N particles in ϕ^4 theory

ETMC Meeting Fall 2019

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in cooperation with
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Motivation — Why ϕ^4-theory?

- **First step** towards lattice QCD
  $\hookrightarrow$ progress in exploration of multihadron matrix elements

- Complex scalar ϕ^4-theory as a **toy model**
  - Weakly coupled model
  - Playground for new developments in multiparticle dynamics
  - Simulation costs cheaper than in lattice QCD

Motivation – Finite Volume Quantities

Access to finite volume quantities via Lüscher formalism

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Access to finite volume quantities via Lüscher formalism

1) **Lüscher threshold expansion** [Huang, Yang, 1957, Lüscher, 1986]

- Two identical particles

- Relates ΔE_2 due to two particle scatt. in finite volume L^3 and a_0

  $a_0 \hat{=}$ low energy S-wave scattering length

- Momenta have discrete values, $\vec{p} = \frac{2\pi}{L}\,\vec{n} \quad \forall \vec{n} \in \mathbb{Z}$

Motivation – Finite Volume Quantities

$2)$ **Expansion in L to $\mathcal{O}(L^{-6})$**

[Beane, Detmold, Savage, 2007, Hansen, Sharpe, 2017, Pang *et al.*, 2019]

- **Two-body sector** — effective range parameter r
- **Three-body sector** — three-body contact interaction η_3 and r

Motivation – Finite Volume Quantities

$2)$ Expansion in L to $\mathcal{O}(L^{-6})$

[Beane, Detmold, Savage, 2007, Hansen, Sharpe, 2017, Pang *et al.*, 2019]

- **Two-body sector** effective range parameter r
- **Three-body sector** three-body contact interaction η_3 and r

Effective range expansion in low energy limit

$$k \cot \delta_0(k) = -\frac{1}{a_0} + \frac{r\,k^2}{2} + \mathcal{O}(k^4)$$

$\hookrightarrow$ r determines behavior of phase shift $\delta_0(k)$ in next leading order

Motivation

- **Try to answer questions**

Is it possible to ...

... determine **correlation functions** for multiparticle states?
$\hookrightarrow$ technical challenge: signal $\leftrightarrow$ thermal pollution

... identify **fundamental scattering parameters** (a_0, r, η_3) consistently?

... determine the three body coupling constant η_3 significantly **different from zero**?

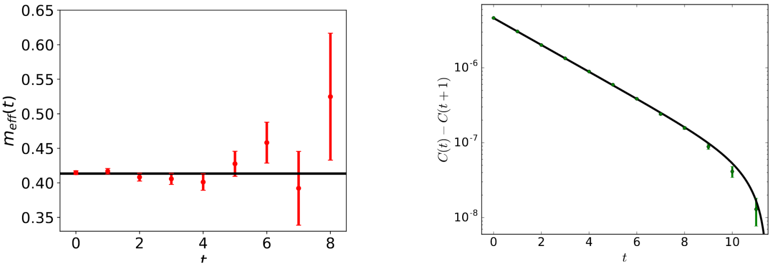
Motivation

Two- and three-body interactions in ϕ^4-theory from lattice simulations
[Romero-López, Rusetsky, Urbach, 2018]

- Compute one- to three-particle energy levels for different lattice volumes $T \cdot L^3$ in complex ϕ^4-theory
- Calculate two- and three-particle energy shifts in dependency on L
- From that: extract a_0, r, η_3

Motivation

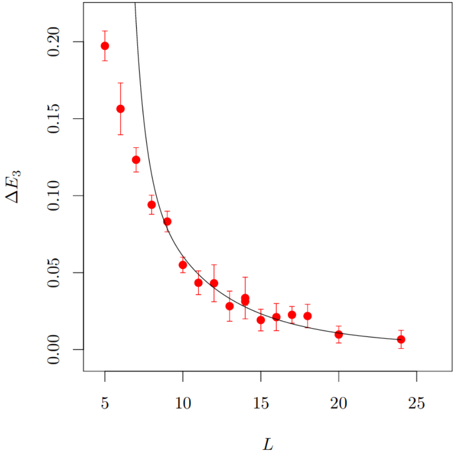
Two particle effective mass and correlation function for $L = 18$



[Romero-López, Rusetsky, Urbach, 2018]

