Three ways of calculating mass spectra for composite particles in the Hamiltonian formalism

Akira Matsumoto (YITP, Kyoto U, RIKEN iTHEMS)
collaboration with
Etsuko Itou (YITP, Kyoto U, RIKEN iTHEMS) and Yuya Tanizaki (YITP, Kyoto U)

arXiv:2307.16655

Quantum Information and Theoretical Physics, 6 Oct. 2023 @YITP

Simulating QFT in Hamiltonian formalism

Lagrangian formalism

- Monte Carlo simulation (Lattice QCD)

  👍 gauge invariance

  👍 well-established algorithms

- tensor network (TRG, HOTRG, ⋯)

Hamiltonian formalism

- tensor network (MPS, PEPS, ⋯)
- quantum computer

  👍 free from the sign problem

  👍 obtain excited states directly

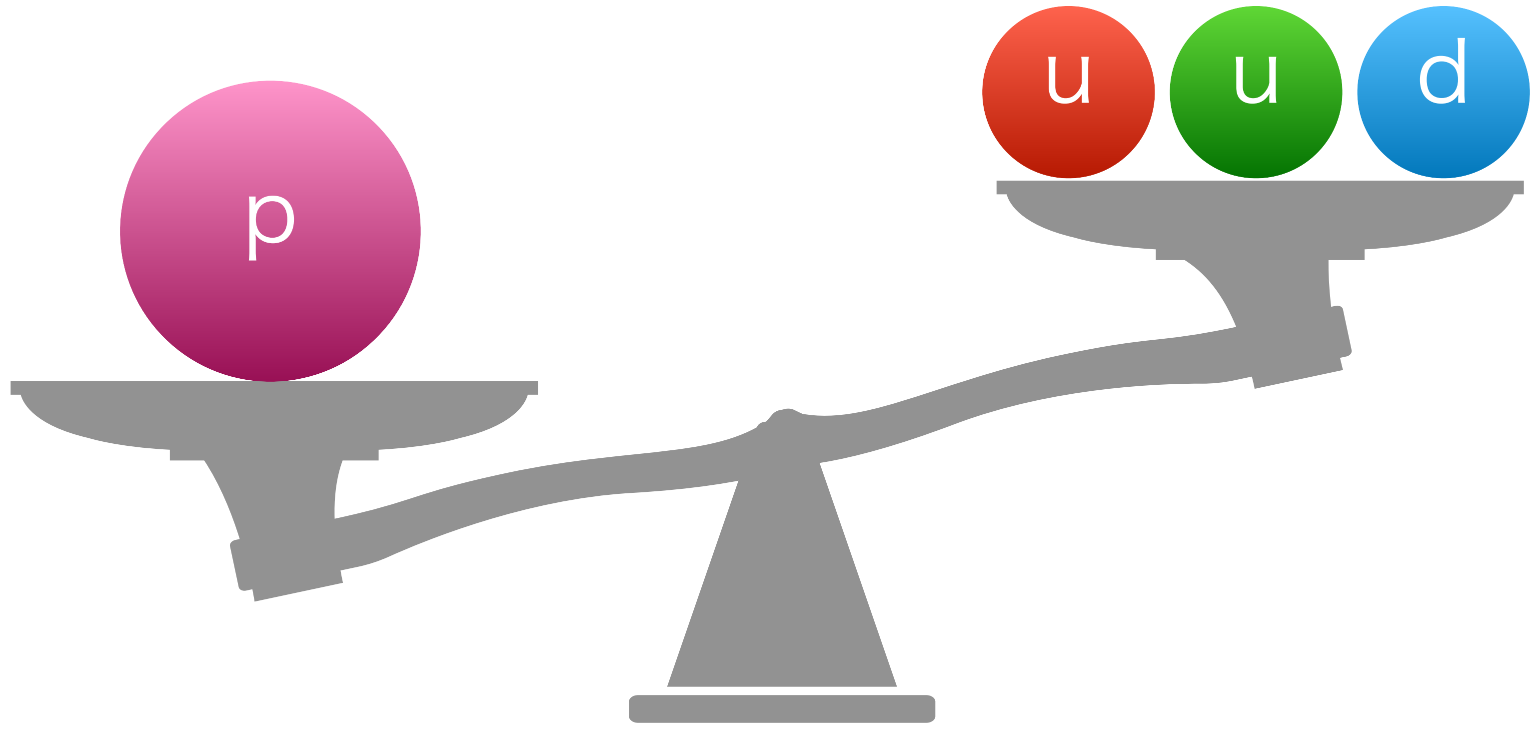
  can be a complementary approach

How to compute physical observables of gauge theory (QCD) efficiently in Hamiltonian formalism?

Mass spectrum of composite particles

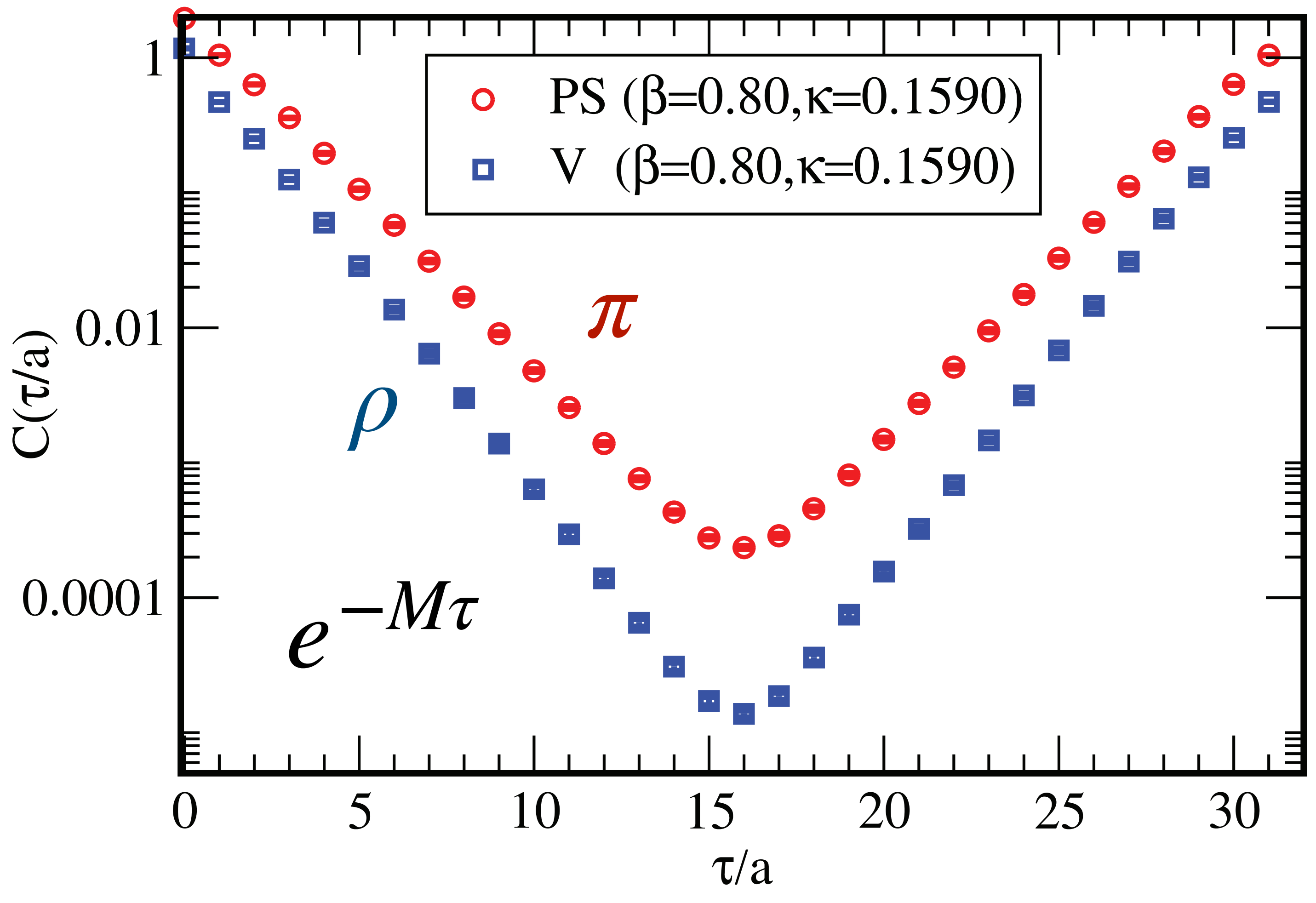
- mass of composite particle in QCD (hadron)

  u/d quark: 2~5 MeV
  proton (uud): 938 MeV >> $2m_u + m_d$



- non-perturbative calculation by lattice Monte Carlo method
  (Lagrangian formalism)

- hadron mass is obtained from imaginary-time correlation fn.
  —> agree with experiments



[Iida et al. (2021)]

