Model Averaging Tool for Parameter Estimation in LFT

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Background

In a typical lattice simulations many quantities can be related to correlation functions through the **spectral decomposition**

$$C(\tau) = \langle O(\tau)O(0)\rangle \xrightarrow{\beta\to\infty} \sum_{n=0}^{\mathrm{N_{state}}} A_n e^{-\tau E_n}. \tag{1}$$

For simplicity we focus on energies $E_n \equiv E_n - E_\Omega$ and overlap factors A_n from two-point correlators. A simple approximation of the first energy is to compute the **effective mass**, $\mathrm{m_{eff}} = \log C(\tau-a) - \log C(\tau+a)/2a$. This requires to truncate the spectral decomposition after the first term introducing **systematic uncertainties** – it neglects excited states. To provide a better estimate the data has to be analysed as a function of truncation $\mathrm{N_{state}}$. Unfortunately, fitting a tower of exponentials is a difficult task and naive minimization routines are likely to fail. Providing guidance to the fit is thus of utmost importance and a natural access point is Bayesian fitting.

Bayes' theorem allows to express the probability of found parameters $\Theta = \{A_n, E_n\}_{n=0}^{\mathrm{N_{state}}}$ – the posterior distribution $\mathrm{p}(\Theta|D)$ – given a data set to fit against $D = \{\tau, C(\tau)\}$,

$$\mathrm{p}(\Theta|D) = \frac{\mathrm{p}(D|\Theta)\,\mathrm{p}(\Theta)}{\mathrm{p}(D)}. \tag{2}$$

This proportionality includes the (maximum) likelihood distribution $\mathrm{p}(D|\Theta) \sim e^{-\chi^2/2}$, and a-priori knowledge on the parameters via the prior distribution $\mathrm{p}(\Theta)$. For our purpose we can ignore the, normalizing, marginal distribution $\mathrm{p}(D)$. From this simple expression we can identify the augmented χ^2 that is minimized to find Θ,

$$\chi^2_{\mathrm{aug}} = \chi^2 + 2\log \mathrm{p}(\Theta) \tag{3}$$

Now expressing **prior knowledge** on the parameters through Θ, σ_Θ allows to guide the fit effectively stabilizing the minimization procedure. A word of caution, any fit that requires guidance to converge explicitly is biased! For the Bayesian approach above, the strength of the bias can be handled by the σ_Θ and needs to be investigated explicitly.

Typical choices of priors can come from analytical arguments, e.g. **non-interacting solutions**. However, if these are not accessible one can use **effective masses** with hand picked ranges, e.g.

$$\mathrm{p}(\Theta = E_0) = \log \mathcal{N}(\mathrm{m_{eff}}, 0.5\mathrm{m_{eff}}). \tag{4}$$

Model Averaging [1, 2, 3]

The truncation of the spectral decomposition (1) naturally induces a systematic uncertainty. There are many ways of estimating how large this uncertainty should be. One way of including an uncertainty estimate into the analysis is to perform **model averaging** under **bootstrap**. Given a set of models m,

$$\left\{ m = \left(\Theta|_{\mathrm{N_{state}}}, D|_{[\tau_s,\tau_e]}\right)\right\}, \tag{5}$$

a model weight can be computed using the **Akaike information criterion**

$$\omega(m) \sim e^{-\frac{1}{2}\mathrm{AIC}(m)}, \tag{6}$$

$$\mathrm{AIC}(m) = \chi^2_{(aug)} - 2|\tau_e - \tau_s| + 2|\Theta|. \tag{7}$$

A simple weighted average $\bar{\Theta}^{(\mathrm{bst})}$, on each bootstrap sample, determines a parameter estimate. Further, using the usual bootstrap deviation over these estimates, $\sigma_\Theta^{\mathrm{bst}}$, then quantifies an uncertainty including statistical and model-systematic deviations.

