Scattering length in the $O(4)$-symmetric non-linear sigma model

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Motivation

Lüscher formalism Lüscher (1990):

- Map from finite volume spectrum to infinite-volume phase shift
- Generalizing to matrix elements Lellouch and Lüscher (2001), three-body scattering Hansen and Sharpe (2017), . . .
- Enormous success in applying the Lüscher formalism, e.g., mesonic sector Briceño et al. (2018), single-baryon sector Lang and Verduci (2013), two-nucleon scattering PACS-CS (2011), . . .

Maiani-Testa method Maiani and Testa (1990):

- Scattering length from Euclidean correlation functions at threshold
- Generalization above elastic threshold Bruno and Hansen (2020)
- Numerical threshold test in two-dimensional ϕ^4 theory Garofalo et al. (2021)

Infinite-volume formalism.

Finite volume effects needs to be studied!

Maiani–Testa threshold expansion

- Euclidean three-point function Maiani and Testa (1990):

$$G_{\mathbf{q}_1\mathbf{q}_2}(t_1, t_2) = \langle\Omega|\phi_{\mathbf{q}_1}(t_1)\phi_{\mathbf{q}_2}(t_2)J(0)|\Omega\rangle$$

$$G_{\mathbf{0},\mathbf{0}}(t_1, t_2) = Z_\pi \frac{e^{-m_\pi(t_1+t_2)}}{4m_\pi^2} f(4m_\pi^2)\left[1 - a_0\sqrt{\frac{m_\pi}{\pi t_2}} + \mathcal{O}(t_2^{-3/2})\right]$$

$$\mathcal{S} = \underbrace{1}_{\propto\ \text{const}} + \underbrace{\mathcal{S}^c}_{\propto\ a_0}$$

- Euclidean four-point function Bruno and Hansen (2020):

$$G_{\mathbf{q}_1'\mathbf{q}_2'\mathbf{q}_1\mathbf{q}_2}(t_1, t_2, t_3) = \langle\Omega|\phi_{\mathbf{q}_1'}(t_1)\phi_{\mathbf{q}_2'}(t_2)\phi_{\mathbf{q}_2}(t_3)\phi_{\mathbf{q}_1}(0)|\Omega\rangle_c$$

$$G_{\mathbf{0},\mathbf{0},\mathbf{0},\mathbf{0}}(t_1, t_2, t_3) = Z_\pi \frac{e^{-m_\pi t_1}}{4m_\pi^2} Z_\pi \frac{e^{-m_\pi(t_2-t_3)}}{4m_\pi^2}$$
$$\times \frac{1}{L^3}\left[32\pi\, m_\pi\, a_0(t_2 - t_3) - 64a_0^2\sqrt{\pi\, m_\pi^3\,(t_2 - t_3)} + \mathcal{O}((t_2 - t_3)^0)\right]$$

$$(\mathcal{S})^2 = \underbrace{\cancel{1}}_{\text{disconnected subtracted}} + \underbrace{2\mathcal{S}^c}_{\propto\ a_0} + \underbrace{(\mathcal{S}^c)^2}_{\propto\ a_0^2}$$

Goal

- Study the Maiani–Testa method for extracting scattering information from Euclidean correlation functions
- Use the $O(4)$ non-linear sigma model as a controlled benchmark for $\pi\pi$-scattering
  $\rightsquigarrow$ compute s-wave scattering lengths in isospin-0 and isospin-2 channels
- Investigate limitations from signal-to-noise problem
- Compare results with Lüscher's finite-volume formalism and perturbation theory

$O(4)$-symmetric scalar field theory

Göckeler et al. (1994), Cianci et al. (2026)

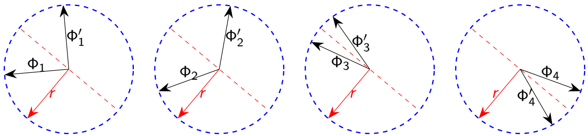
- Four-component real scalar field $\Phi^\alpha(x)$ $(\alpha = 1, 2, 3, 4)$
- $O(4)$-symmetric action with external source term:

$$S\{\Phi, \kappa, \lambda, J\} =$$

$$\sum_{x\in\Lambda} \left\{ -\kappa \sum_{\mu=1}^{4} \left(\Phi^\alpha(x)\Phi^\alpha(x+\hat{\mu}) + \Phi^\alpha(x)\Phi^\alpha(x-\hat{\mu})\right) + \lambda \left(\Phi^\alpha(x)\,\Phi^\alpha(x) - 1\right)^2 + \Phi^\alpha(x)\,\Phi^\alpha(x) - J\,\Phi^4(x) \right\}$$

