

Lattice Spectral Density

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On the extraction of spectral densities from lattice correlators

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Hadronic spectral densities are important quantities whose non-perturbative knowledge allows for calculating phenomenologically relevant observables, such as inclusive hadronic cross-sections and non-leptonic decay-rates. The extraction of spectral densities from lattice correlators is a notoriously difficult problem because lattice simulations are performed in Euclidean time and lattice data are unavoidably affected by statistical and systematic uncertainties. In this paper we present a new method for extracting hadronic spectral densities from lattice correlators. The method allows for choosing a smearing function at the beginning of the procedure and it provides results for the spectral densities smeared with this function together with reliable estimates of the associated uncertainties. The same smearing function can be used in the analysis of correlators obtained on different volumes, such that the infinite volume limit can be studied in a consistent way. While the method is described by using the language of lattice simulations, in reality it is completely general and can profitably be used to cope with inverse problems arising in different fields of research.

Outline

- The need for spectral density
- The difficulties for lattice calculations
- The idea of the Buckus-Gilbert method
- The inspiration from B.-G. to the HLT method
- Some examples
- Summary

The need for spectral density

- Continuum spectrum of the QCD Hamiltonian: the differential cross section for the process $e^+e^- \rightarrow$ hadrons.
- Flavour-changing non-leptonic decay rates of kaons and heavy-flavoured mesons
- Deep inelastic scattering cross-section
- Thermodynamic observables arising in the study of QCD at finite temperature and of the quark-gluon plasma

The difficulties for lattice calculations

- Definition of spectral density

$$C(t) = \sum_n a_n \left[e^{-E_n t} + e^{-E_n (T-t)} \right]$$

$$C(t) = \frac{1}{L^3} \sum_{\vec{x}} T \langle 0 | O(x) \bar{O}(0) | 0 \rangle_L \rightarrow C(t) = \int_0^\infty dE \rho_L(E) e^{-tE}$$

$$\rho_L(E) = \frac{1}{L^3} \sum_{\vec{x}} \langle 0 | O(0, \vec{x}) \delta(E - H_L) \bar{O}(0) | 0 \rangle_L$$

- An inverse Laplace transform is to be performed numerically, which is an ill-posed problem when the measured data are affected by uncertainties.

The difficulties for lattice calculations

An ill-posed question

- Statistical and systematic errors
- Euclidean time-ordered correlators at discrete values
- The volume dependence: a discrete spectrum

$$\rho_L(E) = \frac{1}{L^3} \sum_{\vec{x}} \langle 0 | O(0, \vec{x}) \delta(E - H_L) \bar{O}(0) | 0 \rangle_L$$

$$\rho_L(E) = \sum_n w_n(L) \delta(E - E_n(L))$$

The idea of the Buckus-Gilbert method

- Central idea: to optimise the amount of information that can be extracted from noisy measurements, by focusing on the calculation of smeared spectral densities

$$\rho_L(E) = \sum_n w_n(L) \delta(E - E_n(L)) \Rightarrow \hat{\rho}_L(\sigma, E_\star) = \int_0^\infty dE \Delta_\sigma(E_\star, E) \rho_L(E)$$

smeared spectral densities

$$\rho(E_\star) = \lim_{\sigma \rightarrow 0} \lim_{L \rightarrow \infty} \hat{\rho}_L(\sigma, E_\star)$$

$$C(t) = \int_0^\infty dE \rho_L(E) b_T(t, E), \text{ with } b_T(t, E) = e^{-tE} + e^{-(T-t)E}$$

basis function

The idea of the Buckus-Gilbert method

- Smearred spectral density

$$\hat{\rho}_L^{BG}(E_\star) = \sum_{t=0}^{t_{max}} g_t(E_\star) C(t+1)$$

$$= \int_0^\infty dE \rho_L(E) \Delta^{BG}(E_\star, E)$$

minimizing

$$A_{BG}[g] = \int_0^\infty dE (E - E_\star)^2 \{ \Delta^{BG}(E_\star, E) \}^2$$

with $\int_0^\infty dE \Delta^{BG}(E_\star, E) = 1$

$$R_t = \int_0^\infty dE b_T(t+1, E)$$

$$A_{tr}(E_\star) = \int_0^\infty dE (E - E_\star)^2 b_T(t+1, E) b_T(r+1, E)$$

$$\Delta^{BG}(E_\star, E) = \sum_{t=0}^{t_{max}} g_t(E_\star) b_T(t+1, E)$$

smearing function

$$g(E_\star) = \frac{A^{-1}(E_\star) \mathbf{R}}{\mathbf{R}^T A^{-1}(E_\star) \mathbf{R}}$$