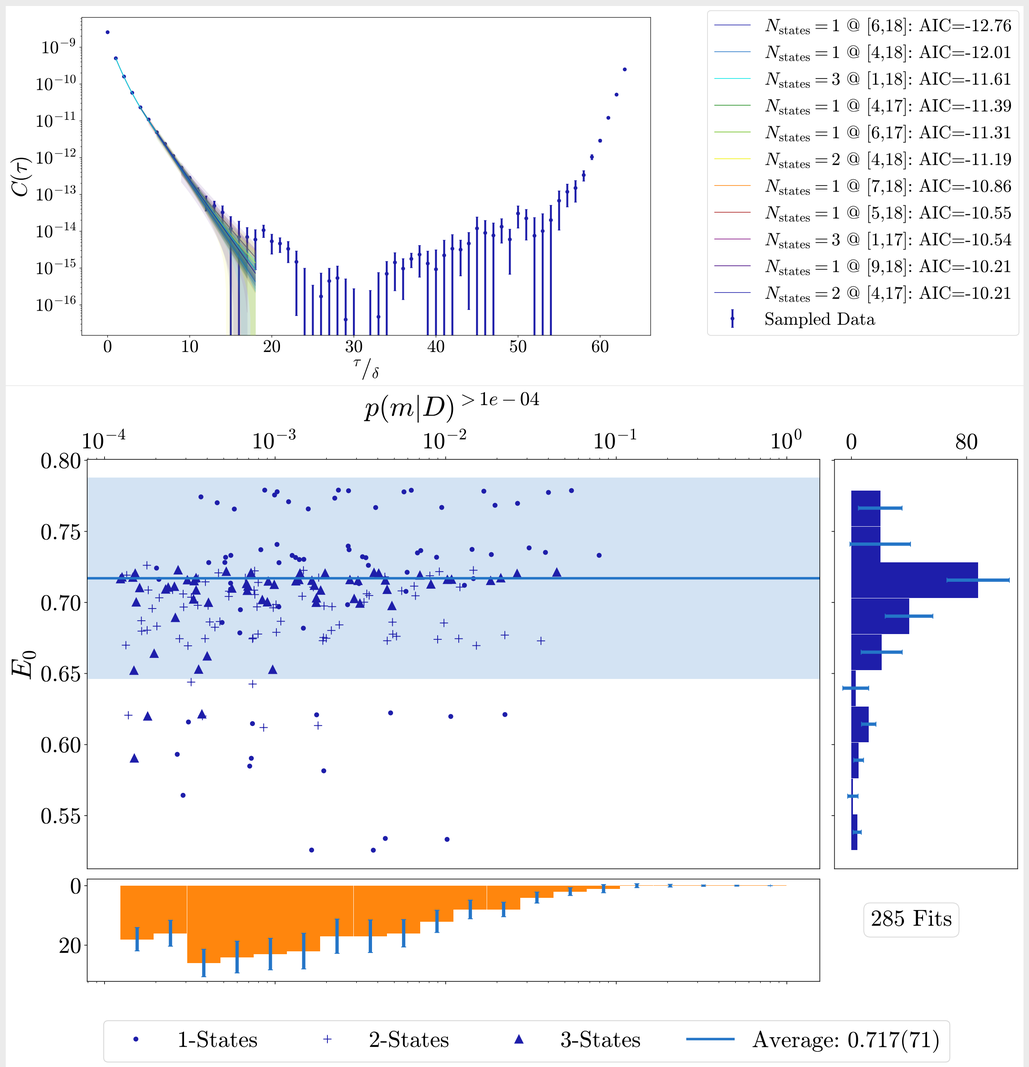
Once a couple of models have been fitted, e.g. when a new state is introduced, one can use the results of the **model average as priors** for the next fits. Typically, the uncertainty is increased compared to the bootstrap deviation to weaken the prior.