- Strong-coupling limit: $\lambda \to \infty$ $\rightsquigarrow$ constraint $\Phi^\alpha(x)\,\Phi^\alpha(x) = 1$
- Symmetry broken phase: $(\kappa, J) = (0.310, 0.005),\ (0.315, 0.010),\ (0.320, 0.020)$
  $\rightsquigarrow$ $m_\sigma / m_\pi \approx 3.12,\ 2.88,\ 3.04$

Numerical methods



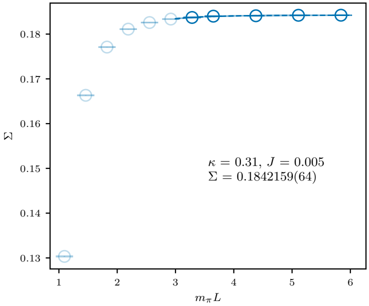
- Multi cluster update for actions with external source — Wolff (1989), Göckeler et al. (1994)
- HMC $\rightsquigarrow$ *constraint* $\Phi^\alpha(x)\,\Phi^\alpha(x) = 1$ leads to $\pi^\alpha(x)\,\Phi^\alpha(x) = 0$ — Engel and Schaefer (2011)

Computational cost $C = t_{\mathrm{site}}\, n_{\mathrm{CPU}}\, 2\tau_{\mathrm{int}}$ with autocorrelation time of $\frac{1}{V}\sum_x \langle \phi^4(x) \rangle$

$L^3 \times T$	C_{cluster} [core-h/site]	C_{HMC} [core-h/site]	$C_{\mathrm{HMC}}/C_{\mathrm{cluster}}$
$12^3 \times 40$	$1.34(26) \times 10^{-8}$	$1.00(39) \times 10^{-7}$	7.5(3.3)
$16^3 \times 32$	$1.44(29) \times 10^{-8}$	$1.14(36) \times 10^{-7}$	7.9(3.6)
$20^3 \times 32$	$1.45(29) \times 10^{-8}$	$1.22(51) \times 10^{-7}$	8.5(3.9)

- For each ensemble generate up to 1 000 000 configurations with multi cluster algorithm and measure every 10 configuration

Measured observables



- Sigma VEV: $\Sigma(L) = \dfrac{1}{\sqrt{2\kappa}\,|\Lambda|} \sum_{x\in\Lambda} \left\langle \Phi^4(x) \right\rangle$

  Infinite-volume correction:

  $\Sigma - \Sigma(L) \propto e^{-m_\pi L}/(m_\pi L)^{3/2}$

- Pion mass: $C_2(t) = \dfrac{1}{3} \sum_{a=1}^{3} \langle \Phi^a(t)\, \Phi^a(0) \rangle = \dfrac{Z_\pi(L)}{2\kappa\, 2m_\pi(L)\, L^3} \left[e^{-m_\pi(L)t} + e^{-m_\pi(L)(T-t)} \right]$

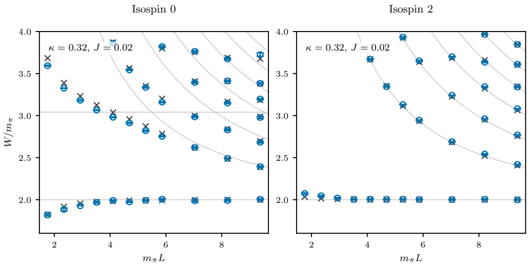
  Infinite-volume corrections:

  $m_\pi - m_\pi(L) \propto e^{-m_\pi L}/(m_\pi L)^{3/2}, \quad Z_\pi - Z_\pi(L) \propto e^{-m_\pi L}/(m_\pi L)^{3/2}$

Two-particle spectrum

- A_1^+-projected two-pion operators: $\mathcal{O}_i^{ab}(t) = \sum_{\mathbf{n}\in\mathbb{Z}_L^3} \delta_{i,|\mathbf{n}|^2}\, \phi^a(-\mathbf{n},t)\,\phi^b(\mathbf{n},t) \;/\; \sum_{\mathbf{n}\in\mathbb{Z}_L^3} \delta_{i,|\mathbf{n}|^2}$
- Connected correlation matrix: $C_{ij}^I(t) = Q^I_{a'b',ab}\,\langle \overline{\mathcal{O}_i^{a'b'}(t)}\,\mathcal{O}_j^{ab}(0)\rangle_c$

