD at $1.22T_c$, finite lattice spacing
- Compare 3 methods:
 - Physics motivated fits
 - Backus-Gilbert method
 - Gaussian Process Regression
- Use 2D correlator data, sum rule, asymptotics

Application 2: Thermal photon rate

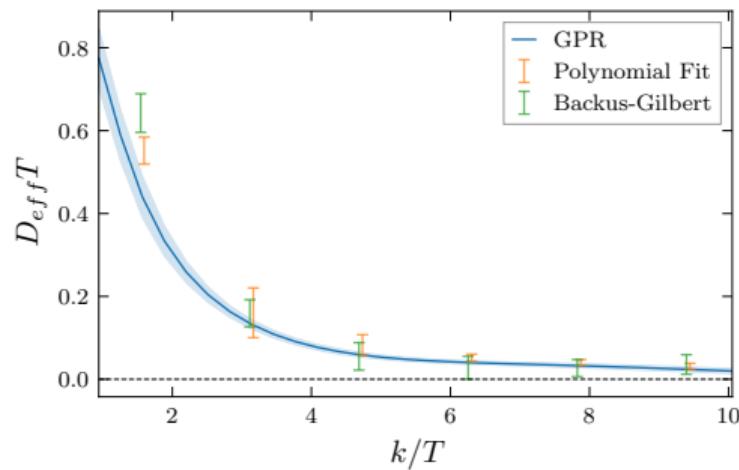


Application 2: Thermal photon rate

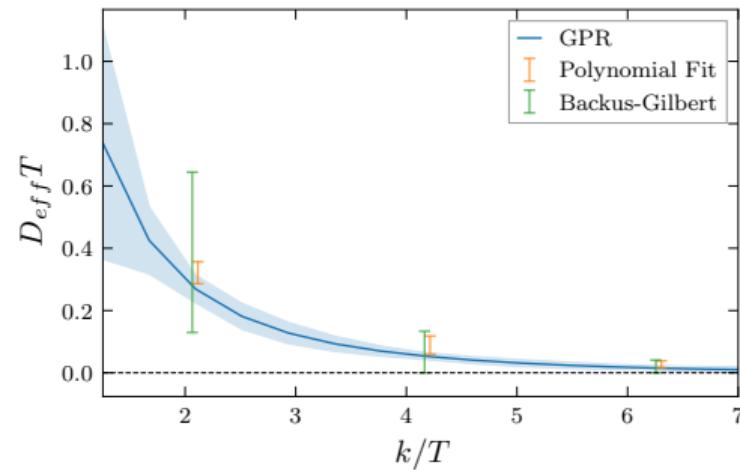


Ali, Bala, Francis, Jackson, Kaczmarek, JT, Ueding, Wink, in preparation

Application 2: Thermal photon rate



(a) $N_f = 0$



(b) $N_f = 2 + 1$, $N_\tau = 32$

Ali, Bala, Francis, Jackson, Kaczmarek, JT, Ueding, Wink, in preparation

- GPs have been shown to be a good method for spectral reconstruction
- Python package coming soon™ with many great features
- Reconstruction in arbitrary dimensions
- Improved the Hyperparameter search
- Inequality constraints, e.g. positivity or monotonicity