Retrieving the optical potential from lattice simulation

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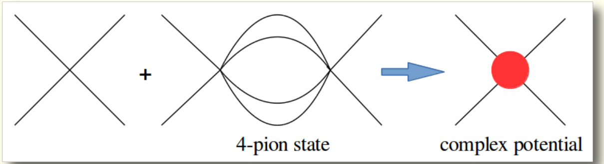
- *ab-initio* calculations of hadron-hadron scattering can be performed on the discretized *Euclidean* space-time in finite volume
- In the single channel case - Lüscher approach Lüscher (1991)
  - For fixed L and P each energy level $\to$ scattering phase in the infinite volume
  - The finite-volume corrections to the scattering phase are exponentially suppressed
  - Mass and width of the resonances are extracted from the measured phase $\rightsquigarrow$ analytical behavior of the scattering has to be known (UChPT,...)
- Multiple two-particle channels - coupled channel Lüscher equation
  Lage, Meißner, Rusetsky (2009), Hansen, Sharpe (2012), ...
  - more unknowns than measurements at a single energy
  - phenomenological parameterizations inevitable (eff.-range exp., K-Matrix...)
    Hadron Spectrum Collaboration (2014-2016)
- Three- or more-particle states Polejaeva, Rusetsky (2012) Hansen, Sharpe (2014)
  - hardly applicable for the data analysis (at the moment!)
  - phenomenological parametrization unclear (at the moment!)

Q But, do we need to resolve into individual channels at all?

- In continuum, effects of **any** inelastic channels can be included via *optical potential* Feshbach (1958), Kerman, McManus, Thaler (1959)
- Example: $\pi\pi$ scattering $(N_f = 2)$
  - above 4π-threshold $\pi\pi$ and $\pi\pi\pi\pi$ states contribute to inelasticity



$\Rightarrow$ $\pi\pi$-scattering amplitude is a ***single-channel*** equation w.r.t the *optical potential*

Q Can we extract such complex valued potential from a set of real energy eigenvalues measured in finite volume?

$\Rightarrow$ YES - this work.

Scattering in the infinite volume

- S-Matrix describes scattering experiments. It is related to the scattering amplitude T via
$$S = \mathbb{1} - iT$$

- Two-particle scattering amplitude can be parametrized by the K-Matrix. Let us start from two two-particle states: $K\bar{K}$ and $\pi\eta$ in S-wave
$$T = \frac{1}{K^{-1} - iDiag\{p_{K\bar{K}}, p_{\pi\eta}\}}$$

  - general derivation requires Feshbach projection operator technique

  Feshbach (1958), ADMMR (2016)

- If we are interested in $K\bar{K}$ scattering (primary channel) then
$$T_{K\bar{K}\to K\bar{K}} = \frac{1}{W^{-1}(E) - ip_{K\bar{K}}} \quad \text{for} \quad W^{-1} = M_{K\bar{K}\to K\bar{K}} - \frac{M^2_{K\bar{K}\to\pi\eta}}{M_{\pi\eta\to\pi\eta} - ip_{\pi\eta}}$$

  - $M := K^{-1}$ is smooth, although K can have poles for $E \in \mathbb{R}$
  - $W \in \mathbb{C}$ contains all inelasticities from the secondary channels and determines the scattering amplitude in this channel!!!

Scattering in the finite volume

Q What is measured in a Lattice simulation?

- Periodic boundary conditions lead to modification of the loop functions:

$$ip \to \frac{2}{\sqrt{\pi}L}\,Z_{00}(1;q^2) \text{ for } q = \frac{pL}{2\pi}$$

- The unitarity cut becomes a set of poles on the real axis

- Energy eigenvalues (E^*) measured on the lattice are energies, for which $T^{-1}(E^*) = 0$ or

$$\frac{2}{\sqrt{\pi}L}\,Z_{00}(1;q^2_{K\bar{K}}(E^*)) = M_{K\bar{K}\to K\bar{K}}(E^*) - \frac{M^2_{K\bar{K}\to\pi\eta}(E^*)}{M_{\pi\eta\to\pi\eta}(E^*) - \frac{2}{\sqrt{\pi}L}\,Z_{00}(1;q^2_{\pi\eta}(E^*))}$$

$\Rightarrow$ for every E^*: $W_L^{-1}(E^*) = \frac{2}{\sqrt{\pi}L}\,Z_{00}(1;q^2_{K\bar{K}}(E^*))$ [$\sim$ cot (*pseudophase*)]

Q How can we retrieve the infinite volume potential?