  $\rightsquigarrow$ For Isospin-0 channel we have to include σ-field $\phi^4(x)$
- GEVP: $C(t)\,v_n(t,t_0) = \lambda_n(t,t_0)\,C(t_0)\,v_n(t,t_0), \quad \lambda_n(t,t_0) \propto e^{-(t-t_0)W_n}$



Lüscher method

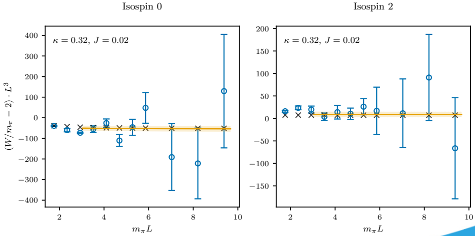
- Lüscher quantization condition Lüscher (1990):

$$\delta_0(k_\nu) = -\tilde{\phi}\left(\frac{k_\nu L}{2\pi}\right) \bmod \pi, \quad \tan\left(-\tilde{\phi}(q)\right) = \frac{q\pi^{3/2}}{\mathcal{Z}_{00}(1;q^2)}, \quad k_\nu = \sqrt{(W_\nu/2)^2 - m_\pi^2}$$

- Expansion of $\mathcal{Z}_{00}(1;q^2)$ around singularity at $q^2 = 0$ Lüscher (1986):

$$\frac{W_0}{m_\pi} = 2 - \frac{4\pi}{m_\pi^2 L^2}\frac{a_0}{L}\left(1 + c_1\frac{a_0}{L} + c_2\frac{a_0^2}{L^2}\right) + \mathcal{O}(L^{-6}), \quad c_1 = -2.837297, \quad c_2 = 6.375183$$

κ	0.310	0.315	0.320
J	0.005	0.01	0.02
a_0^0	0.68(12)	0.57(12)	0.38(10)
a_0^2	-0.119(56)	-0.073(35)	-0.061(41)



Maiani–Testa threshold ratios

- $C_3(t_1,t_2) \equiv Q_{a'b',ab} \left\langle \phi^{a'}(t_1)\, \phi^{b'}(t_2)\, J^{ab}(0) \right\rangle_c \,, \quad J^{ab}(t) \equiv \phi^a(t)\, \phi^b(t)$
- $R_3(t_1,t_2) = \dfrac{1}{n_I} \dfrac{C_3(t_1,t_2)}{C_2(t_1)\, C_2(t_2)} = \dfrac{f(4m_\pi^2)}{Z_\pi} \left[1 - a_0 \sqrt{\dfrac{m_\pi}{\pi t_2}} + \mathcal{O}(t_2^{-3/2})\right] ,$ $\quad n_0 = 3, \;\; n_2 = 6$
- $C_4(t_1,t_2,t_3) \equiv Q_{a'b',ab} \left\langle \phi^{a'}(t_1)\, \phi^{b'}(t_2)\, \phi^b(t_3)\, \phi^a(0) \right\rangle_c$
- $R_4(t_1,t_2,t_3) = \dfrac{1}{n_I} \dfrac{C_4(t_1,t_2,t_3)}{C_2(t_2-t_3)\, C_2(t_1)}$

$$= \frac{1}{L^3} \left[8\pi a_0 (t_2-t_3)\,/\,m_\pi - 16 a_0^2 \sqrt{\pi\,(t_2-t_3)\,/\,m_\pi} + \mathcal{O}\left((t_2-t_3)^0\right)\right]$$

Three-point function

$$R_3(t_1, t_2) = \frac{f(4m_\pi^2)}{Z_\pi}\left[1 - a_0\sqrt{\frac{m_\pi}{\pi t_2}} + \mathcal{O}(t_2^{-3/2})\right], \qquad t_1 = 12$$