Motivation

Fit to the ΔE_3 data in the interval [9,24]



[Romero-López, Rusetsky, Urbach, 2018]

Motivation

- **New** compared to [Romero-López, Rusetsky, Urbach, 2018]
  - Calculation of **four and five particle energy levels**
  - More ensembles $\rightarrow$ more data points
  - Increased number of field configurations

Theoretical Foundations – k Particle Energy Shift

Non-relativistic expansion for k particle scattering

$$\Delta E_k(L) = \frac{4\pi a_0}{M_\phi L^3}\binom{k}{2}\left[1 + c_1\left(\frac{a_0}{\pi L}\right) + c_2(k)\left(\frac{a_0}{\pi L}\right)^2 + c_3(k)\left(\frac{a_0}{\pi L}\right)^3 + \frac{2\pi a_0^2 r}{L^3}\right]$$
$$+ \binom{k}{3}\frac{1}{L^6}\left[\eta_3 + \frac{64\pi a_0^4}{M_\phi}(3\sqrt{3} - 4\pi)\log\left(\frac{M_\phi L}{2\pi}\right)\right] + \mathcal{O}(L^{-7})$$

[Beane, Detmold, Savage, 2007]

$k \;\hat{=}$ number of particles

$E_k \;\hat{=}$ interaction k particle energy

$a_0 \;\hat{=}$ scattering length

$r \;\hat{=}$ effective range

$\eta_3 \;\hat{=}$ three-body contact interaction

Simulation and Analysis – Recipe

A **Field configurations** (Metropolis)

B One to five particle **correlation functions**

C **Corr-fit:** Extract M_ϕ, E_k $\Rightarrow \Delta E_k(L) = E_k(L) - k \cdot M_\phi(L)$

k : Number of particles

D $\Delta E_k(L)$**-fit:** Extract $a_0,\ r,\ \eta_3$

Simulation — Discretized Action

- **Complex ϕ^4-Theory**

$$S[\phi] = \int \mathsf{d}^4x \left[\partial_\mu \phi^* \, \partial^\mu \phi - m^2 \left|\phi\right|^2 - \lambda \left|\phi\right|^4\right]$$

Simulation – Discretized Action

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$$S[\phi] = \int \mathrm{d}^4x \left[\partial_\mu \phi^* \, \partial^\mu \phi - m^2 \, |\phi|^2 - \lambda \, |\phi|^4\right]$$

- **Rescaling**

$$a\,\phi(x) \coloneqq \sqrt{\kappa}\,\phi_x, \qquad (am)^2 \coloneqq \frac{1-2\lambda'-8\kappa}{\kappa}, \qquad \lambda \coloneqq \frac{\lambda'}{\kappa^2}, \qquad a \mathrel{\hat{=}} \text{lattice const.}$$

$\Rightarrow$ Terms depending on $|\phi|$ are converted to binary quadratic form

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Discretized action

$$S = \sum_x \left[\left(-\kappa \sum_\mu \phi_x^*\,\phi_{x+\mu} + c.c.\right) + \lambda' \left(|\phi_x|^2 - 1\right)^2 + |\phi_x|^2\right]$$

$\kappa \mathrel{\hat{=}}$ hopping parameter

Simulation – Discretized Action

Discretized action

$$S = \sum_x \left[\left(-\kappa \sum_\mu \phi_x^* \, \phi_{x+\mu} + c.c. \right) + \lambda' \left(|\phi_x|^2 - 1 \right)^2 + |\phi_x|^2 \right]$$

- **Parameter choice:**

  $$m^2 = -4.9, \quad \lambda = 10.0 \qquad \Rightarrow \qquad \lambda' = 0.253308, \quad \kappa = 0.159156$$

- Small renormalized coupling constant suppresses excited states strongly
- Comparison to previous results

Simulation – Number of Field Configurations with $T = 48$

Finite hyper-cubic lattice

$$V = 48 \times L^3$$

L	n_{conf}	L	n_{conf}
6	100,000	16	100,000
7	100,000	17	100,000
8	100,000	18	100,000
9	100,000	19	100,000
10	100,000	20	80,000
11	100,000	21	70,000
12	100,000	22	50,000
13	100,000	23	50,000
14	100,000	24	30,000
15	100,000		