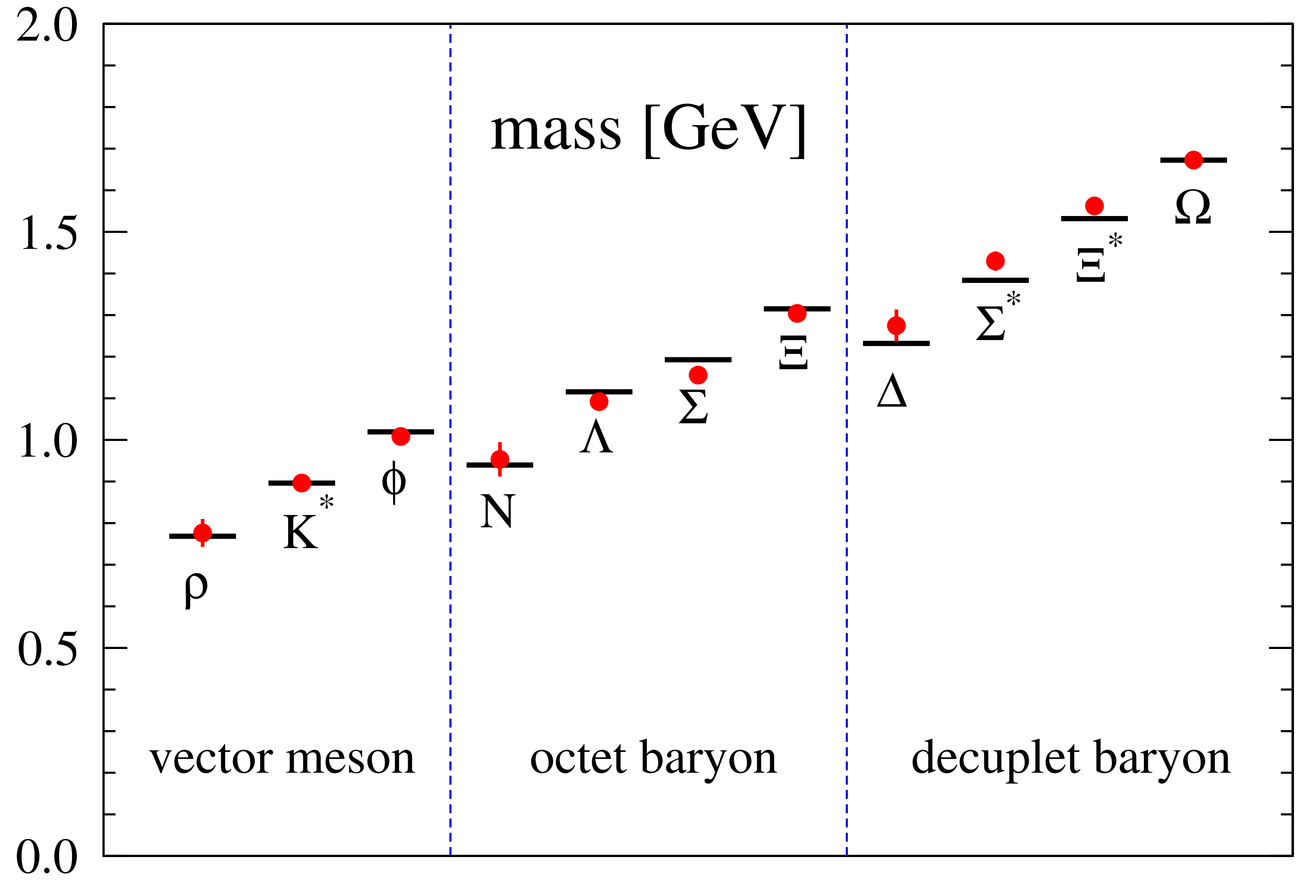


FIG. 24 (color online). Light hadron spectrum extrapolated to the physical point using m_π, m_K and m_Ω as input. Horizontal bars denote the experimental values.

[PACS-CS collab. (2009)]

Composite particles in the 2-flavor Schwinger model

Schwinger model = quantum electrodynamics in 1+1d

- the simplest nontrivial gauge theory sharing some features with QCD

$$\mathscr{L} = -\frac{1}{4g^2}F_{\mu\nu}F^{\mu\nu} + \frac{\theta}{4\pi}\epsilon_{\mu\nu}F^{\mu\nu} + \sum_{f=1}^{N_f}\left[i\bar{\psi}_f\gamma^\mu\left(\partial_\mu + iA_\mu\right)\psi_f - m\bar{\psi}_f\psi_f\right]$$

quantum numbers

- isospin J : SU(2) acting on the flavor doublet
- parity P
- G-parity $G = Ce^{i\pi J_y}$: generalization of C

"mesons"

$\pi = -i\left(\bar{\psi}_1\gamma^5\psi_1 - \bar{\psi}_2\gamma^5\psi_2\right)$: $J^{PG} = 1^{-+}$

$\eta = -i\left(\bar{\psi}_1\gamma^5\psi_1 + \bar{\psi}_2\gamma^5\psi_2\right)$: $J^{PG} = 0^{--}$

$\sigma = \bar{\psi}_1\psi_1 + \bar{\psi}_2\psi_2$: $J^{PG} = 0^{++}$

Short summary

- three distinct methods for computing the mass spectrum

  (1) correlation-function scheme — conventional method in lattice QCD

  (2) one-point-function scheme — make good use of the boundary effect

  (3) dispersion-relation scheme — obtain the excited states directly

- demonstration in the 2-flavor Schwinger model using tensor network (DMRG)

- results of the three methods are consistent with each other

Calculation strategy

- Hamiltonian on the lattice (staggered fermion + open boundary)

$$H = \frac{g^2 a}{2} \sum_{n=0}^{N-2} \left(L_n + \frac{\theta}{2\pi} \right)^2 + \sum_{f=1}^{N_f} \left[\frac{-i}{2a} \sum_{n=0}^{N-2} \left(\chi_{f,n}^\dagger U_n \chi_{f,n+1} - \chi_{f,n+1}^\dagger U_n^\dagger \chi_{f,n} \right) + m_{\text{lat}} \sum_{n=0}^{N-1} (-1)^n \chi_{f,n}^\dagger \chi_{f,n} \right]$$

- solving Gauss law condition to remove L_n

[Kogut & Susskind (1975)]

[Dempsey et al. (2022)]

- gauge fixing to $U_n = 1$

- Jordan-Wigner transformation for Nf=2

$$\chi_{1,n} = \sigma_{1,n}^- \prod_{j=0}^{n-1} (-\sigma_{2,j}^z \sigma_{1,j}^z), \quad \chi_{2,n} = \sigma_{2,n}^- (-i\sigma_{1,n}^z) \prod_{j=0}^{n-1} (-\sigma_{2,j}^z \sigma_{1,j}^z)$$

—> spin Hamiltonian with a finite-dimensional Hilbert space

Density-matrix renormalization group (DMRG)

[White (1992)] [Schollwock (2005)]

variational method to find eigenstates of H using MPS ansatz

- cost function: energy $E = \langle \Psi | H | \Psi \rangle$

- update $A_i(s_i)$ to decrease E

- introduce a cutoff ε to control the accuracy

  singular values smaller than ε are neglected in SVD

  (small ε = large D_i = high accuracy)

$$|\Psi\rangle = \sum_{\{s_i\}} \mathrm{Tr}\left[A_0(s_0)\, A_1(s_1)\ \cdots\right] |\, s_0\, s_1\ \cdots\rangle$$

$A_i(s_i)$: $D_{i-1} \times D_i$ matrix

D_i : bond dimension

- ℓ-th excited state $|\Psi_\ell\rangle$ —> cost function: $\langle \Psi_\ell | H | \Psi_\ell \rangle + W \sum_{\ell'=0}^{\ell-1} \left| \langle \Psi_{\ell'} | \Psi_\ell \rangle \right|^2$

The C++ library of ITensor is used in this work. [Fishman et al. (2022)]

Simulation result ($\theta = 0$)

(1) Correlation-function scheme

(2) One-point-function scheme

(3) Dispersion-relation scheme

Simulation result ($\theta = 0$)

(1) Correlation-function scheme

(2) One-point-function scheme

(3) Dispersion-relation scheme

(1) correlation-function scheme

- spatial correlation: $C_\pi(r) = \langle \pi(x)\pi(y) \rangle$
- effective mass: $M_{\pi,\mathrm{eff}}(r) = -\frac{d}{dr}\log C_\pi(r), \quad r = |x-y|$