- Simple $\lim_{L\to\infty} W_L^{-1}$ is **not** well defined
  $\to$ adiabatic switching of the interaction $\Leftrightarrow$ $E \mapsto E + i\epsilon$ DeWitt (1956)

$$W^{-1}(E) = \lim_{\epsilon\to 0}\lim_{L\to\infty} W_L^{-1}(E + i\epsilon)$$

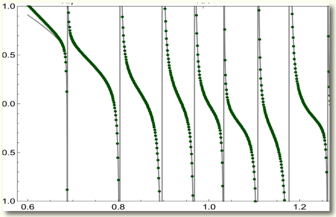
Step-by-step program

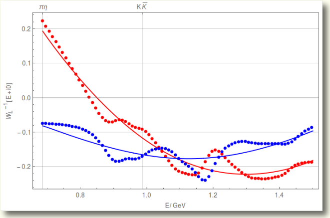
- The input from a lattice simulation (L and P fixed) is

$$\begin{pmatrix} E_1^* & , & \dots \\ W_L^{-1}(E_1^*) = \frac{2}{\sqrt{\pi}L} Z_{00}(1; q^2_{K\bar{K}}(E_1^*)) & , & \dots \end{pmatrix}$$

Step 1. The functional behavior of $W_L^{-1}(E)$ is governed by simple poles + some background

$$\hat{W}_L^{-1}(E) = \sum_i^N \frac{Z_i}{E - Y_i} + D_0 + D_1 E + D_2 E^2 + D_3 E^3$$





Step 2. Perform analytic continuation to the complex plane ⇝ oscillations

Step 3. $L \to \infty$ limit obtained after "smoothing" over the oscillations

Step 4. Perform limit $\epsilon \to 0$

Test of the framework - fit

- UChPT Ansatz to produce synthetic data for the $\pi\eta$-$K\bar{K}$ system. Oller, Oset (1997)
  Fairly large energy range: $E = 2M_K ... 1.7$ GeV, $L = 5M_\pi^{-1}$

Step 1: fit. Do we have enough data to fit $\hat{W}_L^{-1}(E)$?
In the given range ~ 30 energy levels are accessible,
but $\hat{W}_L^{-1}(E)$ has around 36 free parameters: Y_i, Z_i, D_i

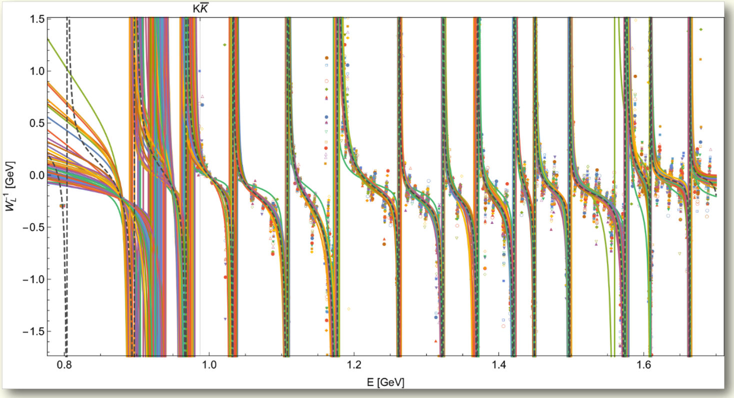
- Levels from lattices of different sizes or reference frames **cannot** be combined directly
- For certain systems twisted boundary conditions is helpful: Bedaque, Chen (2005)
  Twist only the u- and d-quarks by an angle θ
  - $Z_{00}(1; q^2_{K\bar{K}}) \to Z^\theta_{00}(1; q^2_{K\bar{K}})$ "scan function"
  - $Z_{00}(1; q^2_{\pi\eta})$ remains $\Rightarrow$ intrinsic properties of the system unchanged
  - Very economical, if *partial twisting* can be used Agadjanov, Meißner, Rusetsky (2014)
- For six twisting angles 189 energy eigenvalues can (in principle) be obtained