Technical Details

Periodic boundary conditions

$$\phi(x) = \phi(x + aL)$$

Interpolation operator for k-particle state

$$\hat{\mathcal{O}}_{k\phi}(x) = (\phi(x))^k$$

- Transformation $\phi(x) \rightarrow \phi(x)\, e^{\frac{i\pi}{n}}$ is symmetry of S and $\hat{\mathcal{O}}_{k\phi}(x)$ have vanishing vacuum expectation values

  $\Rightarrow$ construct correlator without subtracting vacuum expectation value to the operator previously

Technical Details – Correlation Functions

k-particle correlator

$$C_k(0,t) = \left\langle \hat{\mathcal{O}}'_{k\phi}(t)\, \hat{\mathcal{O}}^\dagger_{k\phi}(0) \right\rangle$$

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Completeness of states relation

$$C_k(t) = \frac{1}{Z} \sum_{m,n} e^{-E_n(T-t)}\, e^{-E_m t}\; \langle n|\hat{\mathcal{O}}_{k\phi}(0)|m\rangle\, \langle m|\hat{\mathcal{O}}^\dagger_{k\phi}(0)|n\rangle$$

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Expand sum in limit $T \to \infty$

$$C_k(t) = A_k^2 \cdot \frac{1}{2}\left(e^{-E_k t} - e^{-E_k(T-t)}\right)$$

$\hookrightarrow$ pollution terms vanish in this limit

Technical Details – Thermal Pollution Terms

- In practice thermal pollution terms have to be taken into account!

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- Expansion of correlation functions in an infinite sum of eigenstates:

$$C_{1/2}(t) = A_{1/2}^2 \cdot \frac{1}{2} \left(e^{-E_{1/2} t} - e^{-E_{1/2}(T-t)} \right)$$

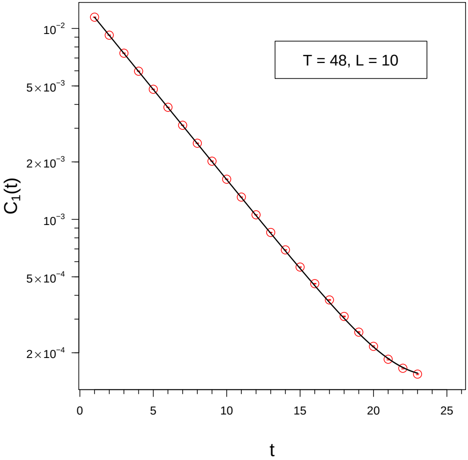
$$C_{3/4}(t) = A_{3/4}^2 \cdot \frac{1}{2} \left(e^{-E_{3/4} t} - e^{-E_{3/4}(T-t)} \right) + A_{3/4}'^2 \cdot \frac{1}{2} \left(e^{-(E_{2/3} - M_\phi) t} - e^{-(E_{2/3} - M_\phi)(T-t)} \right)$$

$$C_5(t) = A_5^2 \cdot \frac{1}{2} \left(e^{-E_5 t} - e^{-E_5 (T-t)} \right) + A_5'^2 \cdot \frac{1}{2} \left(e^{-(E_4 - M_\phi) t} - e^{-(E_4 - M_\phi)(T-t)} \right) + A_5''^2 \cdot \frac{1}{2} \left(e^{-(E_3 - E_2) t} - e^{-(E_3 - E_2)(T-t)} \right)$$

Numerical Results – Correlator Example

One particle correlator

$C_1(t)$-fit $\rightarrow$ $M_\phi \equiv E_1$



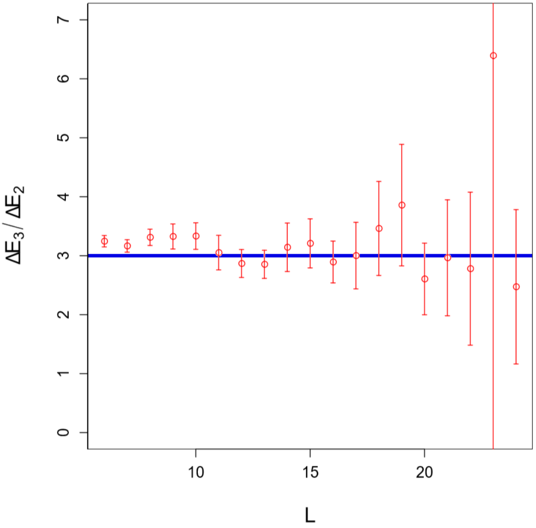
Numerical Results – Energy Shift Ratios

Beane *et al.* formula:

expect for shift ratio

- $\frac{\Delta E_3}{\Delta E_2} = 3 + \mathcal{O}(L^{-5})$
- $\frac{\Delta E_4}{\Delta E_2} = 6 + \mathcal{O}(L^{-5})$
- $\frac{\Delta E_5}{\Delta E_2} = 10 + \mathcal{O}(L^{-5})$