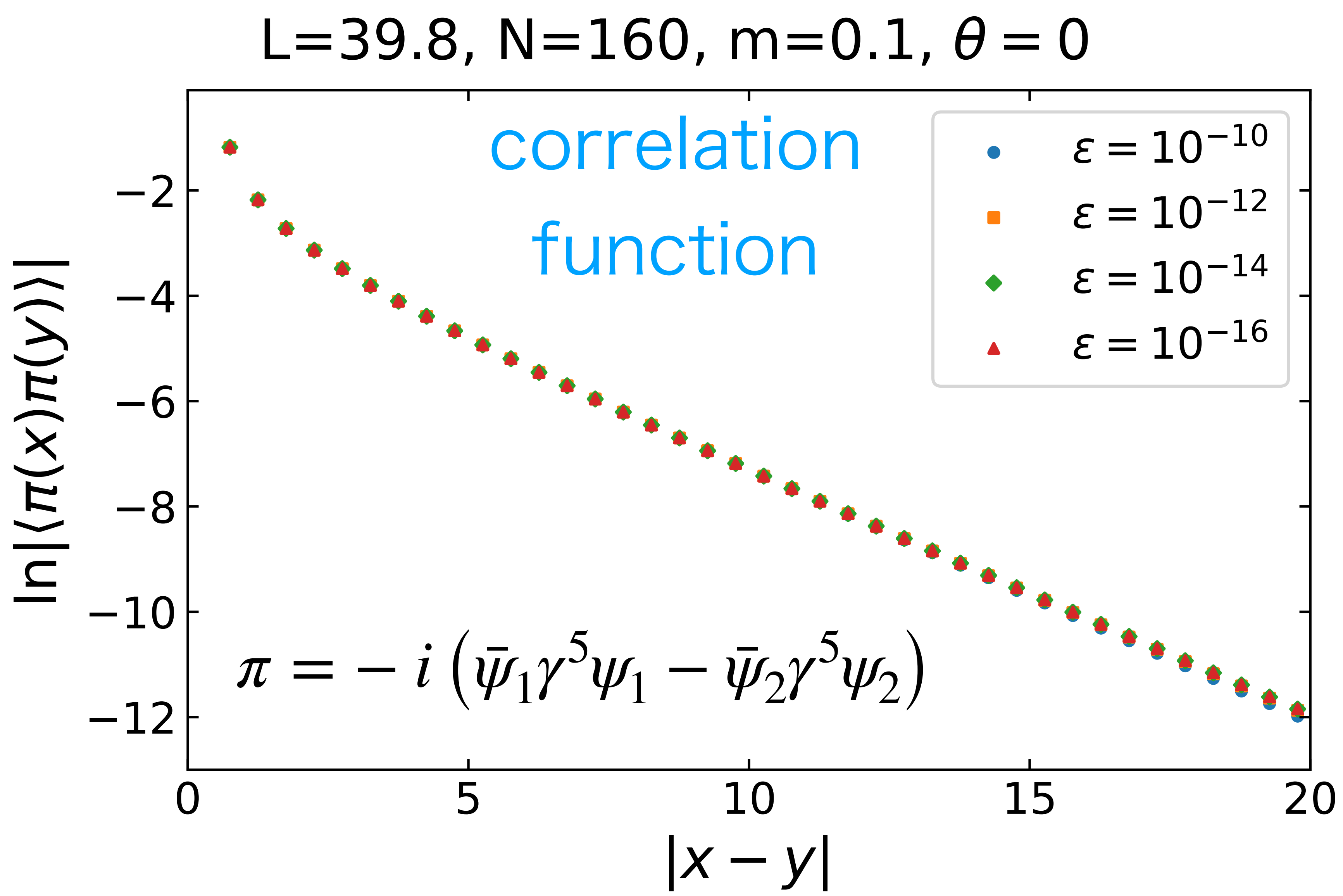
<u>plateau value = pion mass?</u>

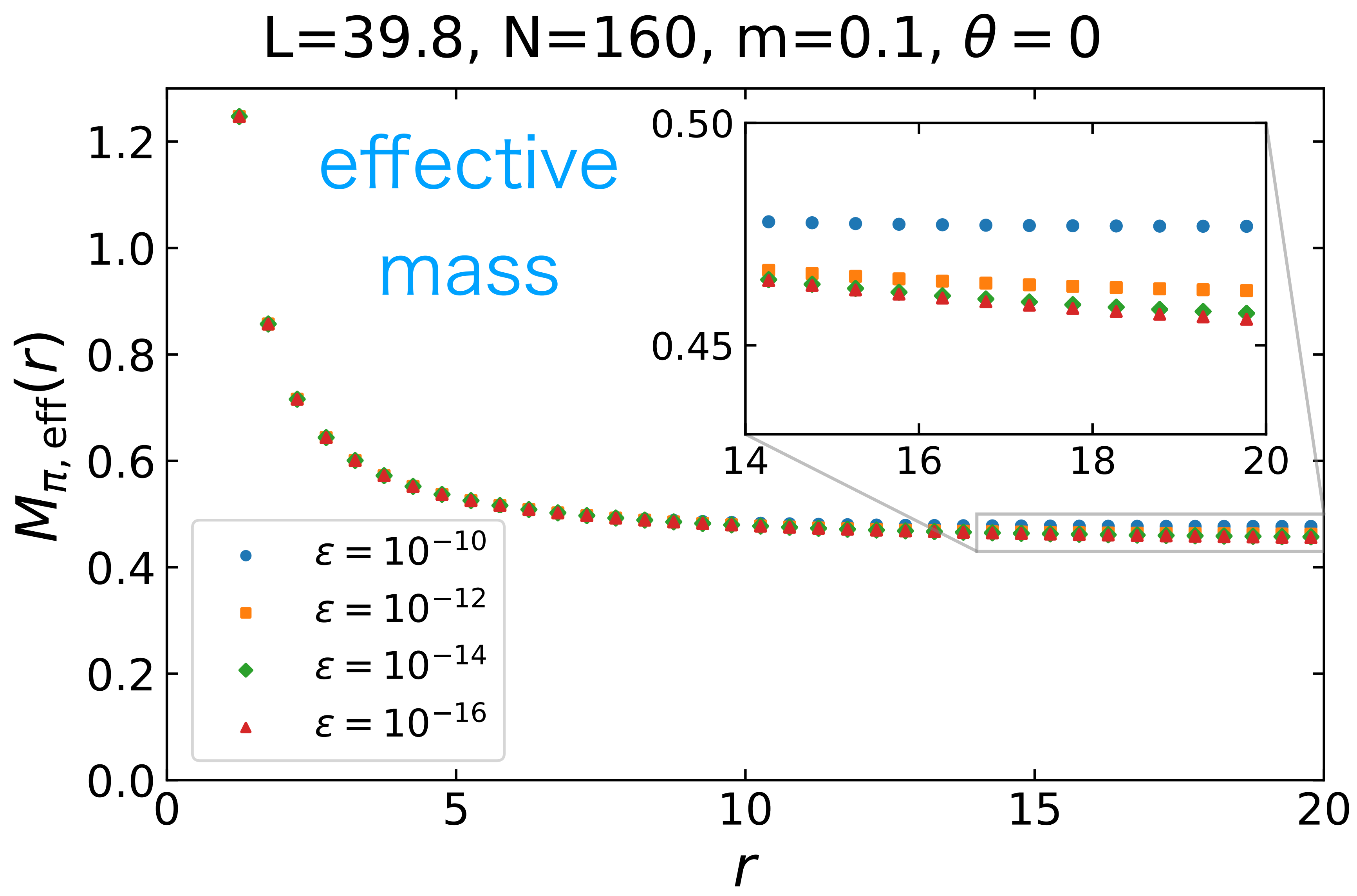
⚠️ plateau behavior gets modified in accurate calc.

$\varepsilon = 10^{-10}$ $(D_i \sim 400)$: $M_{\pi,\mathrm{eff}}(r)$ is almost flat

$\varepsilon = 10^{-16}$ $(D_i \sim 2800)$: $M_{\pi,\mathrm{eff}}(r)$ depends on r

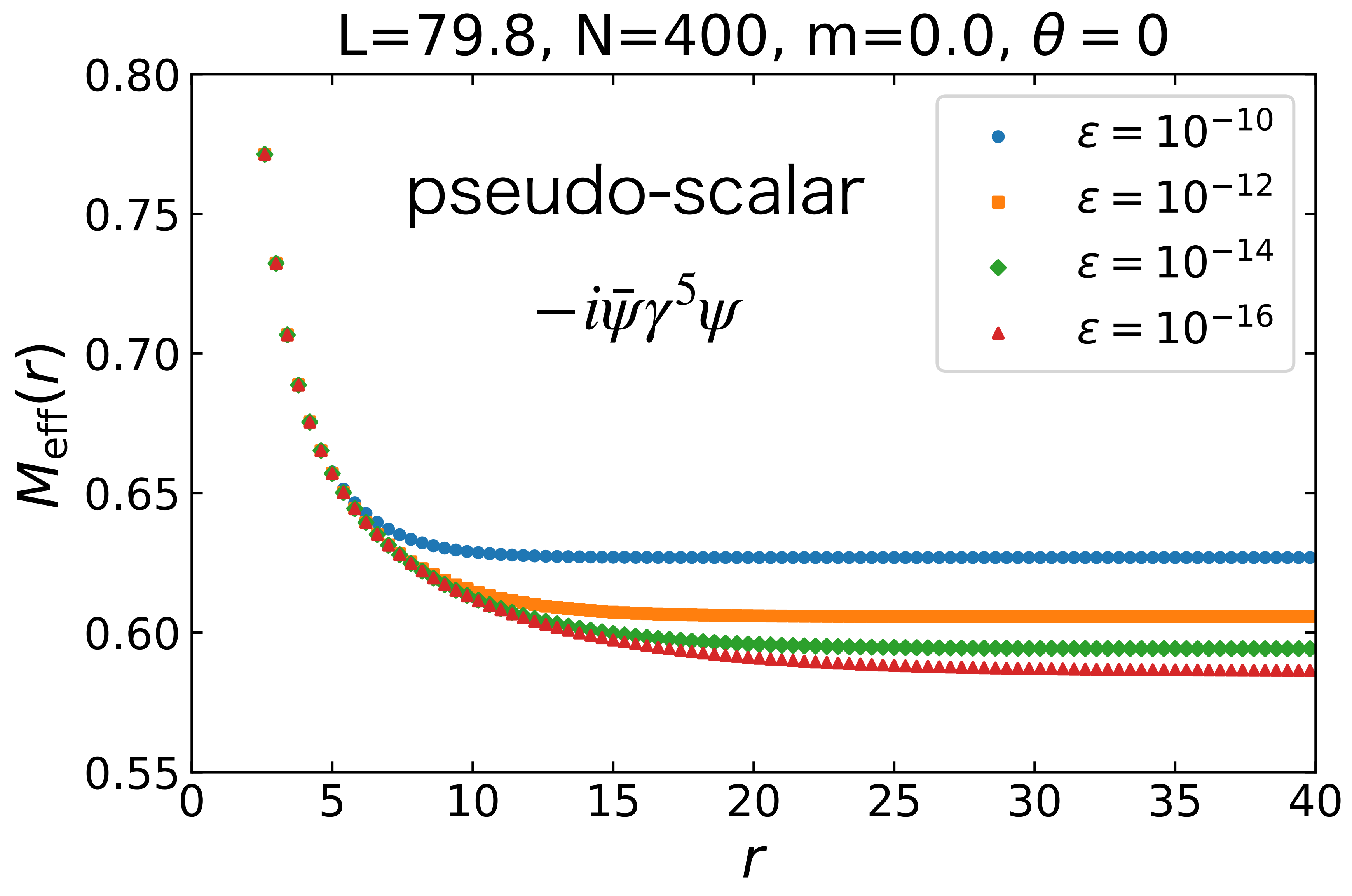
- What's happened?