If you think this is too much, call it 26 per 100 MeV

Test of the framework - fit

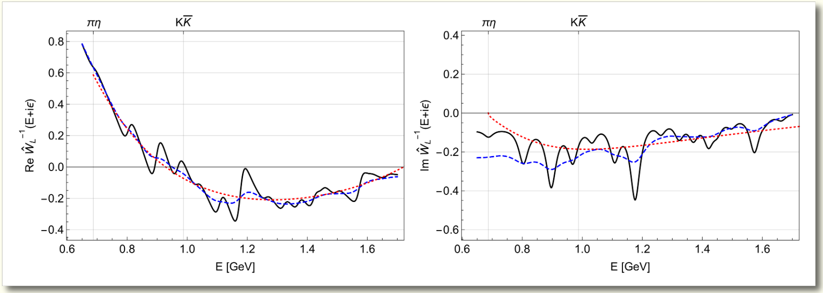
- Realistic simulations have error bars on the energy eigenvalues: ΔE
  - The error bars on $Z^{\theta}_{00}(1; q^2_{K\bar{K}}(E))$ are inclined $\Rightarrow$ what is proper $\chi^2_{\text{d.o.f}}$?
  - In an NLO expansion around the central value

$$\chi^2_{\text{d.o.f.}} = \frac{1}{N-n}\sum_{i=1}^{N}\frac{1}{\Delta E^2}\left(\frac{\hat{W}_L^{-1}(E) - Z^{\theta_i}_{00}(1; q^2_{K\bar{K}}(E))}{\left(\hat{W}_L^{-1}(E) - Z^{\theta_i}_{00}(1; q^2_{K\bar{K}}(E))\right)'}\right)^2_{E=E_i}$$



Test of the framework - smoothing

Step 2: analytical continuation. $\hat{W}_L^{-1}(E) \mapsto \hat{W}_L^{-1}(E + i\epsilon)$



Test of the framework - smoothing

Step 3: $L \to \infty$ limit. Many algorithms exist to smooth over unwanted oscillations.

- Non-parametric method - Gaussian smearing:
  Replace any point of a uniformly distributed data by the weighted $(\exp(-\frac{2x^2}{r^2}))$ *average over its neighboring points within the radius* r.
- Parametric method:
  Fit a general Ansatz, which respects analytical properties. Suppress oscillations, minimizing the modulus of second derivative.
  - Model selection via LASSO method and cross validation

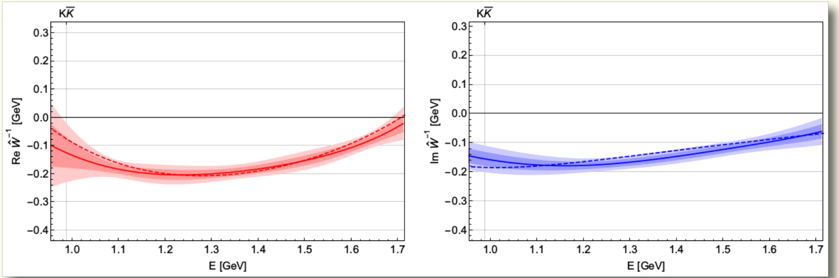
Tibshirani (1996), Ozaki, Sasaki (2013)

Step 4: $\epsilon \to 0$ limit. Gives the infinite volume optical potential!

RECALL: $$S_{K\bar{K}\to K\bar{K}}(E) = 1 - \frac{i}{W^{-1}(E) - ip_{K\bar{K}}}$$

Test of the framework - results

- Repeat the program for re-sampled lattice data sets (~ 1000). Estimate the 1σ and 2σ bands.
  - For $\Delta E = 1$ MeV on the energy eigenvalues



  - Different smoothing methods lead to the same results
  - Uncertainty grows mostly linear with ΔE
  - $\Re(W^{-1}(E))$ is quite stable
  - $\Im(W^{-1}(E))$ is more sensitive, especially when fit misses some poles

Summary and outlook

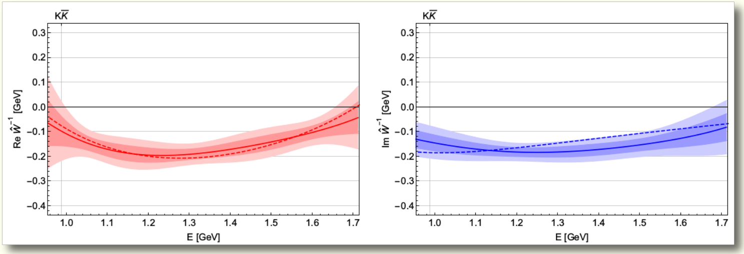
DONE

- A theoretical framework for the extraction of the optical (complex valued) potential from the energy spectrum of LQCD is formulated
- Test on synthetic data reveals possible complications $\rightarrow$ solutions are suggested:
  - use (partially) twisted b.c. to raise the number of extracted energy eigenvalues
  - smoothing methods
  - realistic uncertainty determination