$\hookrightarrow$ **Valid as a first test**, not enough for parameter extraction



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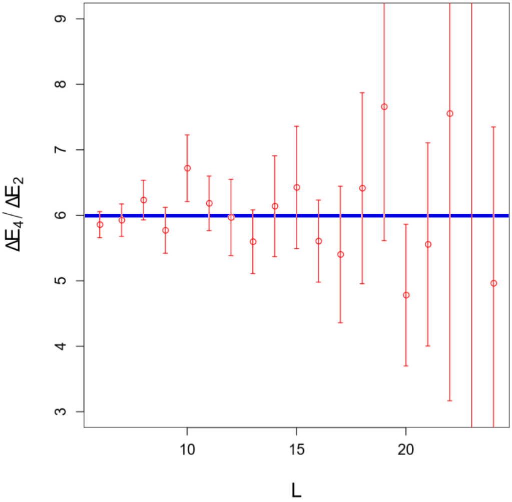

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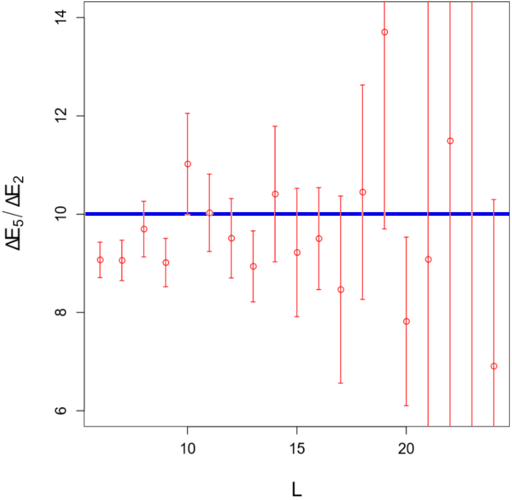

Numerical Results – M_ϕ at Infinite L

L dependence of single particle mass

$$M_\phi(L) = M_\infty + c_M \cdot \frac{K_1(M_\infty L)}{M_\infty L}$$

[Gasser, Leutwyler, 1987, Colangelo *et al.*, 2004, 2005]

$K_\nu(z) \mathrel{\hat{=}}$ modified Bessel function of second kind

$\hookrightarrow$ **asymptotic behavior for large z**

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$K_\nu(z) \hat{=}$ modified Bessel function of second kind

Considering asymptotic behavior of $K_1(z)$

$$M_\phi(L) = M_\infty + c_M \cdot \frac{\exp(-M_\infty L)}{(M_\infty L)^{3/2}}$$

Numerical Results – M_ϕ at Infinite L

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$$M_\phi(L) = M_\infty + c_M \cdot \frac{K_1(M_\infty L)}{M_\infty L}$$

[Gasser, Leutwyler, 1987]

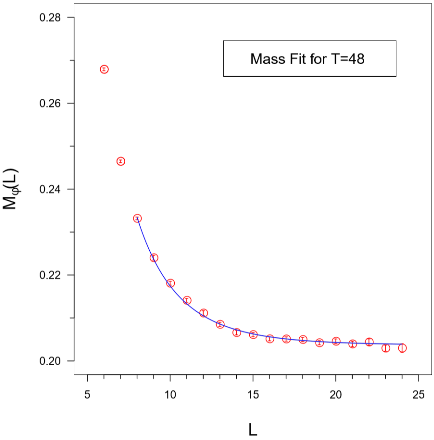
- **Result from fit:**

$$M_\infty = 0.2037(2)$$

- **Result from publication*:**

$$M_\infty = 0.2027(2)$$

*[Romero-López, Rusetsky, Urbach, 2018]