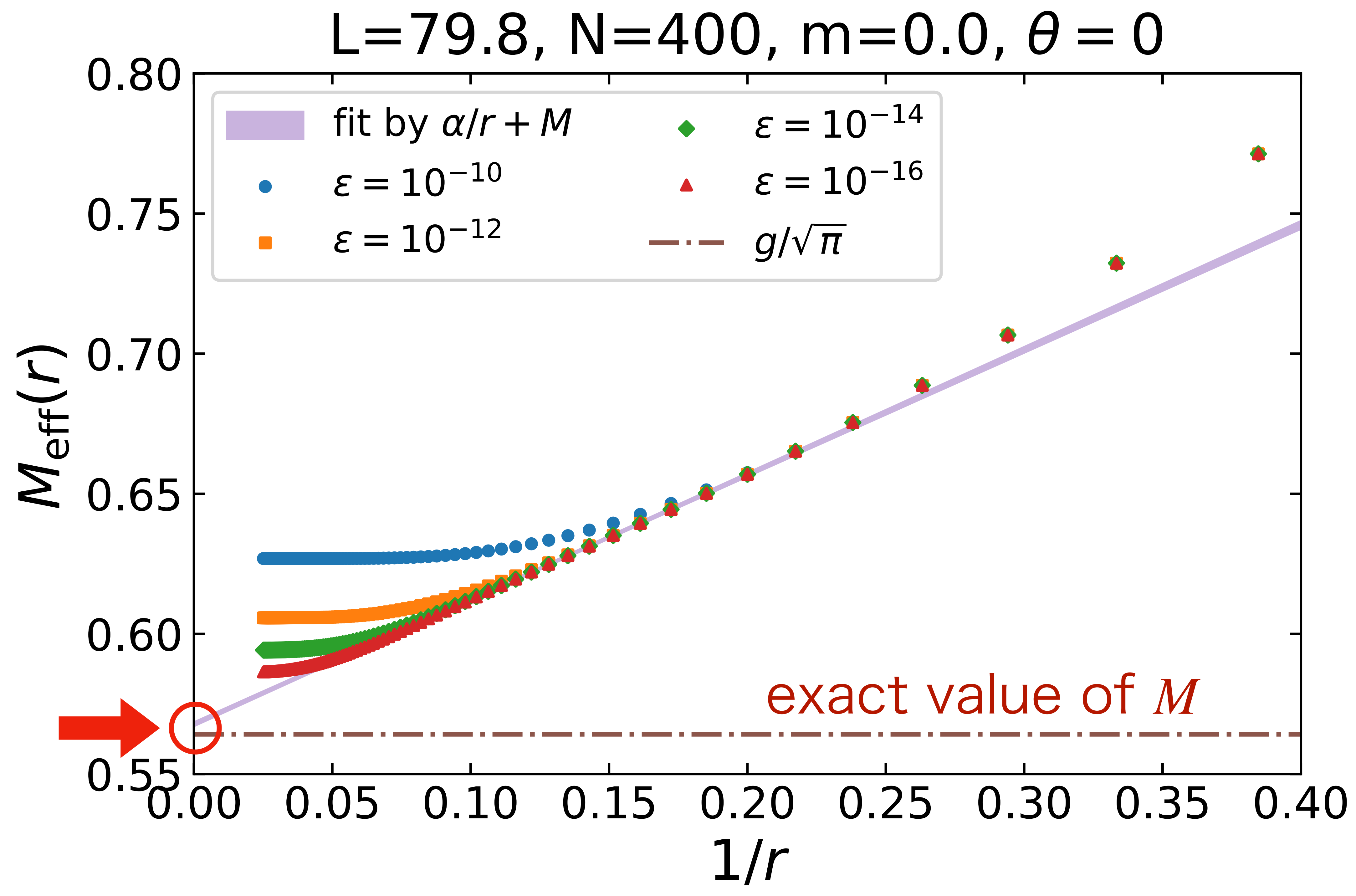


Yukawa-type correlation → 1/r term

- (1+1)d free particle with mass M: $\langle\phi(x,t)\phi(y,t)\rangle \sim \frac{1}{\sqrt{Mr}}e^{-Mr}$ —> $M_{\rm eff}(r) \sim \frac{\alpha}{r} + M$
- massless Nf=1 Schwinger model (exactly solvable)



plot against $\frac{1}{r}$

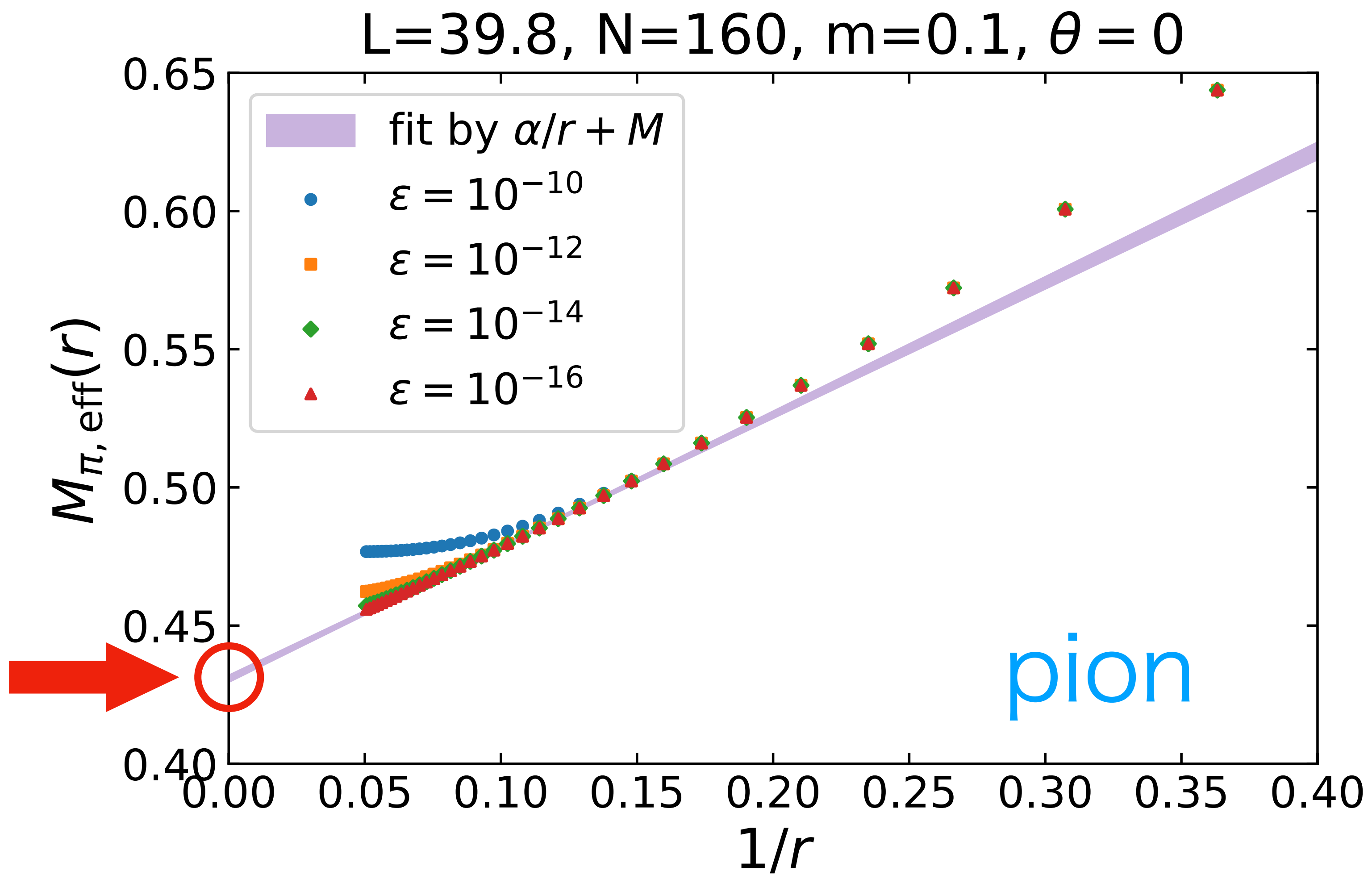


- difficult to reproduce $1/r$ term by MPS
- $r \to \infty$ extrapolation is required

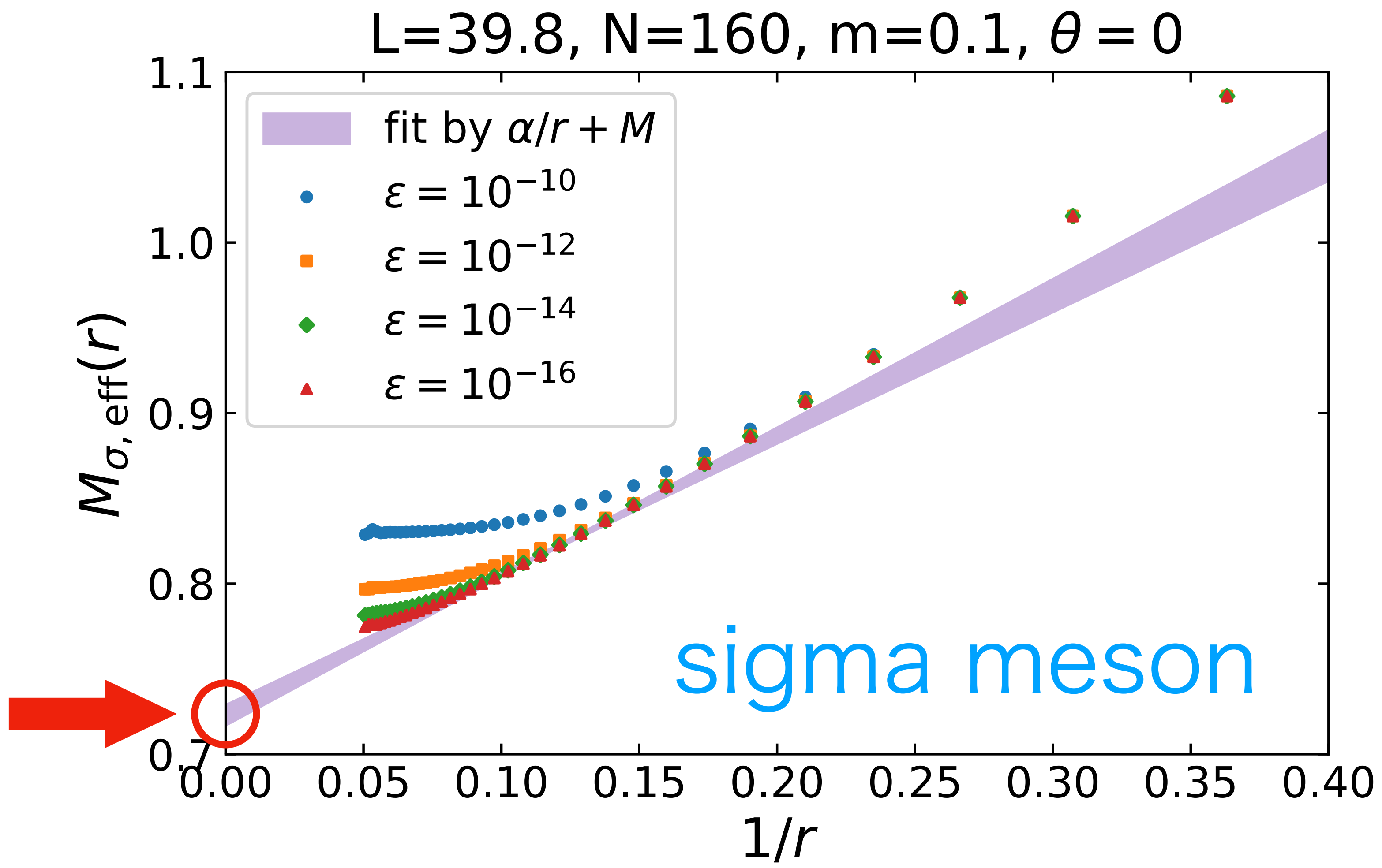
Result of the Nf=2 model

extrapolate the effective mass to $r \to \infty$ using the result for $\varepsilon = 10^{-16}$