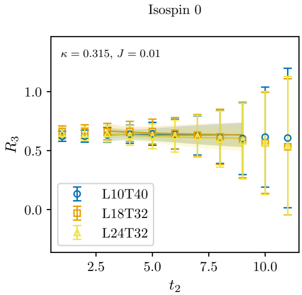
$\kappa = 0.315, \; J = 0.01$

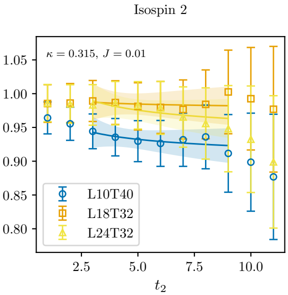
$I = 0$

(L, T)	a_0^0	$f(4m_\pi^2)/Z_\pi$
(10, 40)	−0.05(3.09)	0.63(26)
(18, 32)	−0.1(3.3)	0.66(29)
(24, 32)	−1.0(4.3)	0.55(29)

$I = 2$

(L, T)	a_0^2	$f(4m_\pi^2)/Z_\pi$
(10, 40)	−0.33(69)	0.896(75)
(18, 32)	0.08(70)	0.975(85)
(24, 32)	−0.43(77)	0.928(86)





Four-point function

$$\Delta R_4(t_1,t_2,t_3) = R_4(t_1,t_2+1,t_3) - R_4(t_1,t_2,t_3)$$

$$= \frac{1}{L^3}\left[8\pi a_0/m_\pi - 16 a_0^2\sqrt{\pi/m_\pi}\left(\sqrt{t_2+1-t_3}-\sqrt{t_2-t_3}\right)+\mathcal{O}\left((t_2-t_3)^{-1/2}\right)\right], \quad t_3=3,\ t_1=12$$

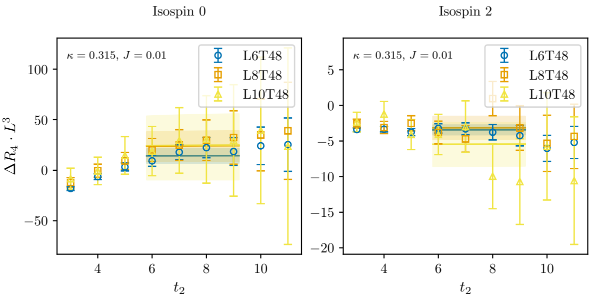
$\kappa = 0.315,\ J = 0.01$

$I = 0$

(L,T)	a_0^0
$(6,48)$	$0.51(26)$
$(8,48)$	$0.84(70)$
$(10,48)$	$0.4(1.2)$

$I = 2$

(L,T)	a_0^2
$(6,48)$	$-0.064(13)$
$(8,48)$	$-0.056(29)$
$(10,48)$	$-0.098(55)$



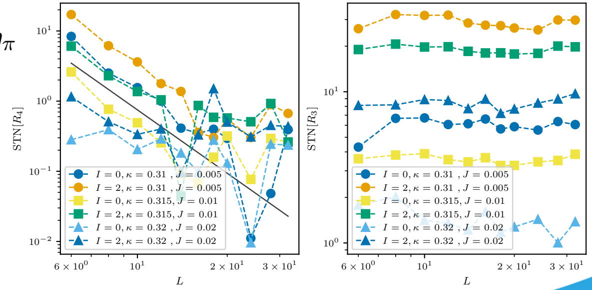
Signal-to-noise scaling

- Connected four-point function: $C_4(t_1, t_2, t_3) \propto L^{-9}/m_\pi$

$$G(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, t_1, t_2, t_3) \equiv \left\langle \phi^{a'}(\mathbf{x}_1, t_1)\, \phi^{b'}(\mathbf{x}_2, t_2)\, \phi^{b}(\mathbf{x}_3, t_3)\, \phi^{a}(\mathbf{x}_4, 0) \right\rangle_c , \quad \mathbf{r}_i = \mathbf{x}_i - \mathbf{x}_4,$$

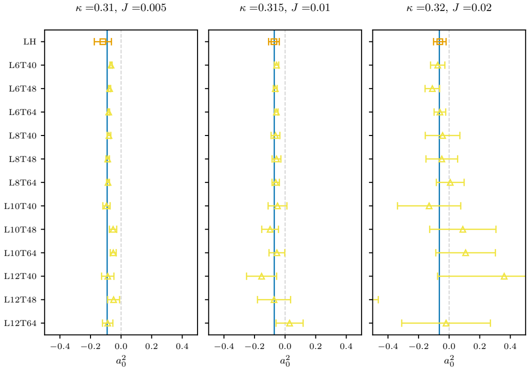
$$\sum_{\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4} \left\langle \phi^{a'}(\mathbf{x}_1, t_1)\, \phi^{b'}(\mathbf{x}_2, t_2)\, \phi^{b}(\mathbf{x}_3, t_3)\, \phi^{a}(\mathbf{x}_4, 0) \right\rangle_c = L^3 \sum_{\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3} G(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, t_1, t_2, t_3)$$