Numerical Results – Fit Strategies

Fit Strategy A

Use parameters a_0, r from two-body sector as input
for analysis of 3-, 4-, 5-body sector

Fit Strategy B

Global fit without any prior knowledge

Numerical Results – Fit Strategy A

Energy shift fits $\Delta E_k(L) = E_k(L) - k \cdot M_\phi(L)$

- Fix $L_{\mathsf{max}} = 24$ and vary L_{min} to determine best fit
- $\Delta E_k(L)$-fit, $k > 2$: Use best fit parameters from $\Delta E_2(L)$-fit as priors

Modified χ^2 function

$$\chi^2 \to \chi^2 + \left(\frac{P_{a_0} - a_0}{\Delta a_0}\right)^2 + \left(\frac{P_r - r}{\Delta r}\right)^2$$

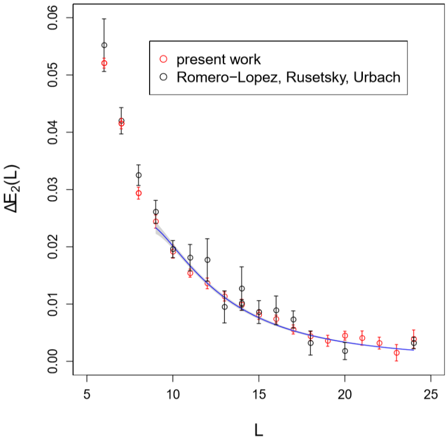
Numerical Results – Fit Strategy A

Two particle case

Expand $\Delta E_2(L)$ to $\mathcal{O}(L^{-6})$

fit interval	a_0	r	p-value
$[9, 24]$	0.43(2)	$-321(18)$	0.43
$[9, 24]$	0.46(3)	$-267(24)$	0.59*

*[Romero-López, Rusetsky, Urbach, 2018]



Numerical Results – Fit Strategy A

Three particle case

Expand $\Delta E_3(L)$ to $\mathcal{O}(L^{-6})$

fit interval	a_0	r	p-value
$[11, 24]$	0.44(2)	$-326(18)$	0.53
$[9, 24]$	0.45(2)	$-267(24)$	0.45*

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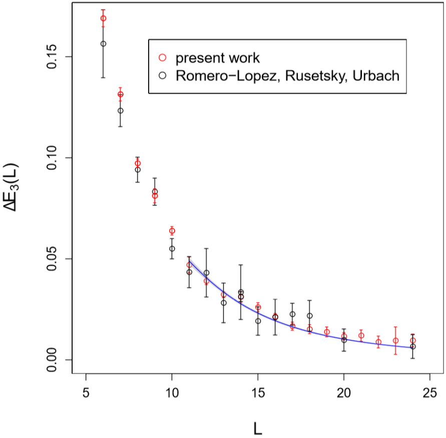
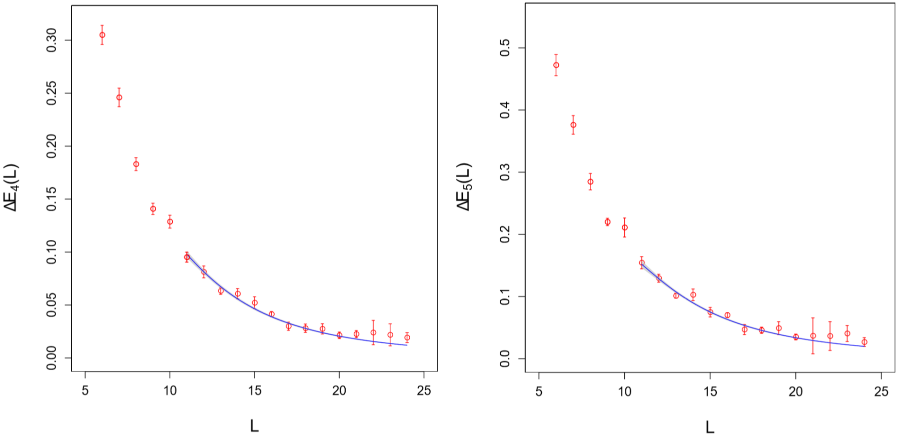