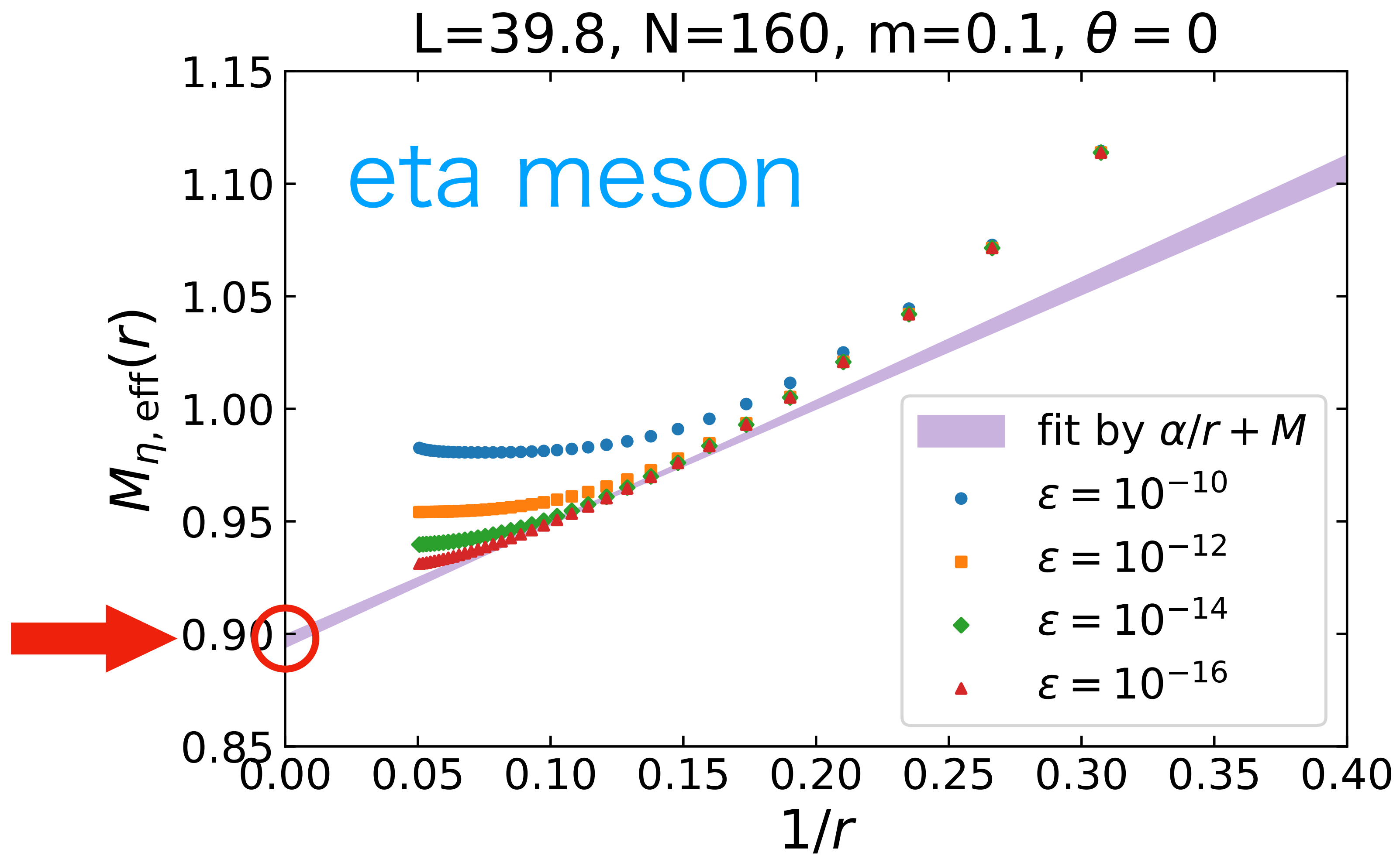
$$\pi = -i\left(\bar{\psi}_1 \gamma^5 \psi_1 - \bar{\psi}_2 \gamma^5 \psi_2\right)$$



$$\sigma = \bar{\psi}_1 \psi_1 + \bar{\psi}_2 \psi_2$$



$$\eta = -i\left(\bar{\psi}_1 \gamma^5 \psi_1 + \bar{\psi}_2 \gamma^5 \psi_2\right)$$



	pion	sigma	eta
M	0.431(1)	0.722(6)	0.899(2)
α	0.477(9)	0.83(5)	0.51(2)

Simulation result ($\theta = 0$)

(1) Correlation-function scheme

(2) One-point-function scheme

(3) Dispersion-relation scheme

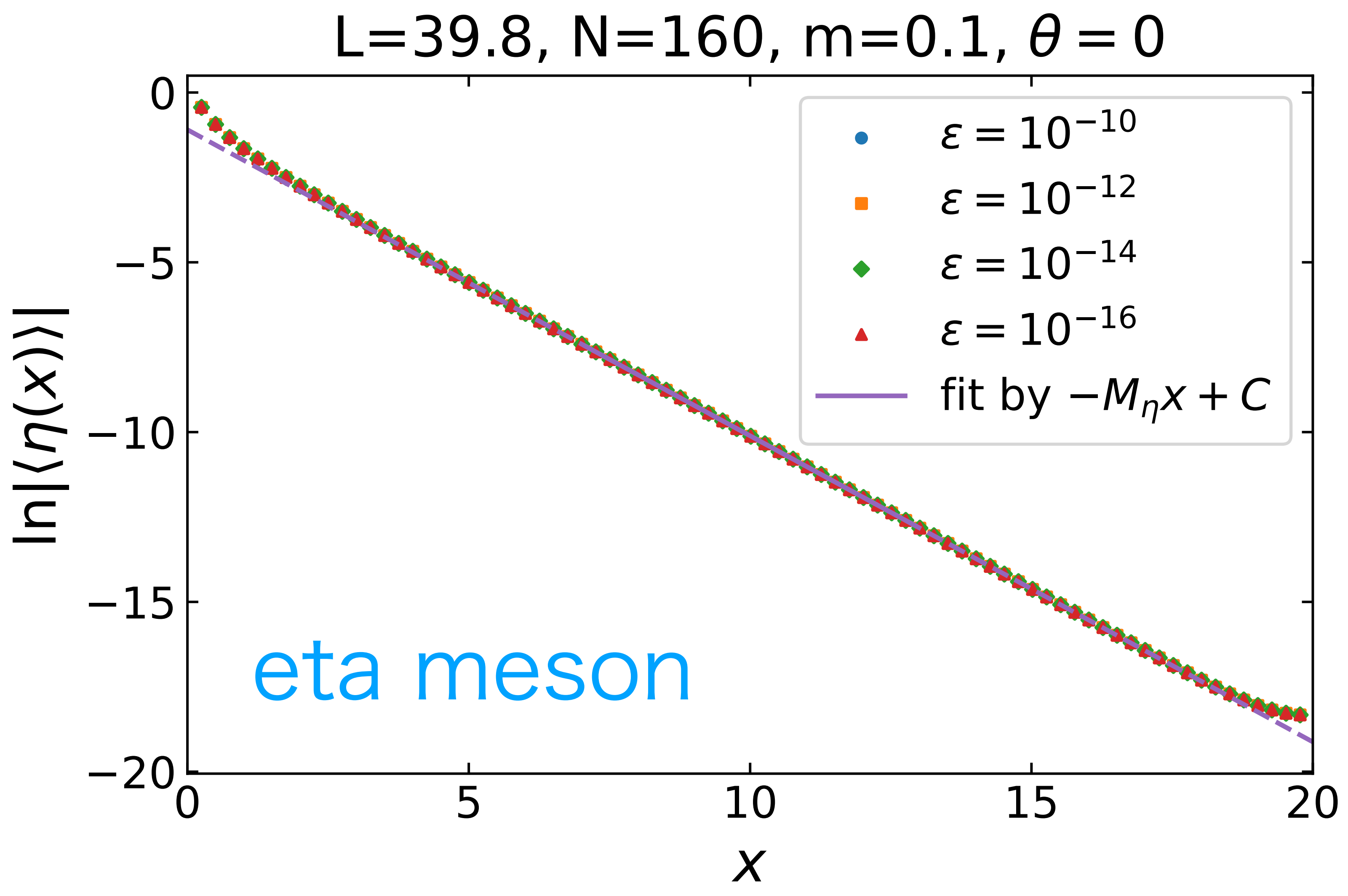
(2) one-point-fn. scheme (eta & sigma)