The idea of the Buckus-Gilbert method

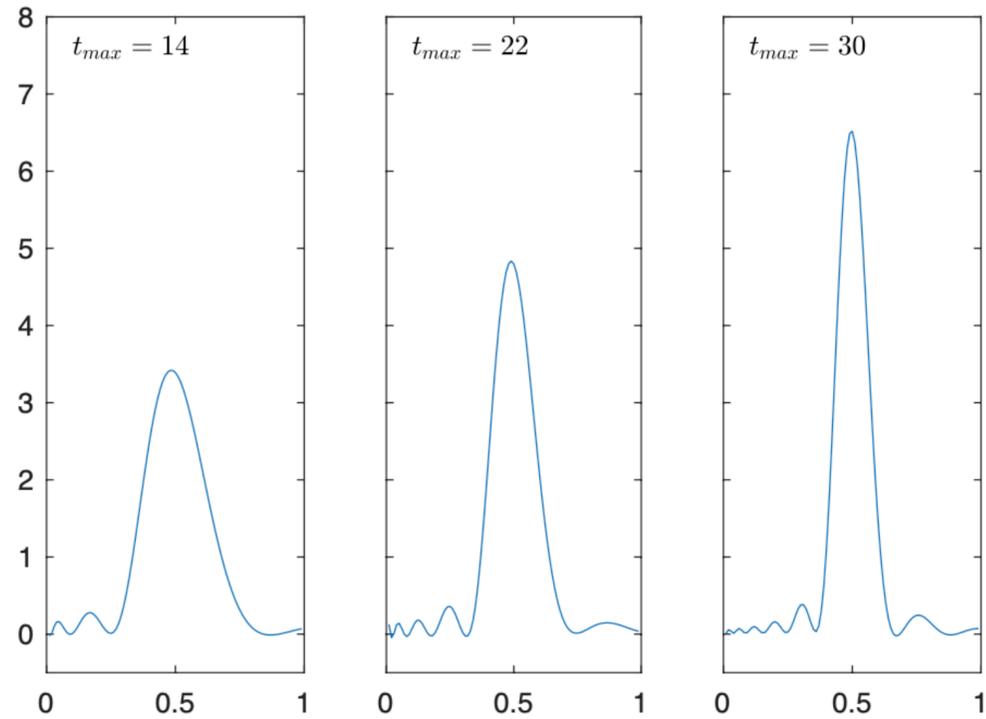


FIG. 1: Smearing functions $\Delta^{BG}(E_*, E)$ obtained by applying the Buckus-Gilbert procedure in the absence of statistical errors with $E_* = 0.5$ and $b_\infty(t, E)$ as basis functions. The different panels correspond to different values of t_{max} . As it can be seen the function $\Delta^{BG}(E_*, E)$ gets more similar to a Dirac δ -function for increasing values of t_{max} .

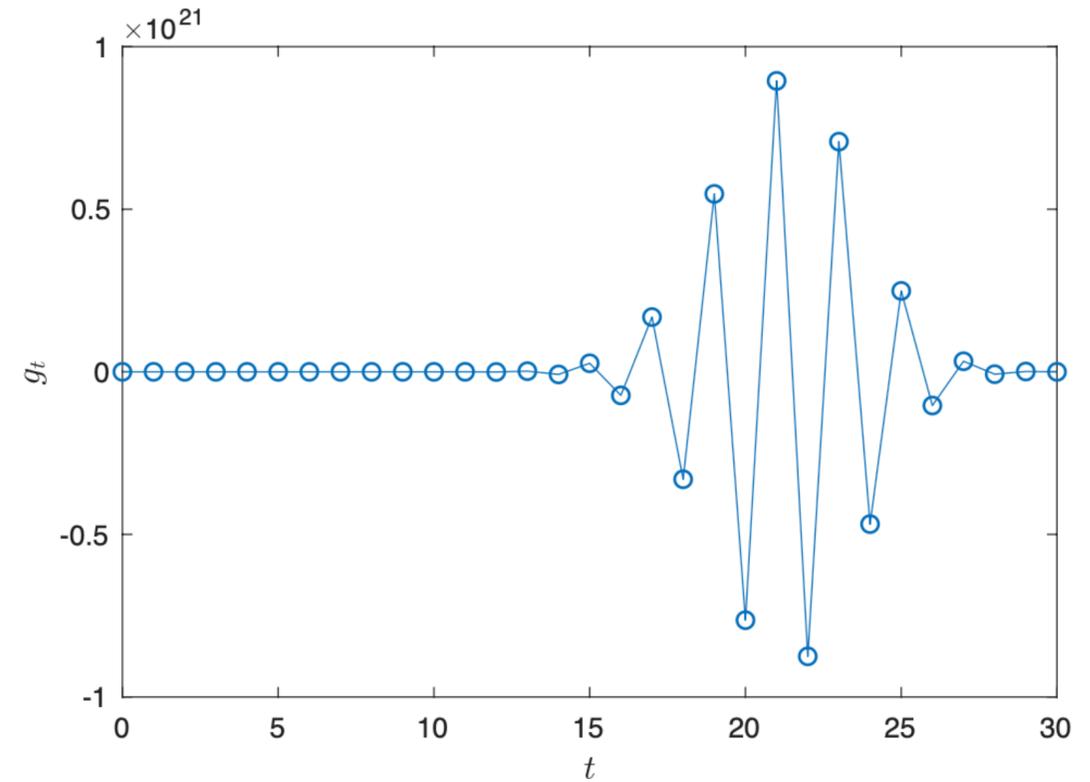


FIG. 2: Values of the coefficients $g_t(E_*)$ corresponding to the smearing function $\Delta^{BG}(E_*, E)$ shown in the right-panel of Figure 1, i.e. the coefficients obtained by applying the Buckus-Gilbert procedure in the absence of statistical errors with $E_* = 0.5$, $b_\infty(t, E)$ as basis functions and $t_{max} = 30$. A typical pattern for these coefficients is that they change sign and for some values of t they have extremely large absolute values (the scale on the y -axis varies between $\pm 10^{21}$).

The idea of the Buckus-Gilbert method

- Consider statistical errors

λ : a free parameter chosen in the range $[0,1]$

$$C_i(t) = \bar{C}(t) + \delta C_i(t)$$

$$B[g] = \mathbf{g}^T \text{Cov} \mathbf{g}$$



minimizing

$$W[\lambda, g] = (1 - \lambda) A_{BG}[g] + \lambda B[g]$$

$$\text{Cov}_{tr} = \frac{1}{N-1} \sum_{i=0}^{N-1} \delta C_i(t+1) \delta C_i(r+1)$$

$$\Rightarrow \mathbf{g}(\lambda, E_\star) = \frac{\mathbf{W}^{-1}(\lambda, E_\star) \mathbf{R}}{\mathbf{R}^T \mathbf{W}^{-1}(\lambda, E_\star) \mathbf{R}} \quad \text{with} \quad \mathbf{W}_{tr}(\lambda, E_\star) = (1 - \lambda) \mathbf{A}_{tr}(E_\star) + \lambda \text{Cov}_{tr}$$

From B.-G. to the HLT method

Smearing function as an input

- The target smearing function becomes an input to the algorithm, for example, a Gaussian function:

$$\Delta_{\sigma}(E_{\star}, E) = \frac{e^{-\frac{(E-E_{\star})^2}{2\sigma^2}}}{\int_0^{\infty} dE e^{-\frac{(E-E_{\star})^2}{2\sigma^2}}}$$

- The method then searches for an optimal approximation of the target smearing function in the space spanned by the basis functions:

$$\bar{\Delta}_{\sigma}(E_{\star}, E) = \sum_{t=0}^{t_{max}} g_t(\lambda, E_{\star}) \underbrace{b_T(t+1, E)}_{\text{basis function}}$$