Four and five particle case

Expand $\Delta E_4(L)$ and $\Delta E_5(L)$ to $\mathcal{O}(L^{-6})$



Numerical Results – Fit Strategy A

Resulting parameters

from $\Delta E_3(L)$-, $\Delta E_4(L)$- and $\Delta E_5(L)$-fit to $\mathcal{O}(L^{-6})$

shift	a_0	r	η_3	p-value
ΔE_3	$0.439(15)$	$-326(18)$	$-3995(3661)$	0.53
ΔE_4	$0.440(14)$	$-326(18)$	$-2715(1686)$	0.47
ΔE_5	$0.436(14)$	$-324(17)$	$-4100(1395)$	0.42

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- Three fits are **consistent** with each other
- Now try a global fit to reduce the errors $\rightarrow$ **Fit Strategy B**

Numerical Results – Fit Strategy B

Global fit model

$$\chi^2_{\mathsf{global}}(\vec{p}) = \sum_{k=2}^{5} \sum_{i \in D_k} \frac{\left[\Delta E_{k,\mathsf{data}}(L_i) - \Delta E_k(L, \vec{p})\right]^2}{\left[\Delta\left(\Delta E_{k,\mathsf{data}}(L_i)\right)\right]^2}$$

$L \mathrel{\hat{=}}$ independent variable
$\vec{p} \mathrel{\hat{=}}$ vector containing the fit parameter

- Find set of parameters $\{a_0, r, \eta_3\}$ that minimizes $\chi^2_{\mathsf{global}}(\vec{p})$

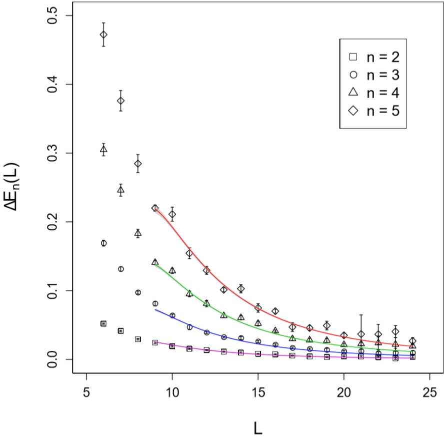
Numerical Results – Fit Strategy B

Global $\Delta E_n(L)$-fit

with $n = 2, 3, 4, 5$ to $\mathcal{O}(L^{-6})$

a_0	r	η_3	p-value
$0.42(1)$	$-287(16)$	$-2805(407)$	0.43

- Fit interval $[L_{\text{min}}, L_{\text{max}}] = [9, 24]$



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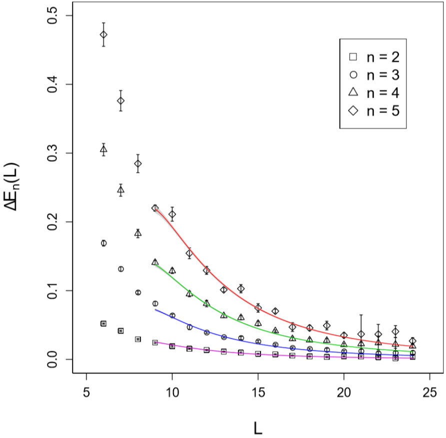
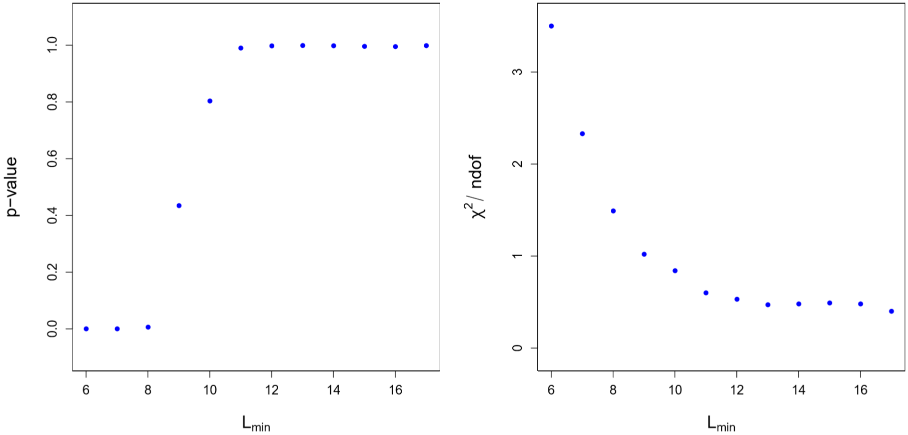
- Find best fit: Fix L_{max}, vary L_{min}