- $\mathrm{StN}[R_4] = R_4/\sigma(R_4) \propto L^{-3}/m_\pi$
- $\mathrm{StN}[R_3] = R_3/\sigma(R_3) \propto L^0$



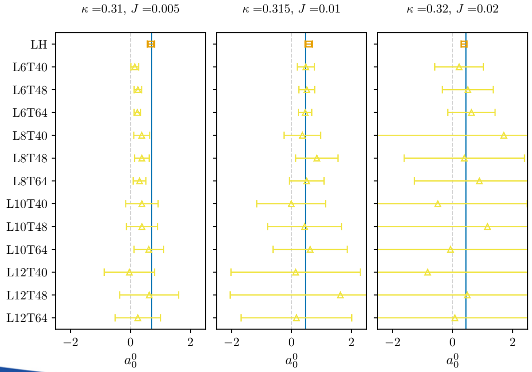
Scattering length a_0^2: Lüscher vs. Maiani-Testa (four-point ratio)

- Perturbation theory and Lüscher method good agreement
- Maiani–Testa method good agreement with other methods



Scattering length a_0^0: Lüscher vs. Maiani-Testa (four-point ratio)

- Perturbation theory and Lüscher method good agreement
- Maiani–Testa method already for $L \gtrsim 10$ no signal
- Possible finite volume effects for small $m_\pi L$

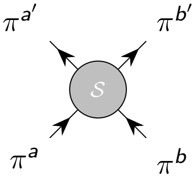


Conclusion and outlook

- Lüscher method gives scattering lengths compatible with perturbation theory
- The Maiani–Testa four-point fits are feasible, but strongly limited by the signal-to-noise problem
- A next step is to apply the Bruno–Hansen method to the isospin-2 channel above threshold Bruno and Hansen (2020)
- Finite-volume effects in the Maiani–Testa correlators should be investigated carefully, especially because the signal-to-noise problem restricts the usable range of volumes
- Variance-reduction methods can improve signal-to-noise, e.g., multilevel algorithms Lüscher (2022), cluster decomposition Liu et al. (2018), Hamiltonian automatic differentiation Catumba and Ramos (2025), . . .

Backup slides

Scattering theory



- Two-pion scattering: $3 \otimes 3 = 1 \oplus 3 \oplus 5$
  $\rightsquigarrow$ Isospin $I = 0, 1$ and 2 channels
- Transition matrix for fixed isospin I:

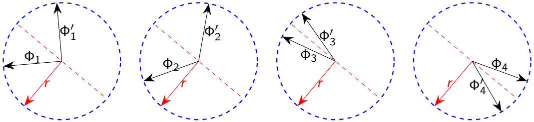
$$T = \sum_{I=0}^{2} Q^I T^I, \qquad T^I = \frac{16\pi W}{k} \sum_{\ell=0}^{\infty} (2\ell+1) P_\ell(\cos\vartheta)\, t_\ell^I(k), \qquad t_\ell^I(k) = \frac{1}{2i}\left(e^{2i\delta_\ell^I(k)} - 1\right)$$

$$Q^0_{a'b',ab} = \frac{1}{3}\delta_{a',b'}\delta_{a,b}, \qquad Q^1_{a'b',ab} = \frac{1}{2}\left(\delta_{a',a}\delta_{b',b} - \delta_{a',b}\delta_{b',a}\right), \qquad Q^2_{a'b',ab} = \frac{1}{2}\left(\delta_{a',a}\delta_{b',b} + \delta_{a',b}\delta_{b',a}\right) - Q^0_{a'b',ab}$$

- Low-energy expansion of the s-wave phase shift $\delta_0^I(k)$:

$$\boxed{a_0^I = \lim_{k\to 0} \frac{1}{2ik}\left(e^{2i\delta_0^I(k)} - 1\right)}$$

Multi-cluster update Göckeler et al. (1994)



1. Chose a random unit vector $\mathbf{r} \in \mathbb{R}^4$.
2. For each nearest-neighbor pair (x, y), a bond is activated with probability

$$p_{\mathbf{r}}(x,y) = \max\Big\{0, 1 - \exp\Big[-4\kappa\,(\mathbf{r}\cdot\Phi(x))(\mathbf{r}\cdot\Phi(y))\Big]\Big\}\,.$$