From B.-G. to the HLT method

minimizing

$$W[\lambda, g] = (1 - \lambda)A[g] + \lambda \frac{B[g]}{C(0)^2} \quad \leftarrow B[g] = \mathbf{g}^T \text{Cov } \mathbf{g}$$

$$A[g] = \int_{E_0}^{\infty} dE \left| \underbrace{\bar{\Delta}_{\sigma}(E_{\star}, E)}_{\text{basis function}} - \underbrace{\Delta_{\sigma}(E_{\star}, E)}_{\text{target smearing function}} \right|^2$$

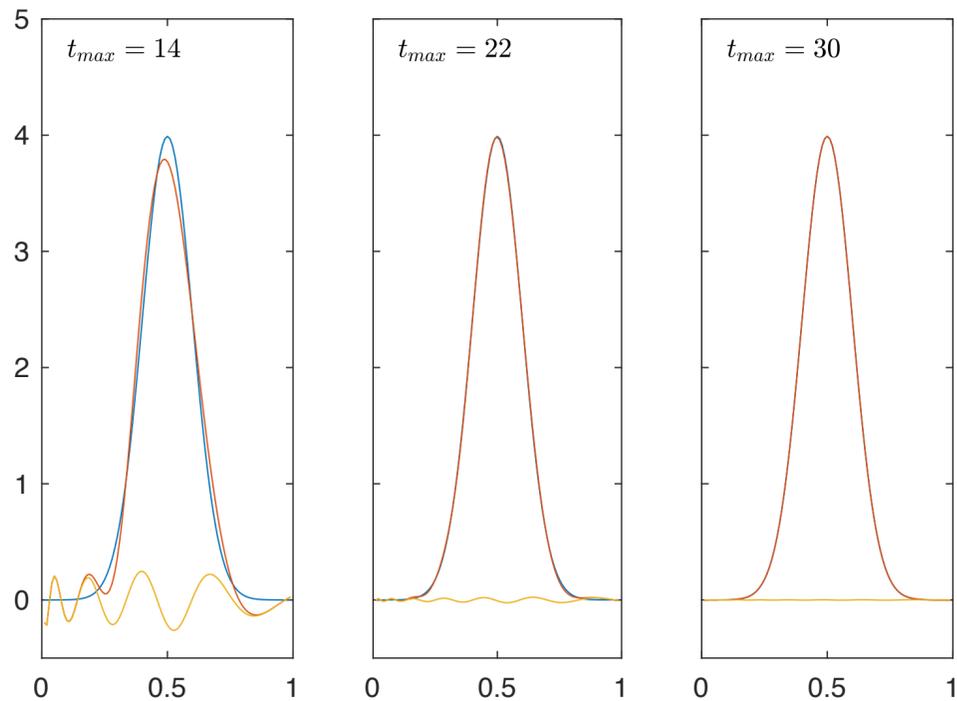
$$f_t(\lambda, E_{\star}) = (1 - \lambda) \int_{E_0}^{\infty} dE b_T(t + 1, E) \Delta_{\sigma}(E_{\star}, E)$$

$$\Rightarrow \mathbf{g}(\lambda, E_{\star}) = \mathbf{W}^{-1}(\lambda) \mathbf{f}(\lambda, E_{\star})$$

$$+ \mathbf{W}^{-1}(\lambda) \mathbf{R} \frac{1 - \vec{R}^T \mathbf{W}^{-1}(\lambda) \vec{f}(\lambda, E_{\star})}{\mathbf{R}^T \mathbf{W}^{-1}(\lambda) \mathbf{R}} \quad \left| \begin{array}{l} \mathbf{W}_{tr}(\lambda) = (1 - \lambda) \mathbf{A}_{tr} + \lambda \frac{\text{Cov}_{tr}}{C(0)^2} \\ \mathbf{A}_{tr} = \int_{E_0}^{\infty} dE b_T(t + 1, E) b_T(r + 1, E) \end{array} \right.$$

From B.-G. to the HLT method

Basis function: exp



Basis function: cosh

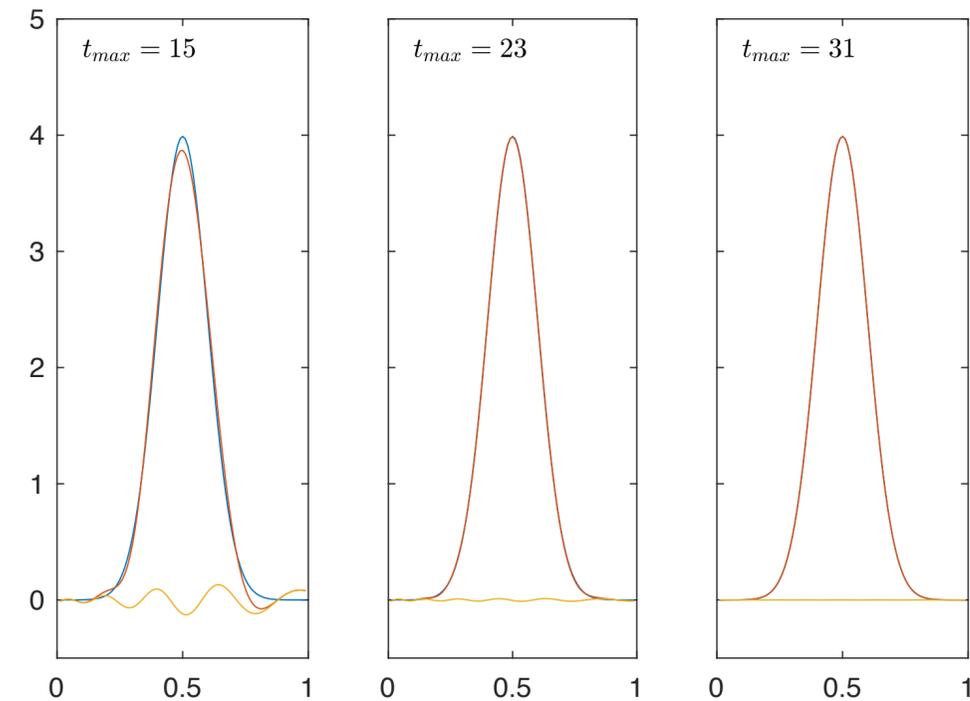


FIG. 3: Comparison of the target smearing function $\Delta_\sigma(E_\star, E)$ (blue curves) at $E_\star = 0.5$ and $\sigma = 0.1$ with the functions $\bar{\Delta}_\sigma(E_\star, E)$ (red curves) obtained with our method. In each row the different panels correspond to different values of t_{max} . The panels in the first row correspond to the choice of $b_\infty(t, E)$ as basis functions while the panels in the second row to the choice of $b_T(t, E)$ with $T = 2(t_{max} + 1)$. In all plots the yellow curve shows the difference, and as expected, it goes to zero in the limit of large t_{max} .