Numerical Results – Fit Strategy B

Quality of the Global Fit

p-value and reduced χ^2 as a function of L_{min}



Comparison of Results

Comparison of the results obtained from the different fits and from [Romero-López, Rusetsky, Urbach, 2018]

fit	interval	a_0	r	η_3	D
ΔE_2	[9,24]	0.43(2)	$-321(18)$	$-$	$-$
ΔE_3	[11,24]	0.44(2)	$-326(18)$	$-3995(3661)$	$-21256(3342)$
ΔE_4	[11,24]	0.44(1)	$-326(18)$	$-2715(1686)$	$-22026(2936)$
ΔE_5	[11,24]	0.44(1)	$-324(17)$	$-4100(1395)$	$-20665(2802)$
1^{st} global	[9,24]	0.42(1)	$-287(16)$	$-2805(407)$	$-15708(1702)$
2^{nd} global	[n, 24],	0.39(1)	$-246(17)$	$-1303(1126)$	$-10983(1333)$
ΔE_2	[9,24]	0.46(3)	$-267(24)$	$-$	$-$ *
ΔE_3	[9,24]	0.45(2)	$-267(24)$	$-$	$-17814(4378)$*

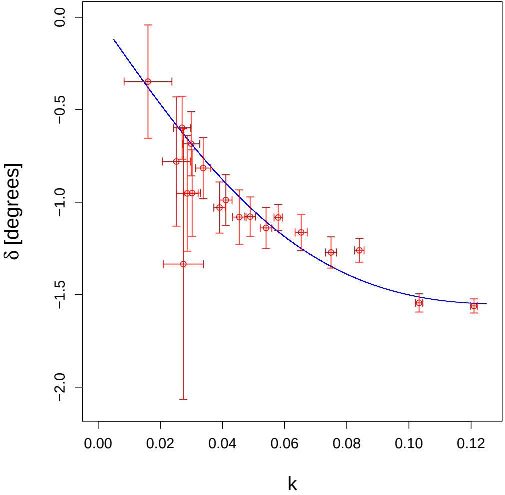
*[Romero-López, Rusetsky, Urbach, 2018]

Numerical Results – Phase Shift

S-wave phase shift
[Lüscher, 1991]

$$\cot\delta = \frac{Z_{00}(1,q^2)}{\pi^{3/2}\,q}, \qquad q = \frac{L\,k}{2\pi}$$

with $E_2 = 2\sqrt{k^2 + M(L)^2}$



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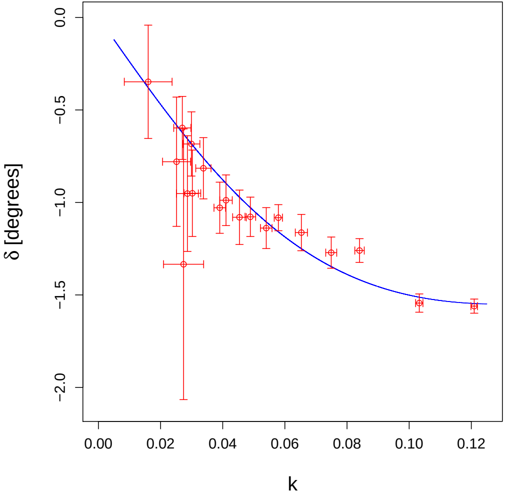
Effective range expansion

$$k\,\cot\delta(k) = -\frac{1}{a_0} + \frac{r\,k^2}{2} + \mathcal{O}(k^4)$$

a_0, r from 1st global



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- **Differences due to**
  - More ensembles $\rightarrow$ more data points
  - Increased number of field configurations

- **Initital questions:**

  Is it possible to ...

  ... determine **correlation functions** for multiparticle states?
  Yes

  ... identify **fundamental scattering parameters** (a_0, r, η_3) consistently?
  Yes

  ... determine the three body coupling constant η_3 significantly **different from zero**?
  Yes

Outlook

- Investigate excited states
- Investigate moving frames
- Compare with perturbative results in ϕ^4-theory
- Explore effect of relativistic corrections in $\Delta E_k(L)$ formula

Thanks for your attention.