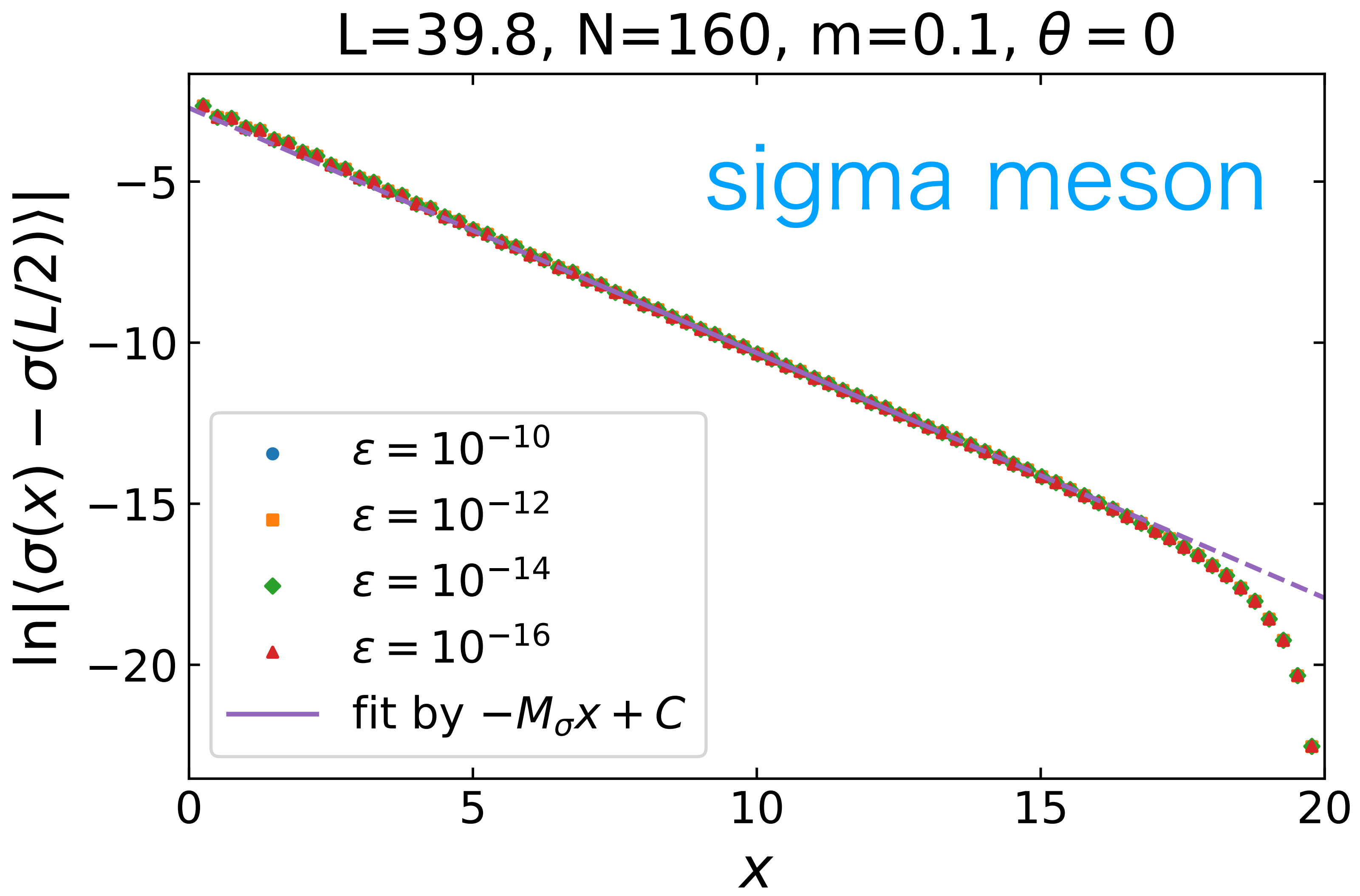
- At $\theta = 0$, the open boundary can be a source of iso-singlet states. (~wall source)

- one-point function: $\langle \mathcal{O}(x) \rangle \sim \langle \mathrm{bdry} \,|\, \mathcal{O}(x) \,|\, 0 \rangle \sim e^{-Mx}$

- ε-dependence is NOT observed
  —> systematic error from
  truncating D_{eff} is sufficiently small

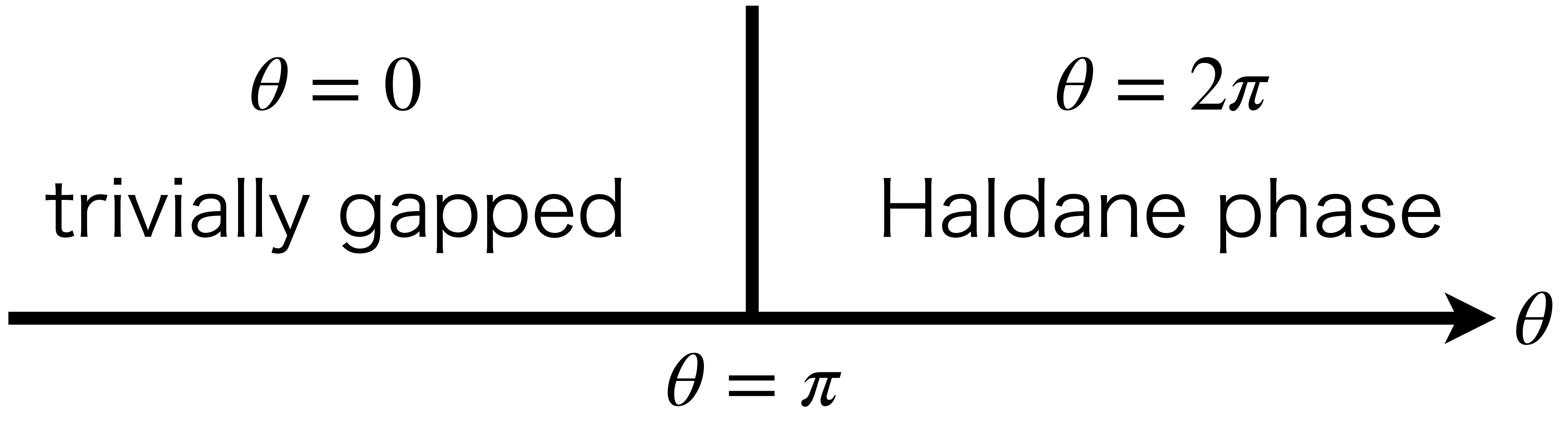
- eta: $M = 0.9014(1),\ C = -1.096(1)$
- sigma: $M = 0.761(2),\ C = -2.71(2)$





(2) pion: tricky case

⚠️ $\langle \pi(x) \rangle = 0$ at $\theta = 0$ (trivially gapped phase)

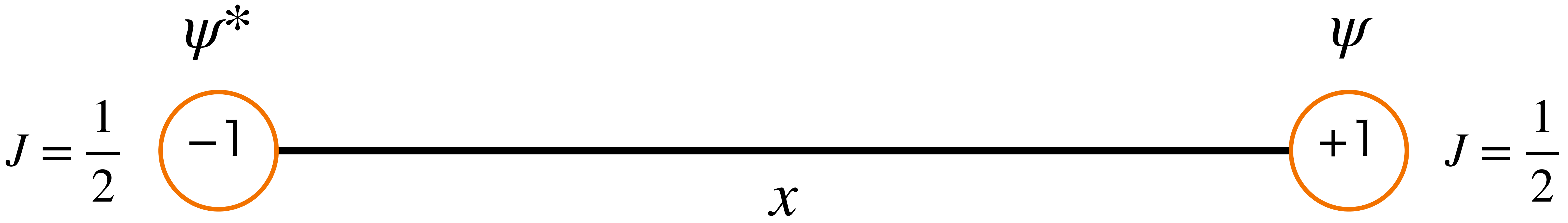


cf.) similar SPT phase
to anti-ferro. Heisenberg chain

[Chen et al. (2011)]
[Kapustin (2014)]

setting $\theta = 2\pi$ —> introducing a background electric field

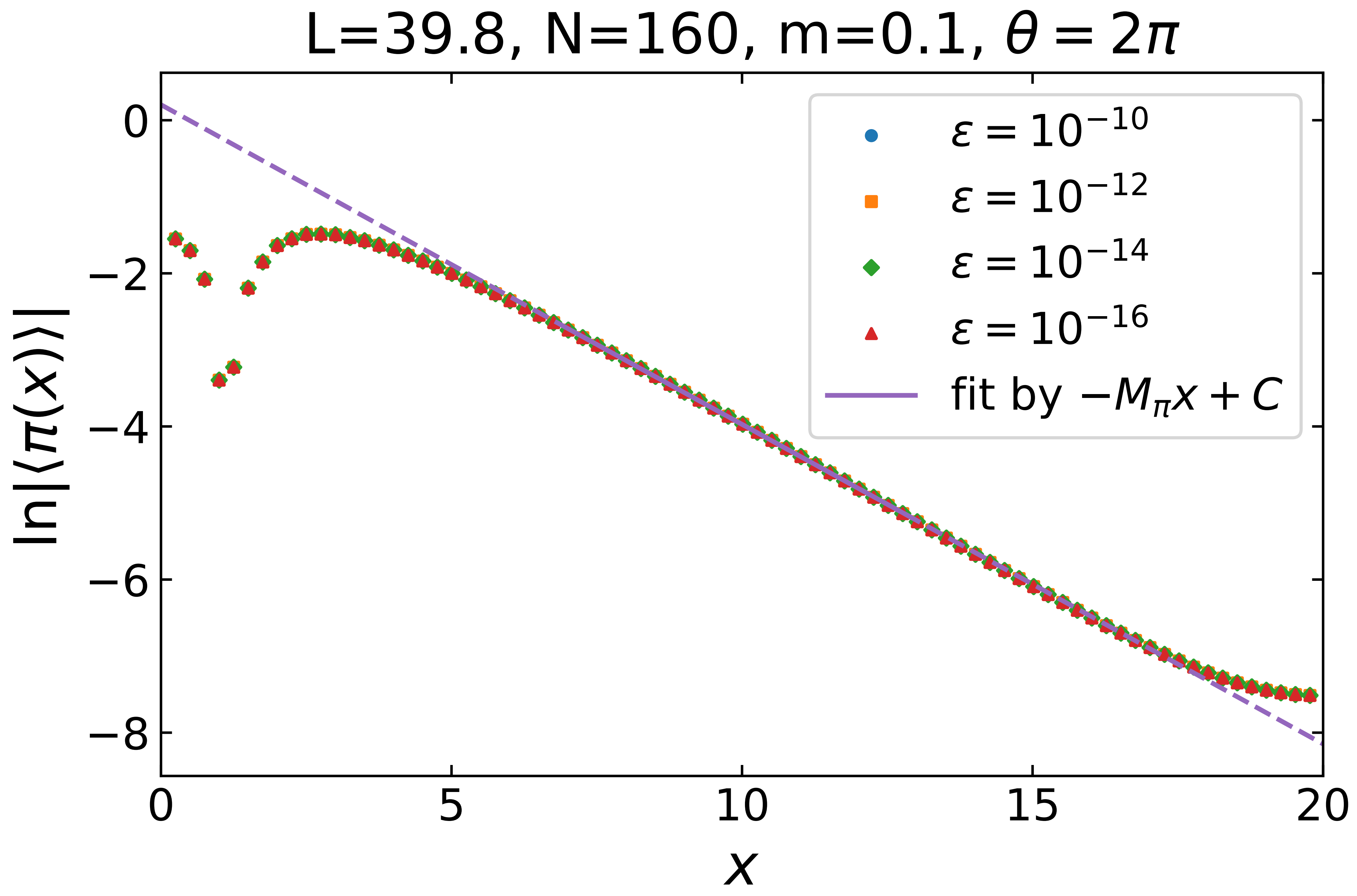
- Dirac fermions with charge ± 1 are induced as edge modes
- isospin 1/2 at the boundary —> a source of iso-triplet mesons