- In the Backus–Gilbert method, by changing t_{max} , one gets a different (sharper) function.
- In the HLT method, by increasing t_{max} , one gets a better approximation of the target smearing function.

From B.-G. to the HLT method

- Difference between the target and the approximated smearing functions

$$\delta_\sigma(E_\star, E) = 1 - \frac{\bar{\Delta}_\sigma(E_\star, E)}{\Delta_\sigma(E_\star, E)}$$

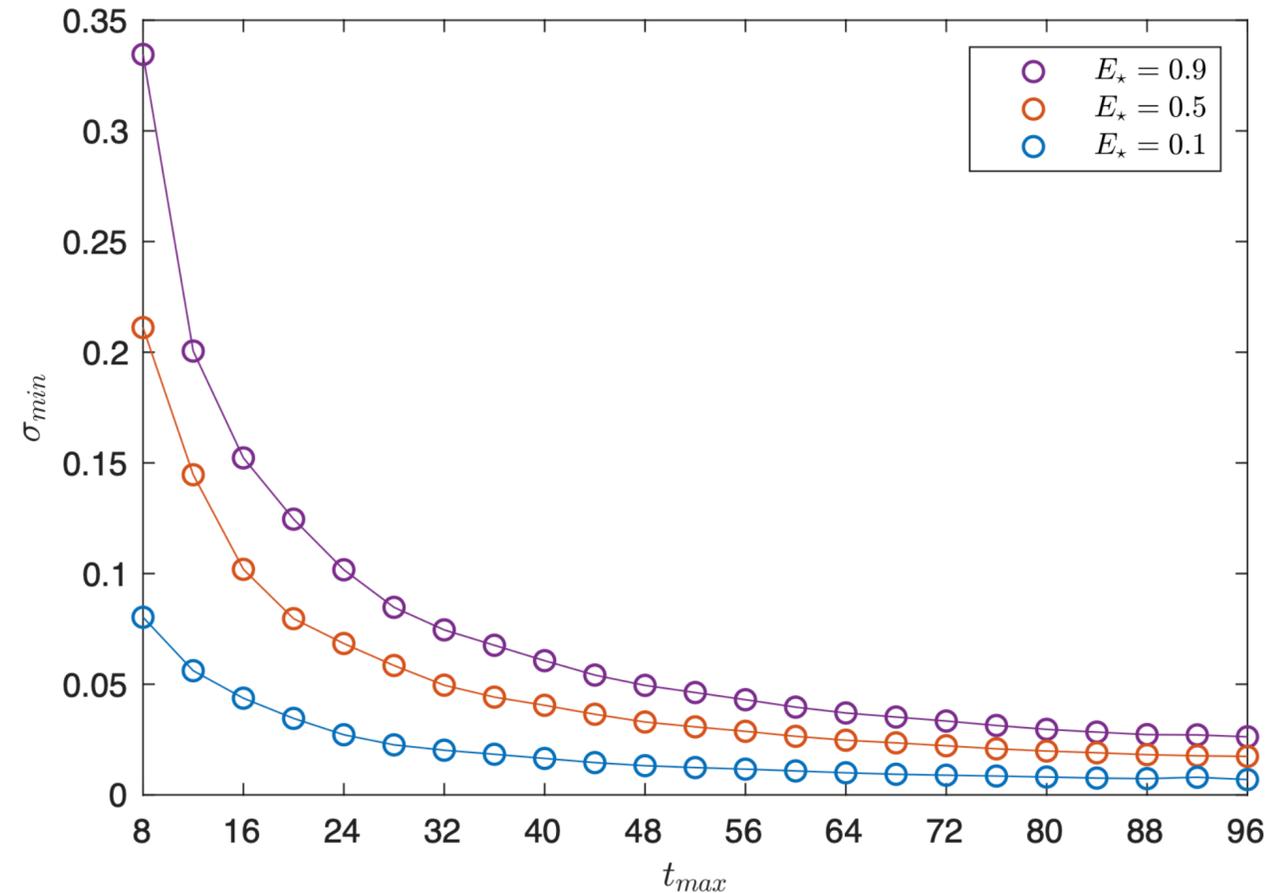


FIG. 4: Solution to the equation $\delta_\sigma(E_\star, E_\star) = 0.05$ as a function of t_{max} for three different values of E_\star in the case where $B[g] = 0$. The solution indicates the smallest possible choice of σ ensuring that the relative error on the target smearing function is below 5%.