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Appendix – Comparison of Results

- **Fit model in** [Romero-López, Rusetsky, Urbach, 2018] **for** $\Delta E_3(L)$**-fit:**

$$\Delta E_3(L) = \frac{12\pi a_0}{M_\phi L^3}\left\{1 + d_1\left(\frac{a_0}{\pi L}\right) + d_2\left(\frac{a_0}{\pi L}\right)^2 + \frac{3\pi a_0}{M_\phi^2 L^3} + \frac{6\pi a_0^2 r}{L^3} + d_3\left(\frac{a_0}{\pi L}\right)^3 \log\left(\frac{M_\phi L}{2\pi}\right)\right\} - \frac{D}{48 M_\phi^3 L^6} + \mathcal{O}\left(L^{-7}\right)$$

- Convert η_3 to D via

$$D \approx 576\pi a_0 M_\phi^2 \left\{\frac{3\pi a_0}{M_\phi^2} + 4\pi a_0^2 r + c_{\text{num}}\left(\frac{a_0}{\pi}\right)^3\right\} - 48 M_\phi^3 \eta_3$$

Numerical Results – Energy Shift Ratios

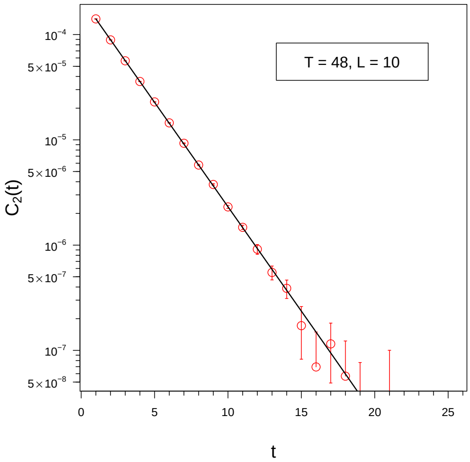

Figure: Two particle correlator fit

Numerical Results – Distribution of Fit Parameters

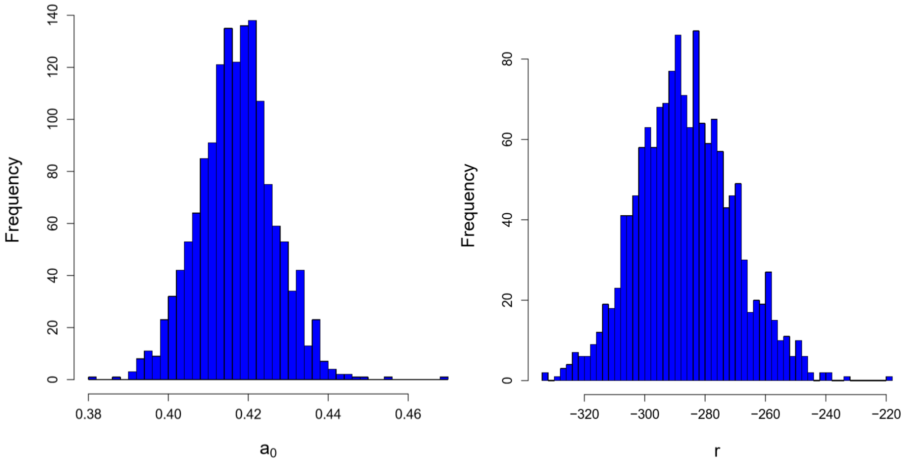

Figure: Distribution of the a_0 (left) and r (right) bootstrap samples obtained from the global fit

Numerical Results – Distribution of Fit Parameters

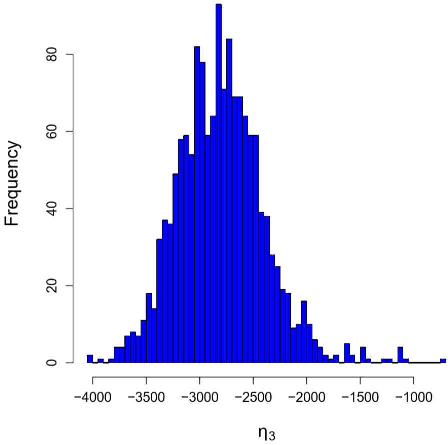

Figure: Distribution of the η_3 bootstrap samples obtained from the global fit