(2) one-point-fn. scheme (pion)

- generate the ground state at $\theta = 2\pi$
- one-point function: $\langle \pi(x) \rangle \sim e^{-Mx}$

- $M = 0.4175(9), \quad C = 0.203(9)$
- ε-dependence is NOT observed



	pion	sigma	eta
M	0.4175(9)	0.761(2)	0.9014(1)

Simulation result ($\theta = 0$)

(1) Correlation-function scheme

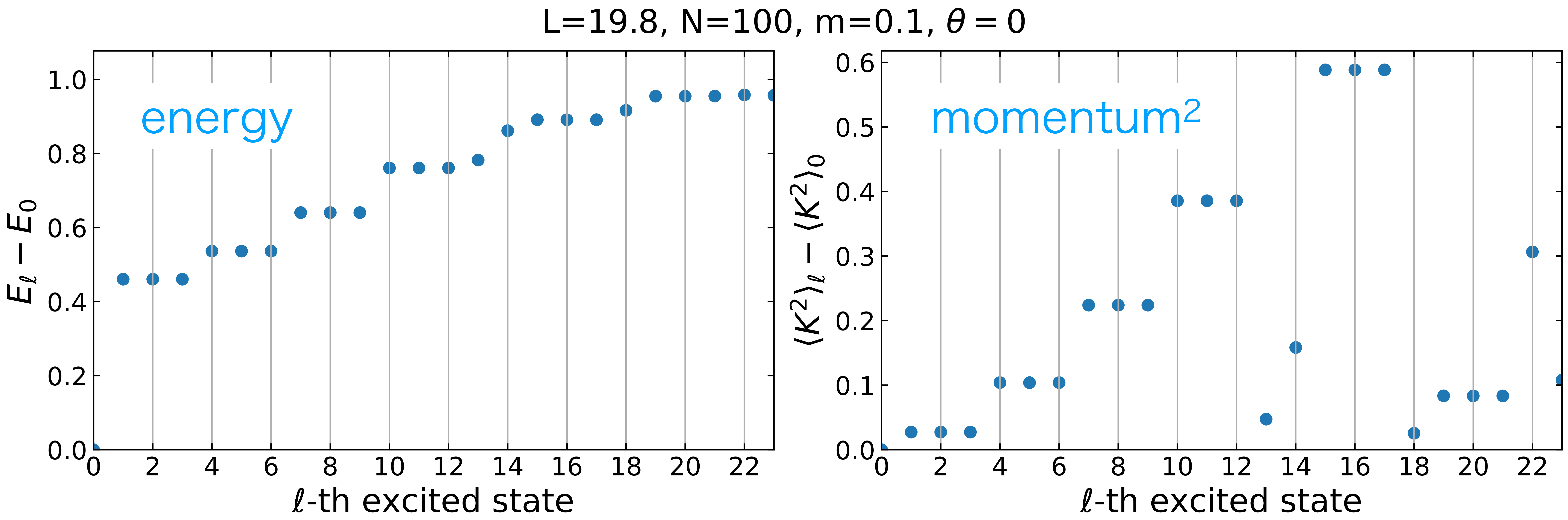
(2) One-point-function scheme

(3) Dispersion-relation scheme

(3) Dispersion-relation scheme

- energy gap: $\Delta E_\ell = E_\ell - E_0$ momentum square: $\Delta K_\ell^2 = \langle K^2 \rangle_\ell - \langle K^2 \rangle_0$
- triplets —> pion? singlets —> sigma or eta meson?

identify the states by measuring quantum numbers: $\mathbf{J}^2, \ J_z, \ G = Ce^{i\pi J_y}$



Quantum numbers

- triplets: $\mathbf{J}^2 = 2, \ \ J_z = (0, \pm 1), \ \ G > 0$

  —> pion ($J^{PG} = 1^{-+}$)

- singlets: $\mathbf{J}^2 = 0, \ \ J_z = 0,$

  $G > 0 \ (\ell = 13{,}14{,}22)$ —> sigma meson ($J^{PG} = 0^{++}$)

  $G < 0 \ (\ell = 18{,}23)$ —> eta meson ($J^{PG} = 0^{--}$)

triplets

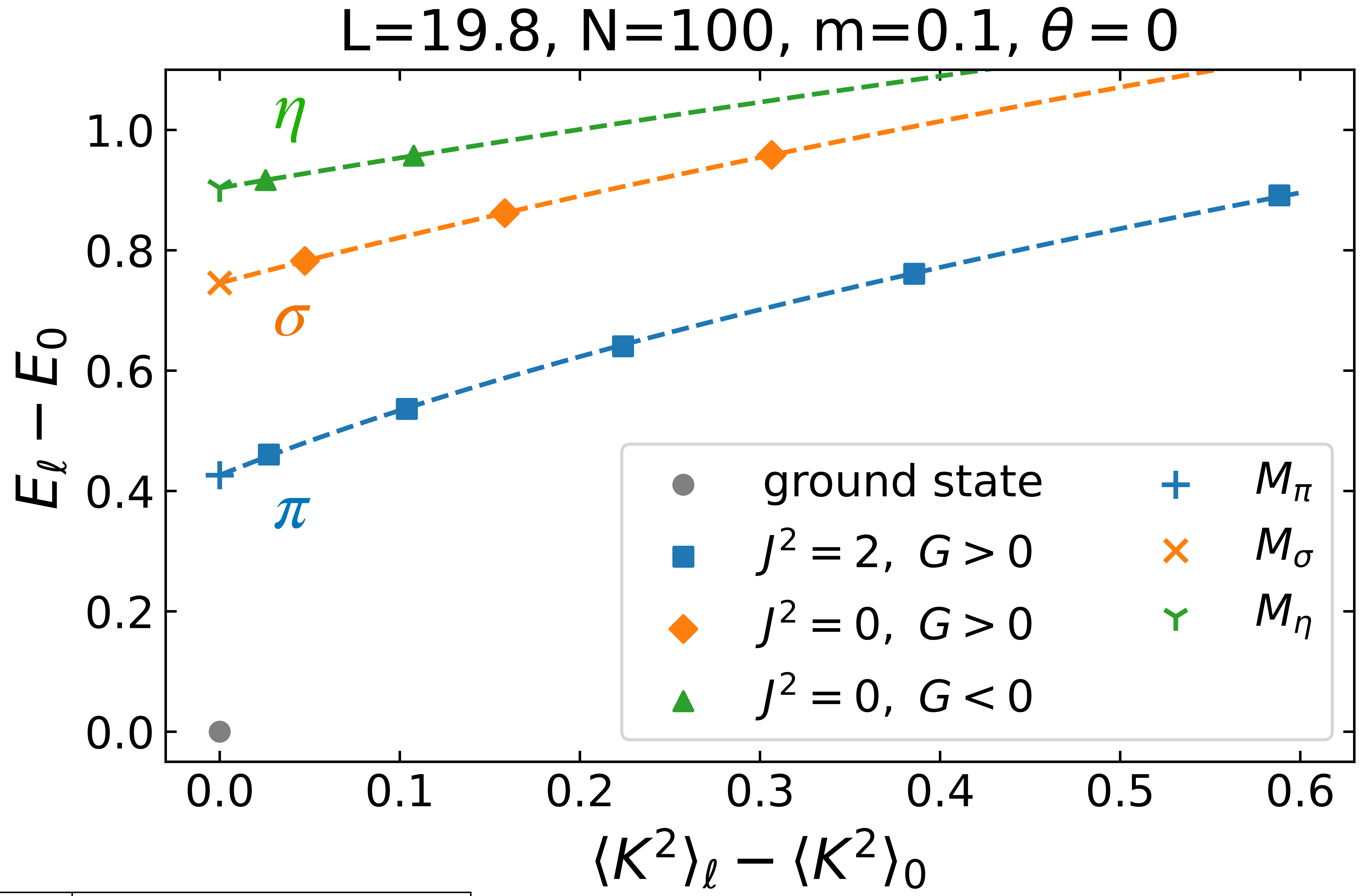
ℓ	$\boldsymbol{J}^2$	J_z	G
1	2.00000004	0.99999997	0.27872443
2	2.00000012	-0.00000000	0.27872416
3	2.00000004	-0.99999996	0.27872443
4	2.00000007	0.99999999	0.27736066
5	2.00000006	0.00000000	0.27736104
6	2.00000009	-0.99999998	0.27736066
7	2.00000010	1.00000000	0.27536687
8	2.00000002	0.00000000	0.27536702
9	2.00000007	-0.99999998	0.27536687
10	2.00000007	0.99999998	0.27356274
11	2.00000005	0.00000001	0.27356277
12	2.00000007	-0.99999999	0.27356274
15	1.99999942	0.99999966	0.27173470
16	2.00000052	0.00000000	0.27173482
17	2.00000015	-1.00000003	0.27173470
19	2.00009067	1.00004377	0.27717104
20	2.00002578	-0.00000004	0.27717020
21	2.00003465	-1.00001622	0.27717104

singlets

ℓ	$\boldsymbol{J}^2$	J_z	G
0	0.00000003	-0.00000000	0.27984227
13	0.00000003	0.00000000	0.27865844
14	0.00000003	0.00000000	0.27508176
18	0.00000028	0.00000006	-0.27390909
22	0.00001537	0.00000115	0.26678987
23	0.00003607	-0.00000482	-0.27664779