From B.-G. to the HLT method

- Choosing the trade-off parameters, λ

$$W(\lambda, E_\star) = W[\lambda, g(\lambda, E_\star)]$$

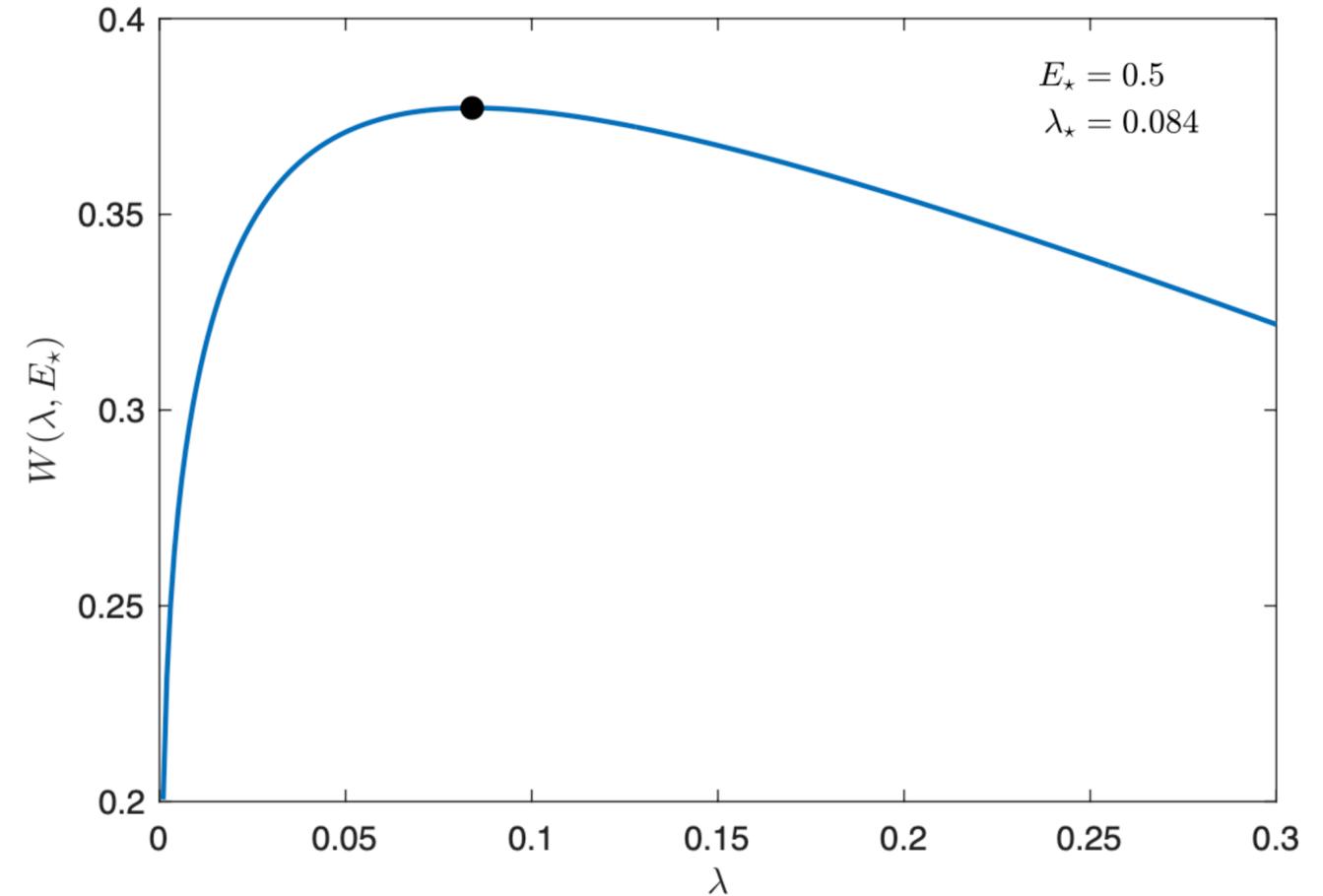
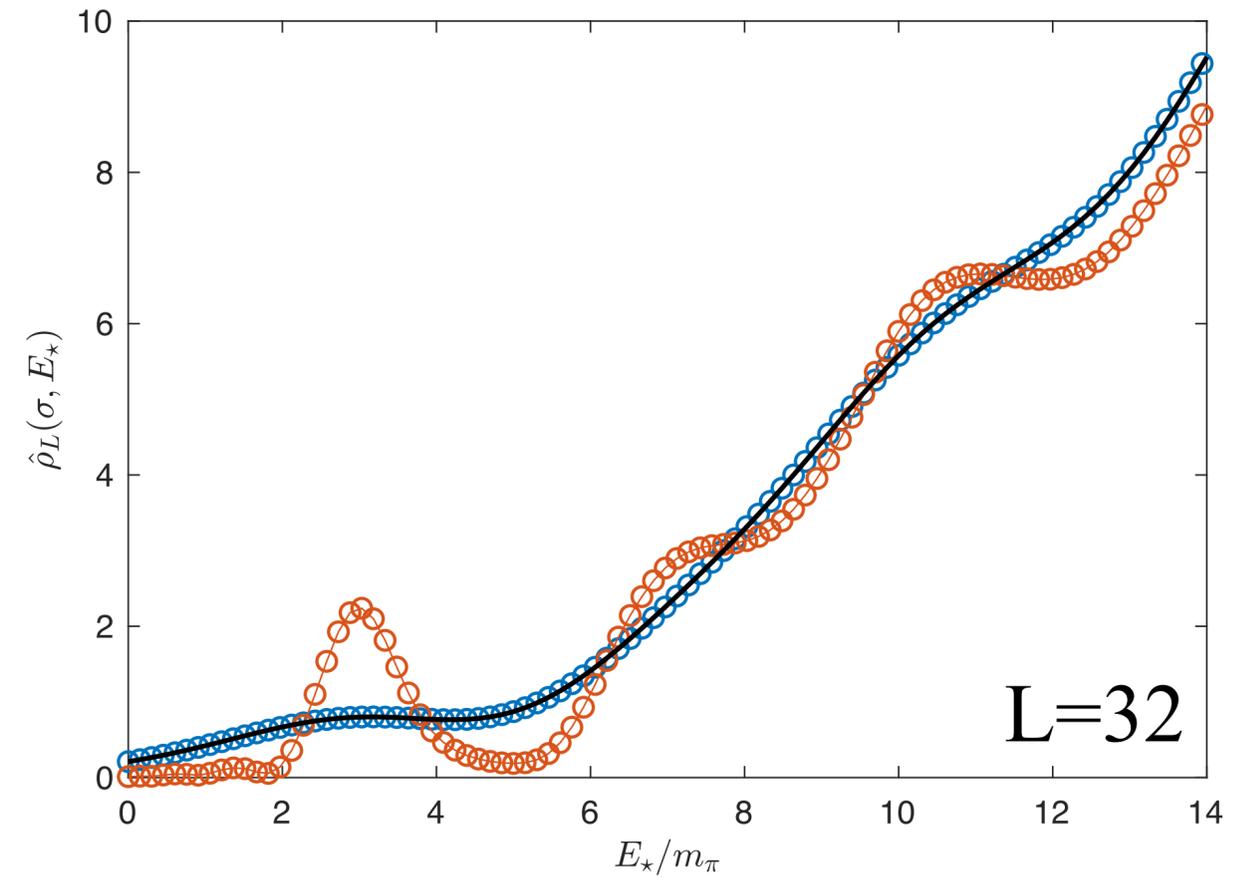
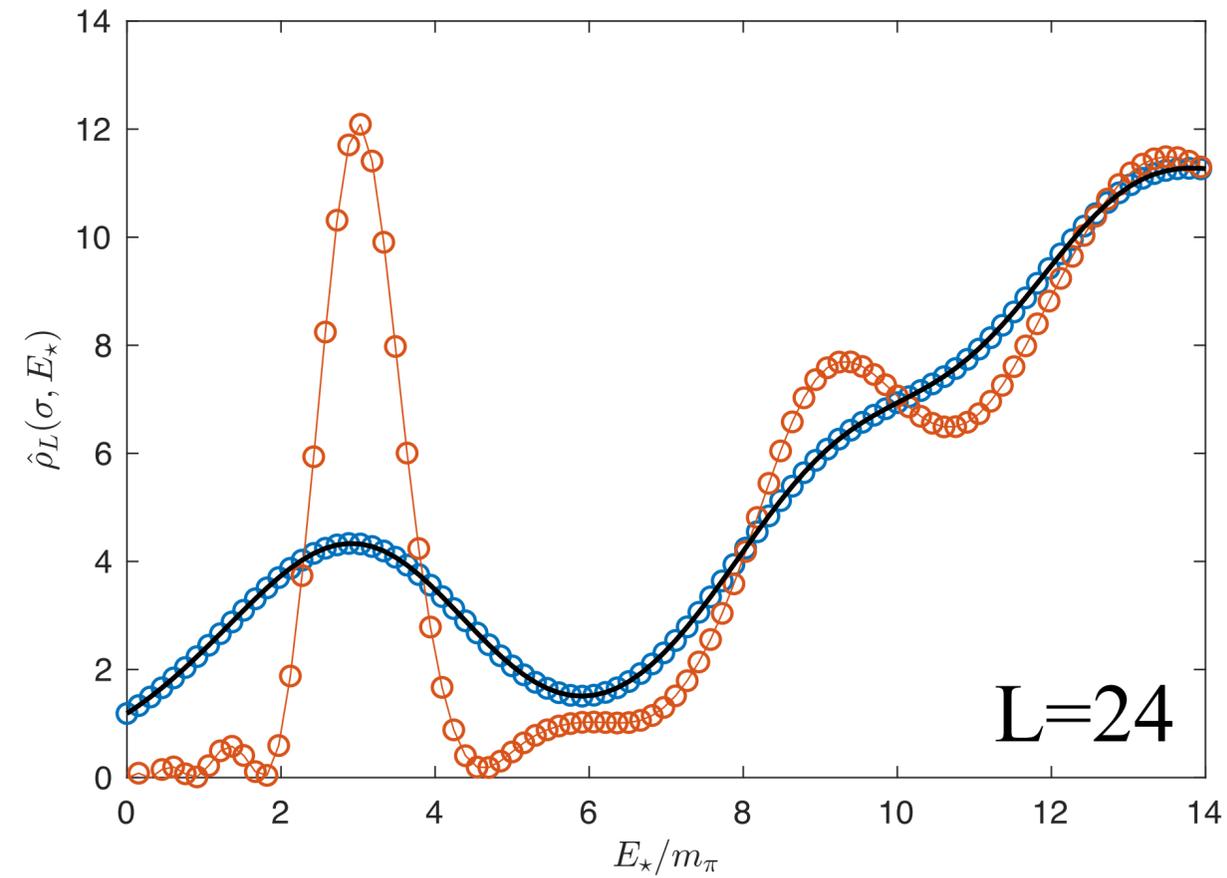


