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

Jonas Turnwald

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CRC-TR 211
Strong-interaction matter under extreme conditions

Why Spectral Reconstruction?

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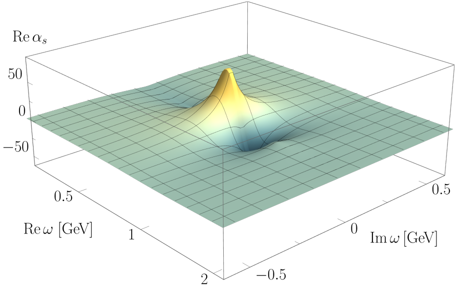
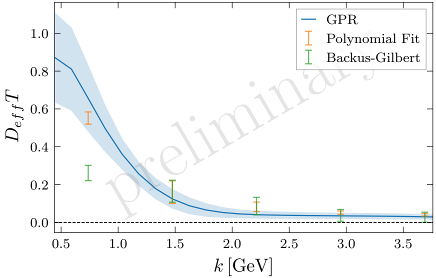


(c) Strong coupling in the complex plane



(d) Thermal Photon rate

Källén-Lehmann spectral representation

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

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Gaussian Process Regression

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

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

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- Finite dimensional subset of the GP at distinct points $\omega_1, ..., \omega_N$

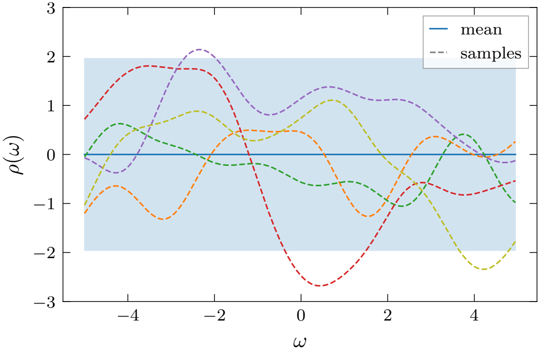
$$\begin{pmatrix} \rho(\omega_1) \\ \vdots \\ \rho(\omega_N) \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \mu(\omega_1) \\ \vdots \\ \mu(\omega_N) \end{pmatrix}, \begin{pmatrix} C(\omega_1, \omega_1) & \dots & C(\omega_1, \omega_N) \\ \vdots & \ddots & \vdots \\ C(\omega_N, \omega_1) & \dots &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

Gaussian Process Regression

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

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

RBF Kernel



Gaussian Process Regression - Prediction

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

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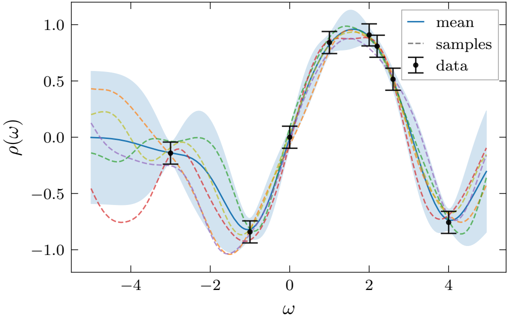
GP Posterior has closed analytic form

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

Gaussian Process Regression - Prediction



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

Spectral Reconstruction with GPR

- Linear transformations preserve Gaussian statistics

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

Horak, Pawlowski, Rodríguez-Quintero, JT, Urban, Wink, Zafeiropoulos, PRD 105 (2022)

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- Joint prior over observations on G and predictions ρ

$$\begin{pmatrix} \rho \\ G \end{pmatrix} \sim \mathcal{N}\begin{pmatrix} \mu & C & C \circ \mathcal{K}^\top \\ \mathcal{K} \circ \mu ' & \mathcal{K} \circ C & \mathcal{K} \circ C \circ \mathcal{K}^\top + \sigma_n^2 \mathbb{1} \end{pmatrix}$$

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- Works for **every** type of linearly connected data, e.g. derivative or normalization data

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Kernel eigenfunctions and spectral function asymptotics