3. Connected components of the resulting bonds are identified with a union-find algorithm.
4. For each cluster c, all spins in the cluster are reflected,

$$\Phi(x) \to \Phi(x) - 2(\mathbf{r}\cdot\Phi(x))\,\mathbf{r}, \qquad x \in c,$$

with probability

$$w_{\mathbf{r}}(c) = \left[1 + \exp\left(2Jr_4 \sum_{x\in c} \mathbf{r}\cdot\Phi(x)\right)\right]^{-1}.$$

HMC algorithm with constraint

Engel and Schaefer (2011)

- Constraint $\Phi^\alpha(x)\,\Phi^\alpha(x) = 1$ leads to $\pi^\alpha(x)\,\Phi^\alpha(x) = 0$:

$$\frac{\partial \Phi}{\partial t} = \pi\,, \quad \frac{\partial \pi}{\partial t} = -\tilde{\nabla}_\Phi S[\Phi]\,, \qquad \tilde{\nabla}_\Phi S[\Phi] = (1 - \Phi\,\Phi^T)\nabla_\Phi S[\Phi]$$

- Molecular dynamics update:

$$\begin{pmatrix} \Phi_{i+1} \\ \pi_{i+1} \end{pmatrix} = \begin{pmatrix} \cos(\alpha) & \frac{1}{|\pi_i|}\sin(\alpha) \\ -|\pi_i|\sin(\alpha) & \cos(\alpha) \end{pmatrix} \begin{pmatrix} \Phi_i \\ \pi_i \end{pmatrix}\,, \qquad \alpha = \Delta t\,|\pi_i|$$

Phase shift and sigma resonance

- Perturbation theory (one-loop order):

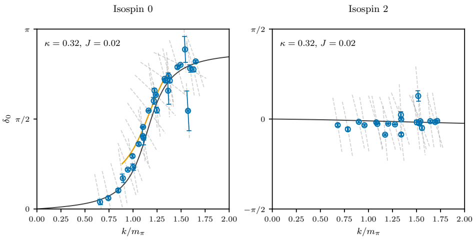
Göckeler et al. (1994)

$$\delta_0^0 = \delta_r^0 + \delta_s^0\,, \quad \tan\left(\delta_s^0\right) = g_R \frac{1}{16\pi} \frac{m_\sigma^2 - m_\pi^2}{m_\sigma^2 - W^2} \frac{k}{W}\,, \quad \delta_r^0 = \delta_0^2 - g_R \frac{1}{16\pi} \frac{k}{W}\,,$$

$$\delta_0^2 = \frac{g_R}{96\pi} \frac{m_\sigma^2 - m_\pi^2}{kW} \log\left(\frac{4k^2 + m_\sigma^2}{m_\sigma^2}\right) - \frac{g_R}{24\pi} \frac{k}{W}\,, \qquad g_R = 3 Z_R \frac{m_\sigma^2 - m_\pi^2}{\Sigma^2}$$

- Relativistic Breit–Wigner fit for $\pi/4 \le \delta_0^0 \le 3\pi/4$:

$$\tan\left(\delta_0^0(k) - \tfrac{\pi}{2}\right) = \frac{W^2 - m_\sigma^2}{m_\sigma \Gamma_\sigma}$$



Measured observables and simulation details

- Simulated lattice sizes (L, T) for each parameter set: $(6, 40)$, $(8, 40)$, $(10, 40)$, $(12, 40)$, $(14, 32)$, $(16, 32)$, $(18, 32)$, $(20, 32)$, $(24, 32)$, $(28, 40)$ and $(32, 40)$
- Discard 10 000 sweeps for thermalization. Production runs consist of 1 000 000 update sweeps for $L \leq 24$ and 500 000 sweeps for $L > 24$. Measurements taken every 10 sweeps.