Result of dispersion relation

- plot ΔE_ℓ against ΔK_ℓ^2 for each meson
- fit the data points by $\Delta E = \sqrt{b^2 \Delta K^2 + M^2}$



	pion	sigma	eta
M	0.426(2)	0.7456(5)	0.9037
b	1.017(4)	1.087(2)	0.9622

Summary

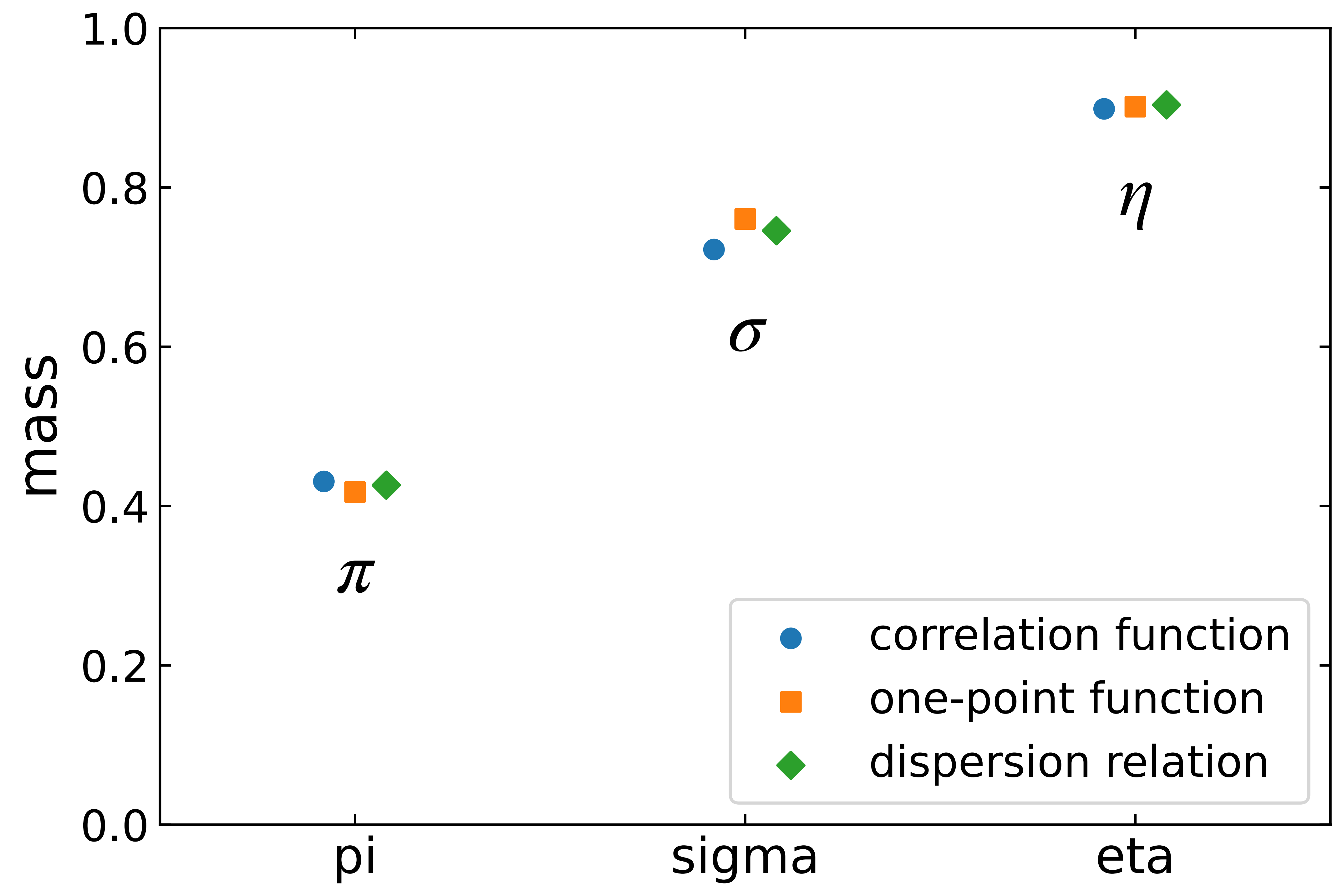
- The three results are consistent with each other and look promising.
- consistent with predictions by bosonization

✔ $M_\pi < M_\sigma < M_\eta$ —> U(1) problem

✔ $M_\eta \sim \mu \quad (\mu = g\sqrt{2/\pi} \sim 0.8)$

✔ $M_\sigma / M_\pi = \sqrt{3}$ within 5% deviation

[Coleman (1976)] [Dashen et al. (1975)]



	correlation func.	one-point func.	dispersion
M_σ/M_π	1.68(2)	1.821(6)	1.75(1)

Discussion

(1)correlation-function scheme

👍 generic method applicable to any case

😥 sensitive to the bond dimension of MPS —> 😊 quantum computation

(2)one-point-function scheme

👍 needs to increase NEITHER the bond dimension NOR the system size

😥 only the lowest state of the same quantum number as the boundary

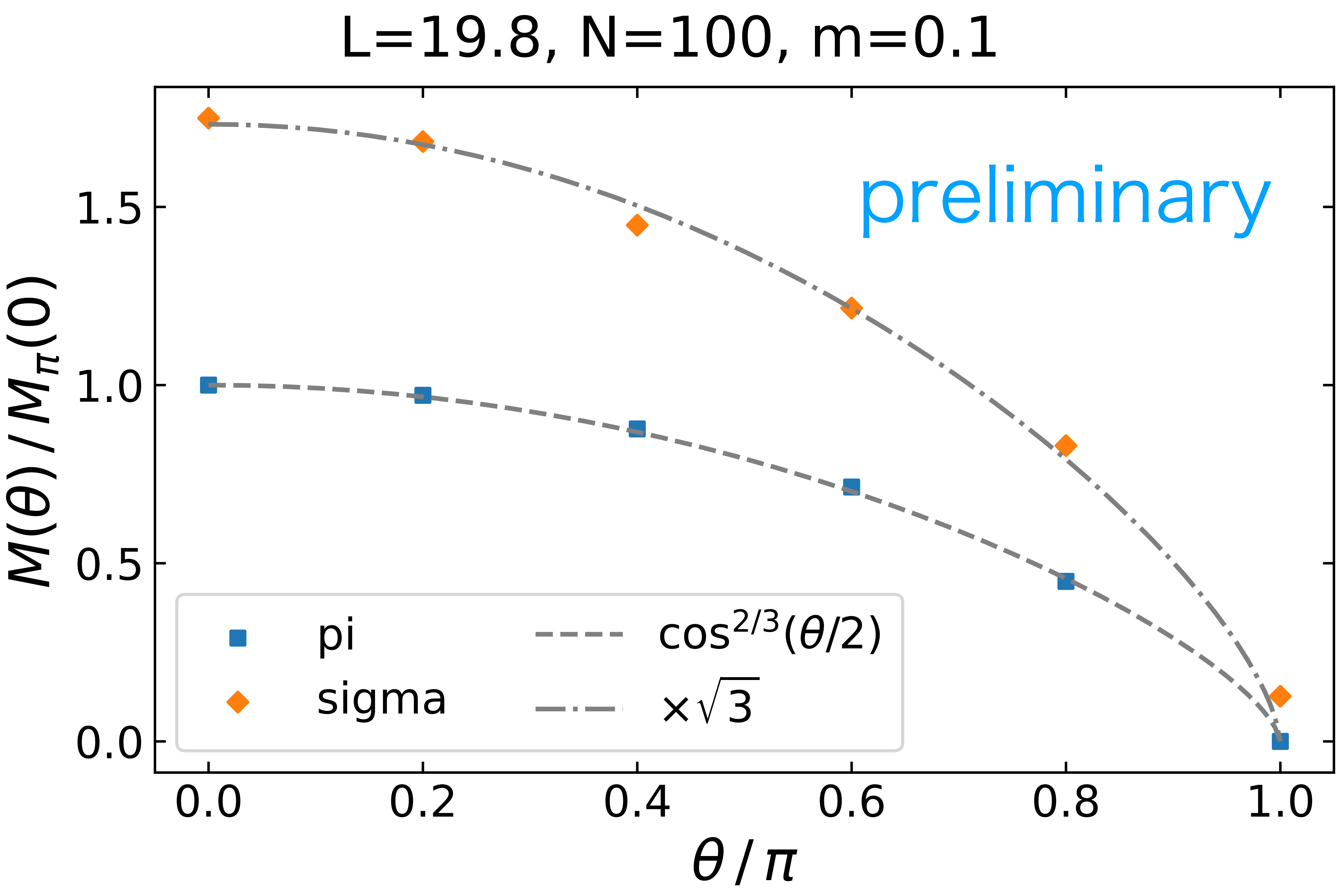
(3)dispersion-relation scheme

👍 obtain various states heuristically / directly see wave functions

😥 computational cost to generate many excited states

Application to $\theta \neq 0$

(3) dispersion-relation scheme



Monte Carlo result

[Fukaya & Onogi (2003)]