FIG. 5: The function $W(\lambda, E_\star)$ in the case of the lattice QCD correlator discussed in section V at $E_\star = 0.5$. This function has a characteristic shape exhibiting a maximum at the optimal value λ_\star of the trade-off parameter where the deterministic and error functionals are equally important in the minimization procedure.

Some examples

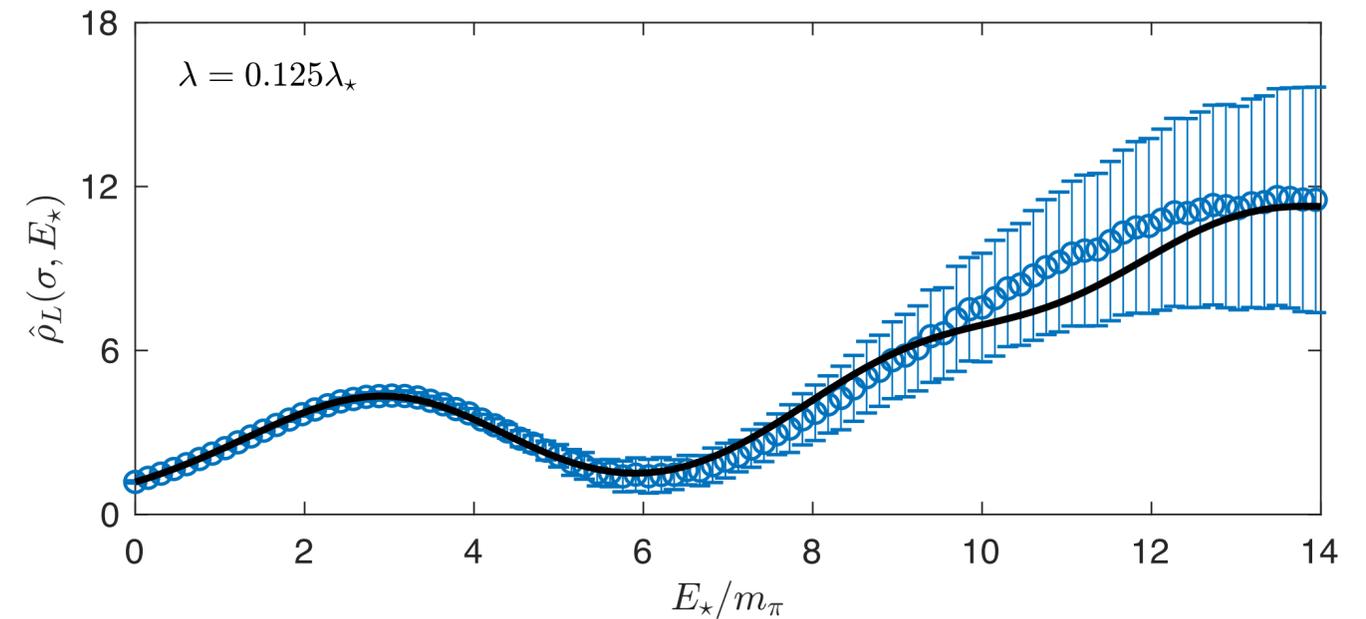
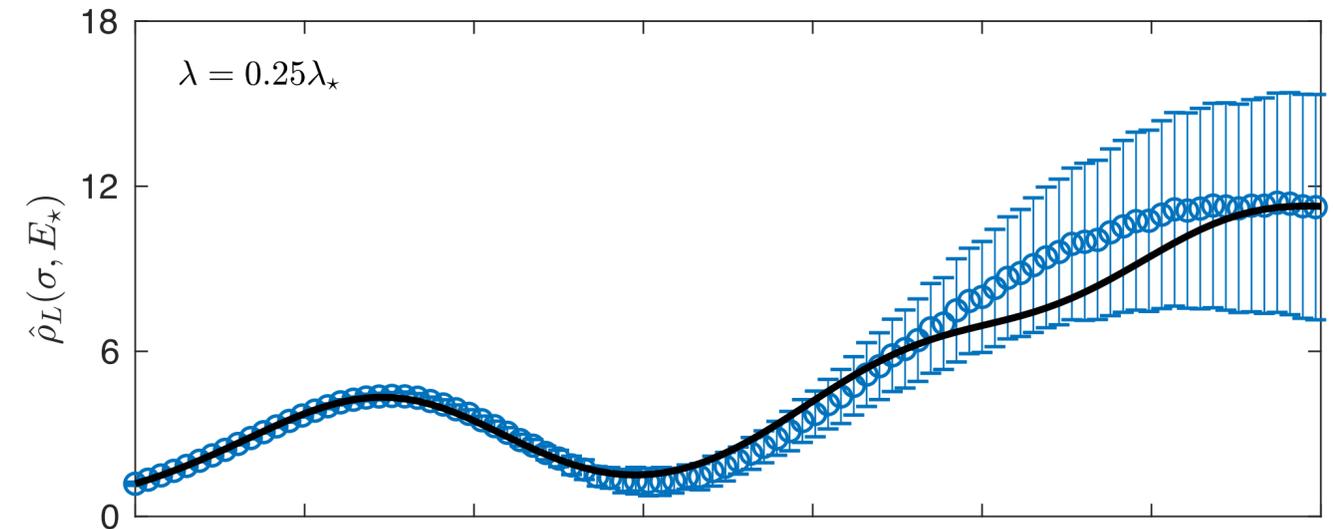
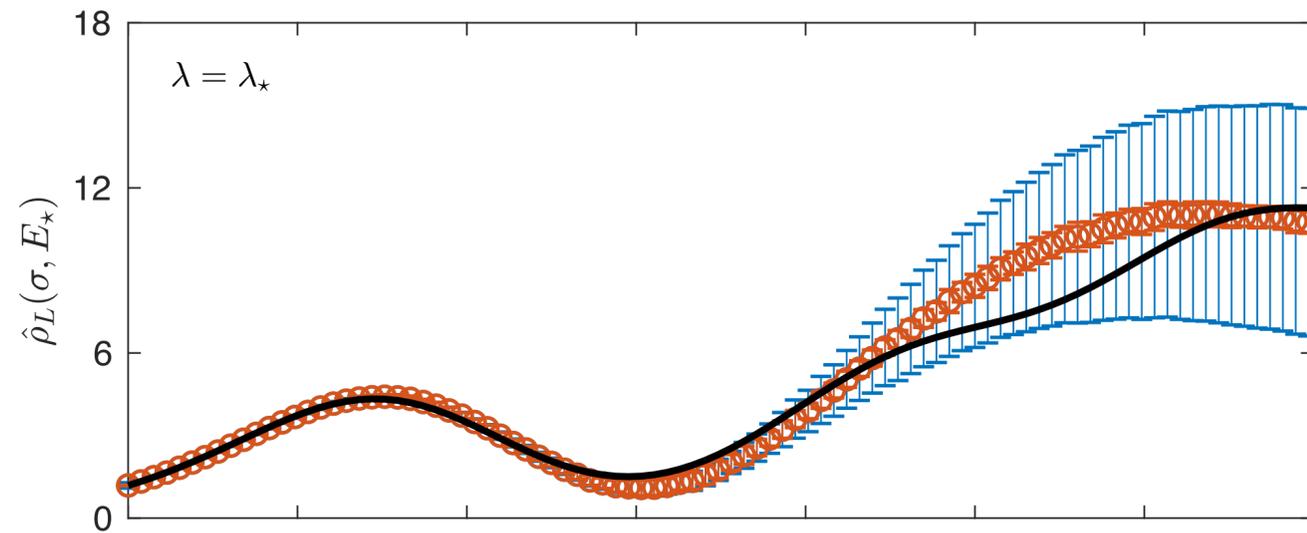
No errors