κ	0.310	0.315	0.320
J	0.005	0.010	0.020
m_π	0.18250(39)	0.22755(37)	0.29313(45)
Z_π	0.9628(14)	0.9574(14)	0.9509(17)
Σ	0.1842159(64)	0.2356064(30)	0.2806728(28)
m_σ	0.52596(28)	0.71091(62)	0.89134(95)
Γ_σ	0.0691(13)	0.1252(27)	0.2045(34)
g_R	20.833(28)	23.735(47)	26.122(63)

Cluster decomposition

Liu et al. (2018)

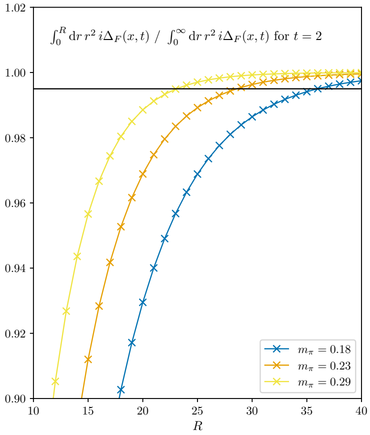
Consider two-point correlator with cutoff R:

$$C_2(t, R) = \frac{1}{V} \sum_{\mathbf{x}} \sum_{|\mathbf{r}|<R} \left\langle \mathcal{O}^\dagger(\mathbf{x}+\mathbf{r}, t)\, \mathcal{O}(\mathbf{x}, 0) \right\rangle$$

- Scalar field Feynman propagator:

  $i\Delta_F(x) = r^2\, \mathrm{K}_1\left(m_\pi \sqrt{r^2+t^2}\right) / \sqrt{r^2+t^2}$
- $\int_0^R \mathrm{d}r\, r^2\, i\Delta_F(x,t)\ /\ \int_0^\infty \mathrm{d}r\, r^2\, i\Delta_F(x,t) \approx 0.9295$

  for $R = 20,\ m_\pi = 0.18$ and $t = 2$
- Requires $m_\pi R \approx 8$ to get 99.5% of signal



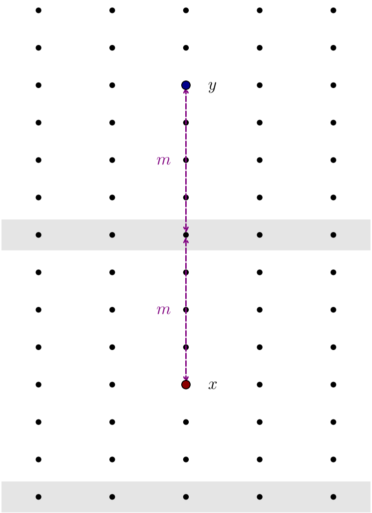
Multilevel algorithm

Lüscher (2022)

Construct observable $\mathcal{O}'$ such that $\langle \mathcal{O}' \rangle = \langle \mathcal{O} \rangle$ and $\sigma(\mathcal{O}') \ll \sigma(\mathcal{O})$.

- Perform N two-level updates:
  1. Perform n_0 global updates
  2. Perform n_1 local updates
- $[\phi(x)]_k = \frac{1}{n_1} \sum_{j=1}^{n_1} \phi_{n_0+k(n_0+n_1)+j}(x)$
- $\langle \phi(x)\, \phi(y) \rangle = \frac{1}{N} \sum_{k=1}^{N} [\phi(x)]_k \, [\phi(y)]_k$

$\Rightarrow$ Improve statistical error from $\propto e^{2m\,|x-y|}$ to $\propto e^{m\,|x-y|}$

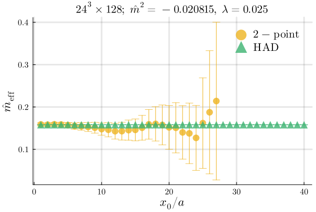


Hamiltonian automatic differentiation

Catumba and Ramos (2025)

Reduce two-point function $\sum_{\mathbf{x}} \langle \mathcal{O}^\dagger(x)\, \mathcal{O}(0) \rangle$ to one-point function $\frac{\partial}{\partial J}\big|_{J=0} \langle \mathcal{O}^\dagger(x) \rangle_J$ with $S_J[\phi] = S[\phi] - J \sum_{\mathbf{x}} \mathcal{O}(x)\big|_{x_0=0}$.

- Consider equations of motion for $J = 0 + \varepsilon$: $\dot{\phi}(x) = \pi(x), \quad \dot{\pi}(x) = -\frac{\partial S_J[\phi]}{\partial \phi(x)}$
- Truncate field and momentum to first order (i.e. $\phi(x) = \phi_0(x) + \varepsilon \phi_1(x)$) and solve EOM order by order in ε.
- $\langle \phi(t)\, \phi(0) \rangle = \frac{1}{N} \sum_{k=1}^{N} \phi_{1,k}(t)$



Picture adapted from arXiv:2502.15570