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- The kernel fully characterizes the GP, implicitly controls features of the interpolation

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Kernel eigenfunctions and spectral function asymptotics

- 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

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

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Kernel eigenfunctions and spectral function asymptotics

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

$$C(\omega,\omega') = \theta^{+}(\omega;\mu_{\text{UV}},\ell_{\text{UV}})\,\theta^{+}(\omega';\mu_{\text{UV}},\ell_{\text{UV}})\,\rho_{\text{UV}}(\omega)\,\rho_{\text{UV}}(\omega') \\ + \theta^{-}(\omega;\mu_{\text{UV}},\ell_{\text{UV}})\,\theta^{-}(\omega';\mu_{\text{UV}},\ell_{\text{UV}})\,C_{\text{universal}}(\omega,\omega')$$

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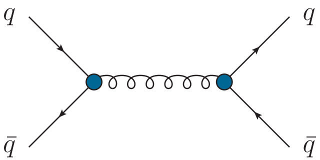
Application 1: Strong coupling at time-like momenta



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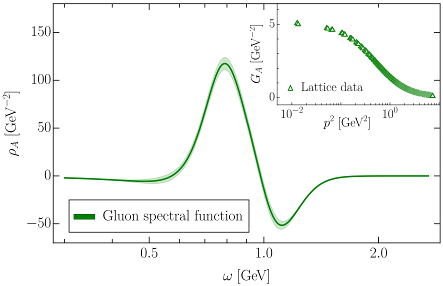
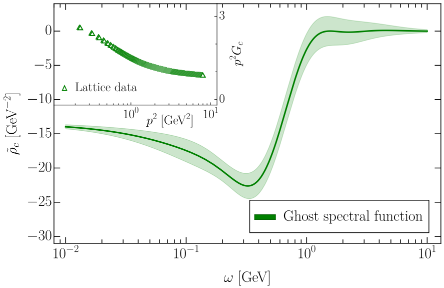
$$\alpha_s(p) = \frac{g_s^2}{4\pi} \frac{1}{Z_A(p) Z_c^2(p)}$$





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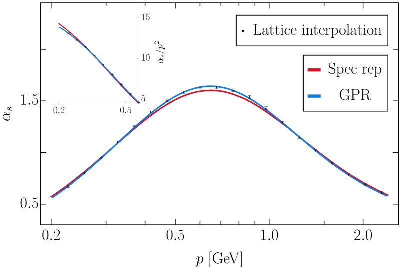
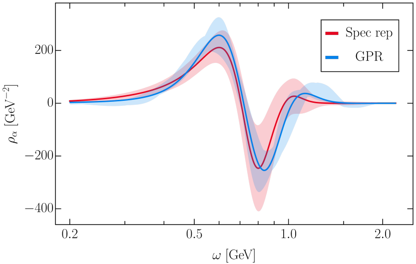


(e) Euclidean strong coupling



(f) Strong coupling spectral function

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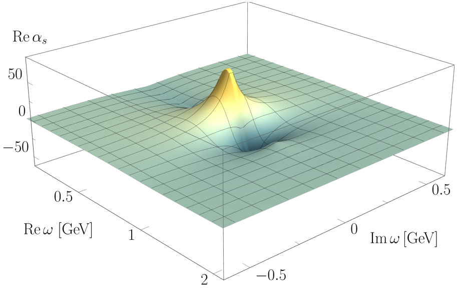

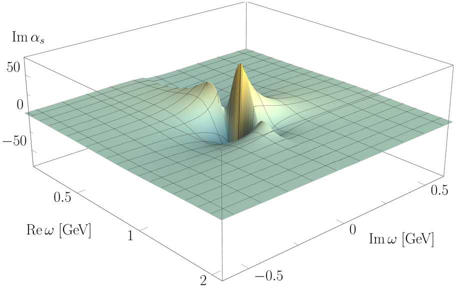

Strong coupling in the complex plane

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Application 2: Thermal Photon Rate

see talk by Dibyendu Bala

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

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Thermal photons are produced at high T from the QGP