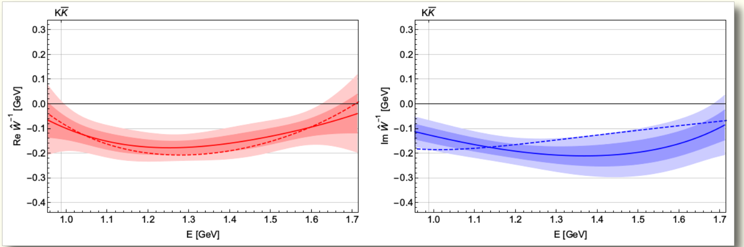
TO DO

- Test on the real lattice data for $\phi^4(D = 1 + 1)$ theory is in preparation
- Application to systems with three-particle intermediate channels is highly tempting
- Similarly, exotic states $Z_c(3900)$ or $Z_c(4025)$ can be studied

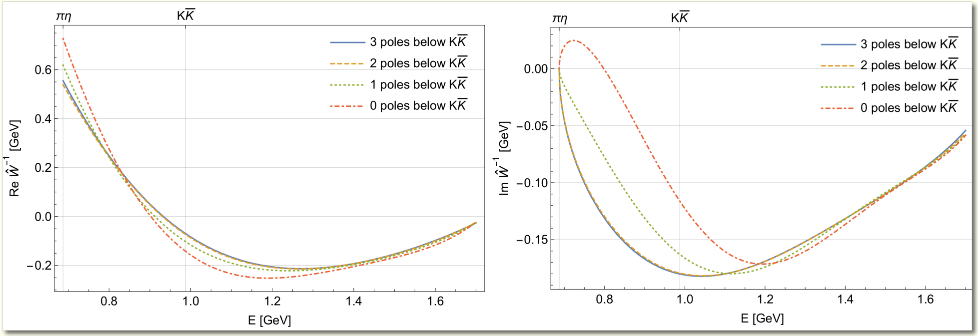
THANK YOU!



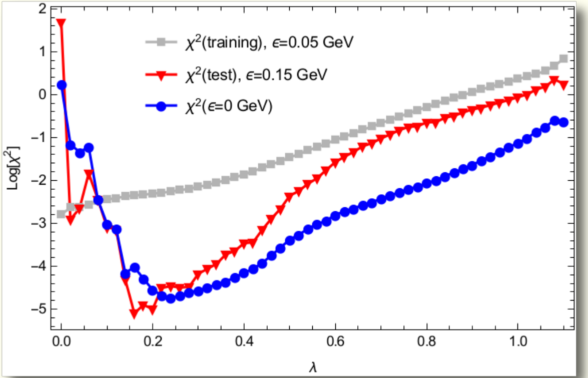
$K\bar{K}$
$K\bar{K}$
$\mathrm{Re}\,\hat{W}^{-1}$ [GeV]
$\mathrm{Im}\,\hat{W}^{-1}$ [GeV]
E [GeV]
E [GeV]



$K\bar{K}$
$K\bar{K}$
$\mathrm{Re}\,\hat{W}^{-1}$ [GeV]
$\mathrm{Im}\,\hat{W}^{-1}$ [GeV]
E [GeV]
E [GeV]



πη
KK̄
3 poles below KK̄
2 poles below KK̄
1 poles below KK̄
0 poles below KK̄
Re Ŵ⁻¹ [GeV]
E [GeV]
Im Ŵ⁻¹ [GeV]
0.6
0.4
0.2
0.0
−0.2
0.00
−0.05
−0.10
−0.15
0.8
1.0
1.2
1.4
1.6



2
1
0
−1
−2
−3
−4
−5
Log[χ²]
χ²(training), ϵ=0.05 GeV
χ²(test), ϵ=0.15 GeV
χ²(ϵ=0 GeV)
0.0
0.2
0.4
0.6
0.8
1.0
λ