- Orange points: BG, Blue point: HLT method

Some examples

with errors and λ dependance



- Orange points: only statistical error, Blue points: adding systematic errors

Some examples

QCD data

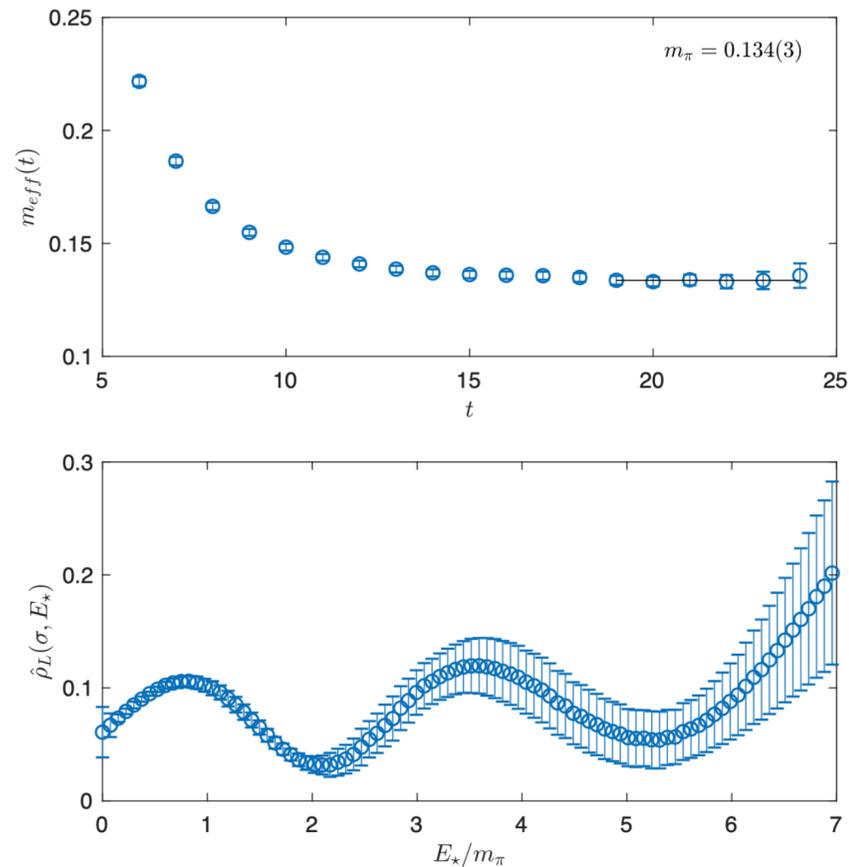


FIG. 10: Extraction of the smeared spectral density from the correlator $C_{\text{QCD}}(t)$ discussed in the text. The top-panel shows the calculation of the pion mass, the lightest state contributing to the spectral density in this case, extracted from a standard effective-mass analysis. The bottom-panel shows the reconstructed smeared spectral density obtained by applying our method with $\sigma = 0.1$, by using $b_T(t, E)$ as basis functions with $T = 48 = (2t_{max} + 1)$, by setting $E_0 = 0.37m_\pi$ and by using the value of λ_* determined at $E_* = 3.7m_\pi$ for all the energies explored. As expected, the smeared spectral density shows a peak in correspondence of $E_*/m_\pi \simeq 1$ and another structure around $E_*/m_\pi \simeq 3$.

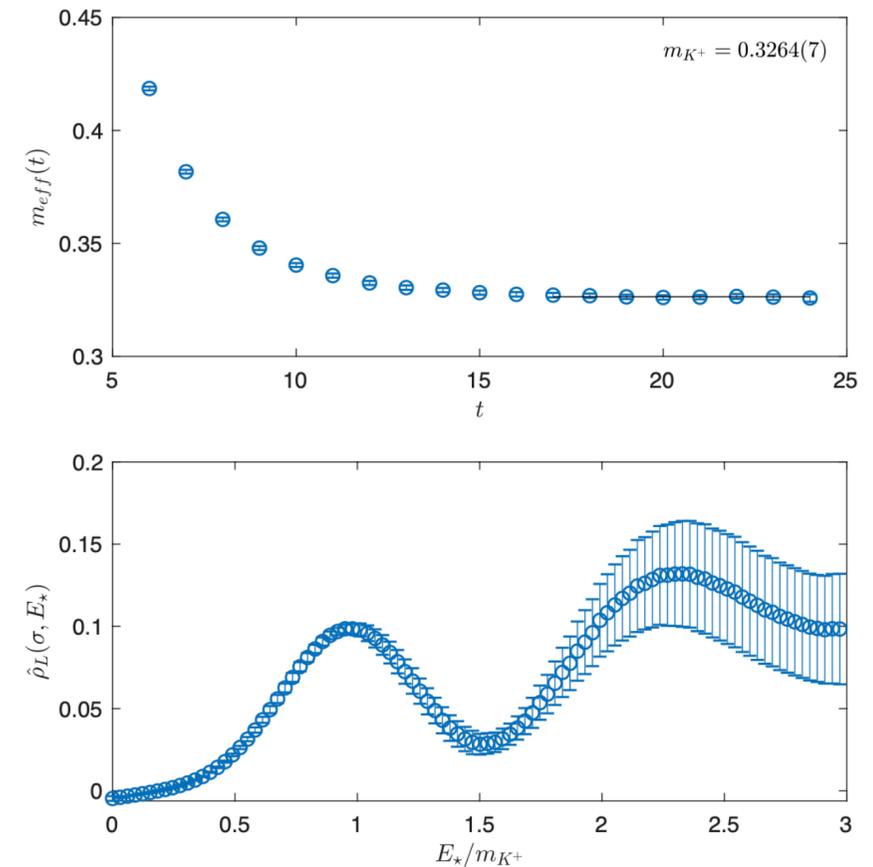


FIG. 11: Extraction of the smeared spectral density from the correlator $C_{\text{QCD}+\text{QED}}(t)$ discussed in the text. The top-panel shows the calculation of the charged kaon mass, the lightest state contributing to the spectral density in this case, extracted from a standard effective-mass analysis. The bottom-panel shows the reconstructed smeared spectral density obtained by applying our method with $\sigma = 0.1$, by using $b_T(t, E)$ as basis functions with $T = 48 = (2t_{max} + 1)$, by setting $E_0 = 0.15m_{K^+}$ and by using the value of λ_* determined at $E_* = 1.5m_{K^+}$ for all the energies explored. As expected, the smeared spectral density shows an isolated peak in correspondence of $E_*/m_{K^+} \simeq 1$ and another structure that starts in proximity of $E_*/m_{K^+} \simeq 2.4$.

Summary

- Buckus-Gilbert method: Smearing function to prob the spectrum density is an output
 - ➔ With large t-max, it goes closer to a delta function
- HLT method: Smearing function is an input to find the best overlap of basis functions
 - ➔ With large t-max, it goes closer to the target smearing function
- Examining the λ and σ parameters