Reconstruction of bottomonium spectral functions in thermal QCD using Kernel Ridge Regression

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Gen 2L Setup

- N_f = 2+1 Wilson quarks
- a_s = 0.1136 fm and a_τ^{-1} = 5.997 GeV
- M_π = 236 MeV
- Anisotropy, ζ = 3.45
- N_s = 32
- 47 MeV $\leq T \leq$ 375 MeV

See arXiv:2007.04188 (hep-lat)

NRQCD

- An effective field theory by expanding dispersion relation in powers of v.
- Terms up to v^4 are included.
- Correlators are generated from an initial value problem.
- All physics is contained within the spectral functions and correlators but former is harder to access.

$$G(\tau) = \int_{\omega_{min}}^{\omega_{max}} \mathrm{d}\omega\, K(\tau,\omega)\rho(\omega)$$

where $K(\tau,\omega) = e^{-\omega\tau}$

- Inversion is an ill-posed problem

Kernel Ridge Regression

- Linear case: $y = \mathbf{w}x \rightarrow$ Kernel case : $y = \mathbf{C}(x, x')\alpha$
- $\mathbf{w} \rightarrow \alpha$
- Relate this to lattice quantities by setting $y \rightarrow \rho(\omega)$ and $x \rightarrow G(\tau)$
- $\rho(\omega)$ can be parameterised by a vector $\mathbf{p}$.
- Kernel function contains "distance" between input data (L1, L2 norms, etc)
- α is determined by minimizing a cost function.

KRR

$$E = (\mathbf{p} - \mathbf{C}\alpha)^2 + \lambda|\mathrm{I}\alpha|^2$$

- λ is regularisation constant to prevent overfitting.
- We can determine α using:

$$\alpha = (\mathbf{C} + \mathrm{I}\lambda)^{-1}\mathbf{p}$$

where

$$C_{ij}(x_i, x_j) = \exp\left\{-\gamma \sum_{\tau} \left[\log(G_i(\tau)) - \log(G_j(\tau))\right]^2\right\}$$

- γ is scale length, determines "strength" of correlations.
- Finally predictions are made using $\mathbf{p} = C(x_{\mathrm{train}}, x_{\mathrm{NRQCD}})\alpha$

For a more thorough explanation see arXiv:1912.12900 [hep-lat]

Considerations

- We have two issues that need considering
- Is the training data appropriate?
- How do we optimize hyperparameters?

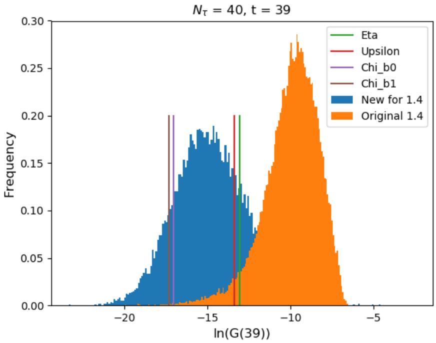
Data Generation

- To train the model we require mock data (spectral functions and corresponding correlators).
- The mock ρ were made from 5 Gaussians over a range of $a_\tau(\omega_{max} - \omega_{min}) = 1.4$.
- 20000 ρ were generated, each with 15 associated parameters.
- Corresponding correlators were calculated from

$$G(\tau) = \Delta\omega \sum_{\omega=\omega_{\min}}^{\omega_{\max}} K(\tau,\omega)\rho(\omega)$$

Data Generation

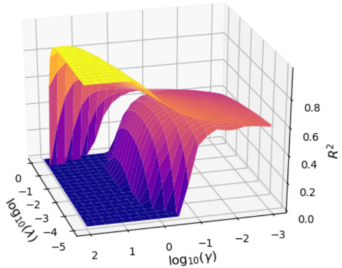
- Does this need improving and can it be improved?
- We compared these mock correlators to NRQCD data and selected the most similar.
- This was done for 4 channels and 10 values of N_τ to obtain a set of 'optimal' parameters for generating ρ.



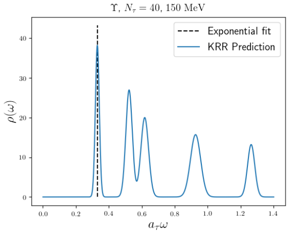
Hyperparameters.

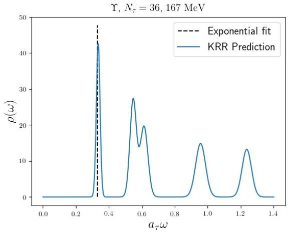
- KRR models are trained using a subset of the mock data.
- A second smaller test set is used to select the hyperparameters
- It is common to minimize the test set error to do this.
- Instead (λ, γ) were chosen by maximising R^2 for the test set, with $|R^2_{train} - R^2_{test}| < 0.01$.

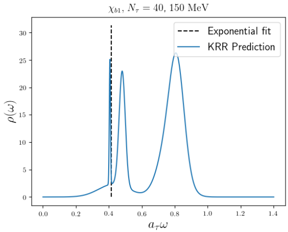
$$R^2 = 1 - \frac{\sum_i |y_i^{true} - y_i^{pred}|^2}{\sum_i |y_i^{true} - \bar{y}^{true}|^2}$$

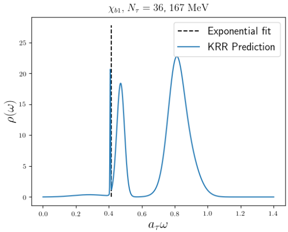


Results (Preliminary)









Summary

- We have compared mock data to actual NRQCD correlators and used this to generate more appropriate training functions.
- An alternate method for optimizing KRR hyperparameters has been discussed
- Groundstate state mass of Υ and χ_{b1} show agreement with exponential fit.

Further work

- Alternative forms for training data (Breit-Wigner functions, continuum, etc.).
- Introducing noise to the training step.

Thank you for listening