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

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With the finite T vector current spectral function defined as

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

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- compute the T-L correlator $\rho_H = 2(\rho_T - \rho_L)$ with suppressed UV ($\sim 1/\omega^4$)

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- $\rho_L(\omega = |\vec{k}|, \vec{k}) = 0 \Rightarrow$ photon rate unchanged

Application 2: Thermal photon rate

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- Lattice data:
  - Pure Gluonic theory at $1.5T_c$, continuum extrapolated
  - $N_f = 2 + 1$ QCD at $1.22T_c$, finite lattice spacing

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- Use 2D correlator data, sum rule, UV asymptotics

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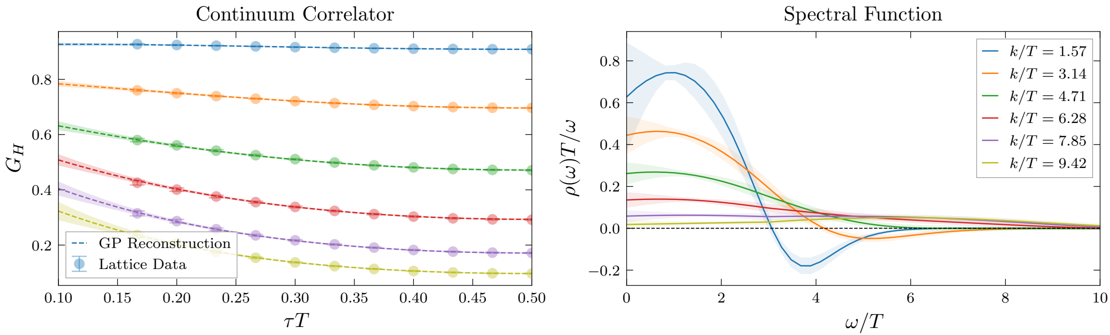

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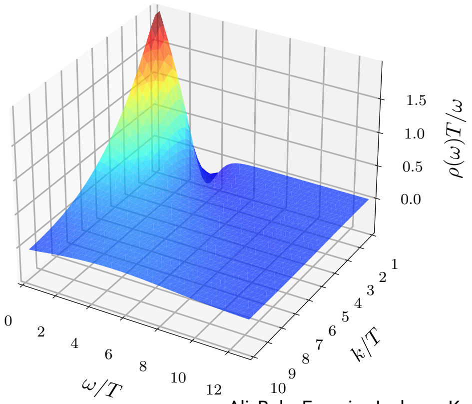

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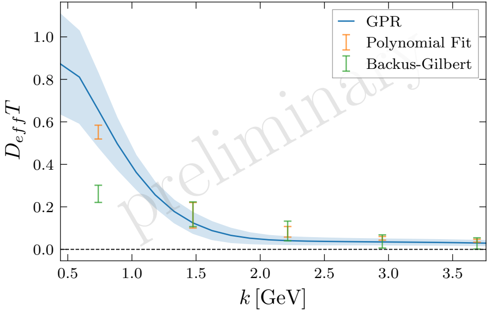
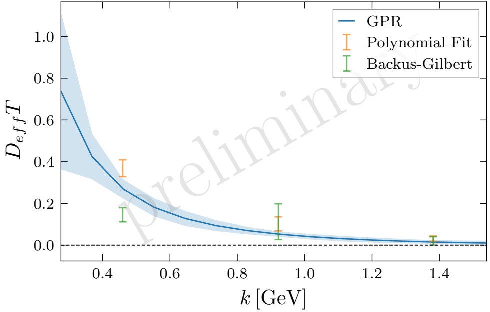


(a) $N_f = 0,\ T = 470\,\text{MeV}$



(b) $N_f = 2 + 1,\ N_\tau = 32,\ T = 220\,\text{MeV}$

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- Python package coming soon(-ish)