Lattice QCD: The Nucleon

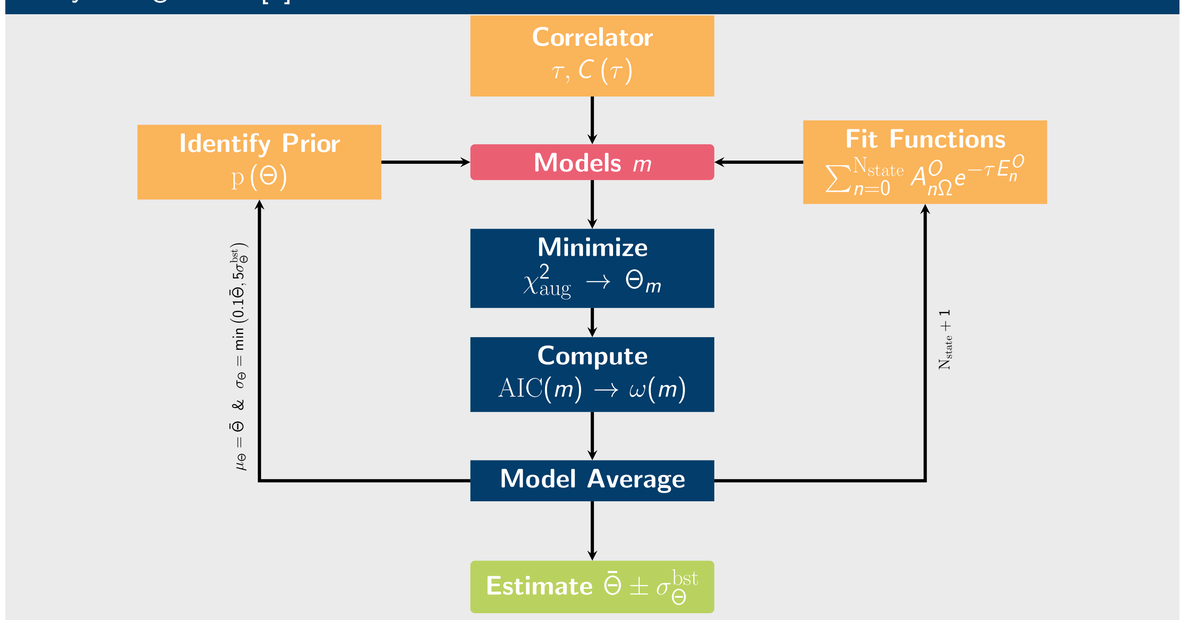
We compute nucleon correlators on one $L^3 \times \mathrm{N_t} = 24^3 \times 64$ ensemble at a lattice spacing of $a \approx 0.125\,\mathrm{fm}$ using a tree-level Symanzik-improved gauge action and 2+1 flavor tree-level improved Wilson Clover fermions coupling via 6-level stout-smearing [4].The ensemble parameters are

β	am_l	am_s	m_π[MeV]	$m_\pi L$	$\mathrm{N_{conf}}$
3.3	−0.1265	−0.057	273(13)	4.15(20)	500

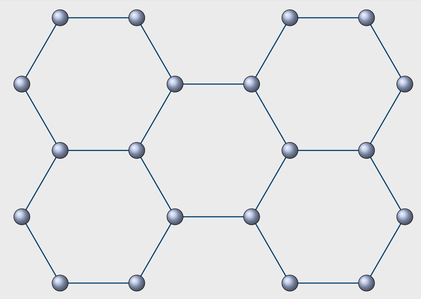
We measure only one smeared source on each configuration. The simple spectral decomposition of (1) is used and the prior is determined by (4). The prior for the overlap is determined by the effective mass and $C(\tau/a = 7)$ with 100% uncertainty. Higher states are fitted by iterative model averaging as described in the algorithm.



Analysis Algorithm [5]



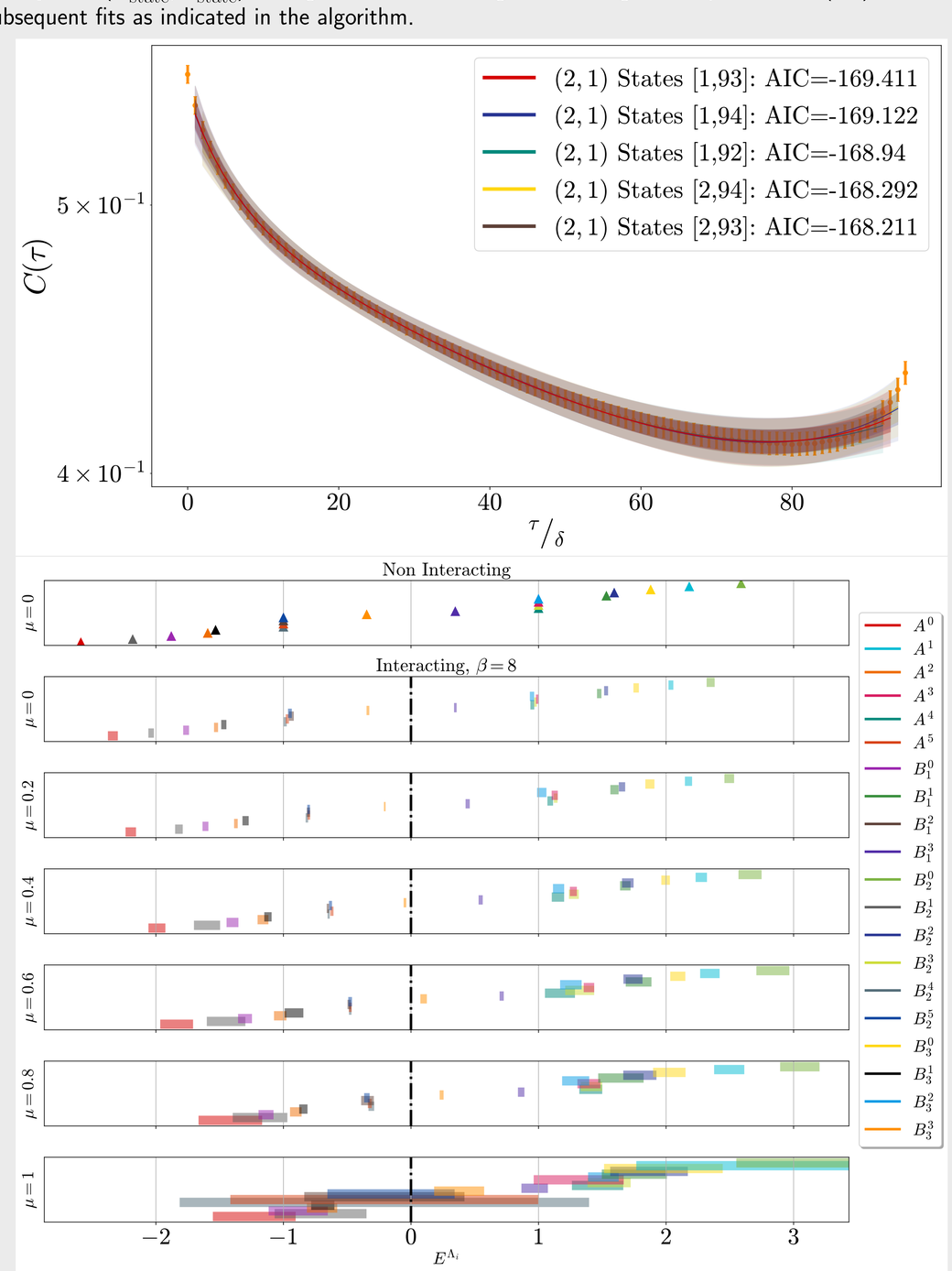
Hubbard Model: Single Particle Spectrum of Perylene [5]



We simulate the single particle spectrum of Perylene described by the Hubbard model,

$$\hat{\mathcal{H}}_{\mathrm{Hubbard}} = -\frac{1}{2}\sum_{x,y\in\Lambda}\left\{\hat{p}^\dagger_x K^{xy}\hat{p}_y - \hat{h}^\dagger_x K^{xy}\hat{h}_y\right\} + \frac{U}{2}\sum_{x\in\Lambda}\hat{\rho}^2_x - \mu\sum_{x\in\Lambda}\hat{\rho}_x, \tag{8}$$

as a function of chemical potential. This parameter scan includes about 2000 single particle correlators $C^{\Lambda_i}(\tau) = \left\langle p^\dagger_{\Lambda_i}(\tau) p_{\Lambda_i}\right\rangle$ to analyse. The data allows to fit forward and backward propagating states which we truncate separately with $(\mathrm{N^L_{state}}, \mathrm{N^R_{state}})$. Using the non-interacting model energies as a prior to the (1,1) state fits, and all subsequent fits as indicated in the algorithm.



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[2] Ethan T. Neil and Jacob W. Sitison. "Model averaging approaches to data subset selection". In: *Physical Review E* 108.4 (Oct. 2023), p. 045308. arXiv: 2305.19417.

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[4] S. Durr et al. "Ab-initio Determination of Light Hadron Masses". In: *Science* 322.5905 (Nov. 2008), pp. 1224–1227. arXiv: 0906.3599.

[5] Marcel Rodekamp et al. *Single Particle Spectrum of Doped* $\mathrm{C_{20}H_{12}}$*-Perylene*. June 2024. arXiv: 2406.06711.

[6] Marcel Rodekamp and Giovanni Pederiva. *Correlator Analyser*. URL: https://github.com/Marcel-Rodekamp/CorrelatorAnalyser.