Computing composite-particle mass spectra in the Hamiltonian formalism

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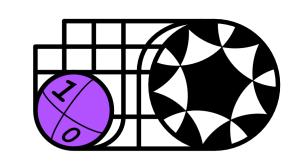
JHEP09 (2024) 155 [2407.11391]

QuantHEP 2025, 29 September 2025 @Lawrence Berkeley National Lab





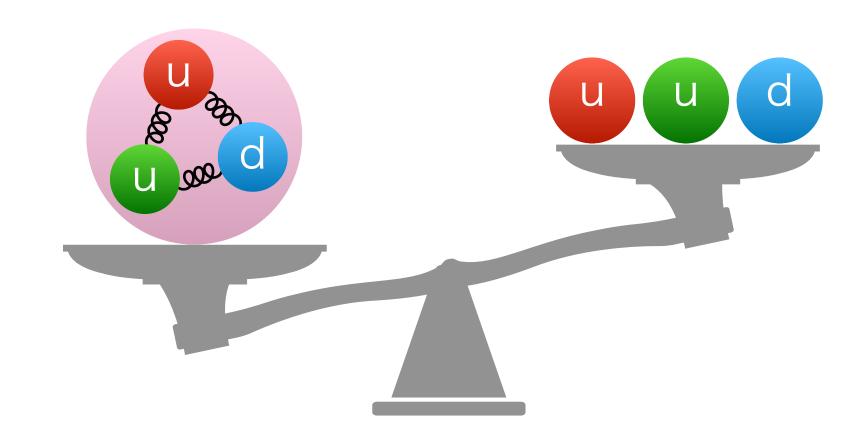




Background: mass spectrum of QCD

- quark confinement in Quantum ChromoDynamics (QCD)
 low-energy d.o.f. are not quarks but composite particles (hadrons)
- hadrons are much heavier than quarks

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u/d quark: m_u \sim 2 MeV, m_d \sim 5 MeV \pi^+ meson (u, d): 140 MeV \gg m_u + m_d proton (u, u, d): 938 MeV \gg 2m_u + m_d
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nonperturbative calc. is essential to understand the properties of hadrons

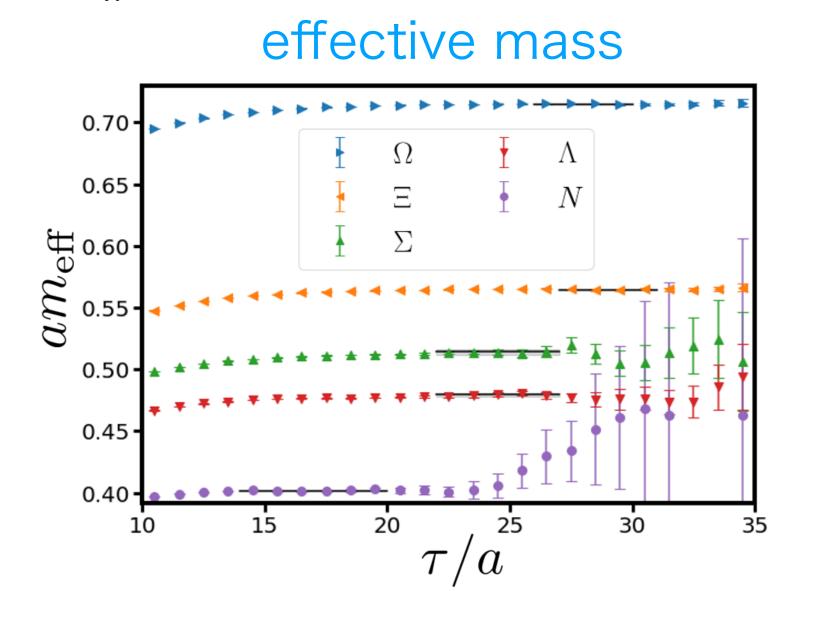
our motivation:

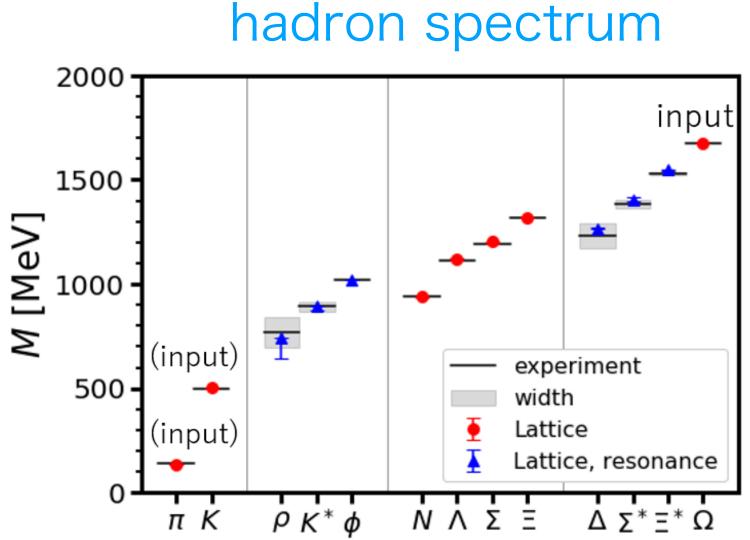
Numerically investigate low-energy spectra of gauge theories such as QCD

Mass spectrum by lattice QCD

- conventional method:
 - Monte Carlo simulation of the lattice gauge theory in Lagrangian formalism
- obtain hadron masses from imaginary-time correlation functions

$$C(\tau) = \sum \langle \mathcal{O}(0,0) \mathcal{O}(x,\tau) \rangle \sim e^{-M\tau} \longrightarrow \text{effective mass: } m_{\text{eff}}(\tau) := -\frac{d}{d\tau} \log C(\tau) \simeq M$$





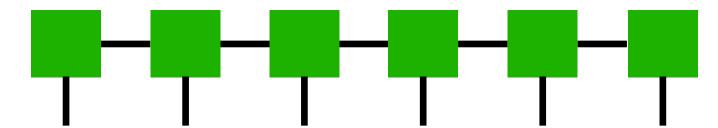
[HAL QCD collab. (2024)]

Hamiltonian formalism

- 100 Monte Carlo method cannot be applied to models with complex actions
 - -> sign problem (finite density QCD, topological term, real-time evolution, ···)
- Tensor network and quantum computing in Hamiltonian formalism can be complementary approaches!
 - tree from the sign problem
 - analyze wave functions directly

aim of this work:

compute the hadron mass spectrum in Hamiltonian formalism that is applicable even when the sign problem arises



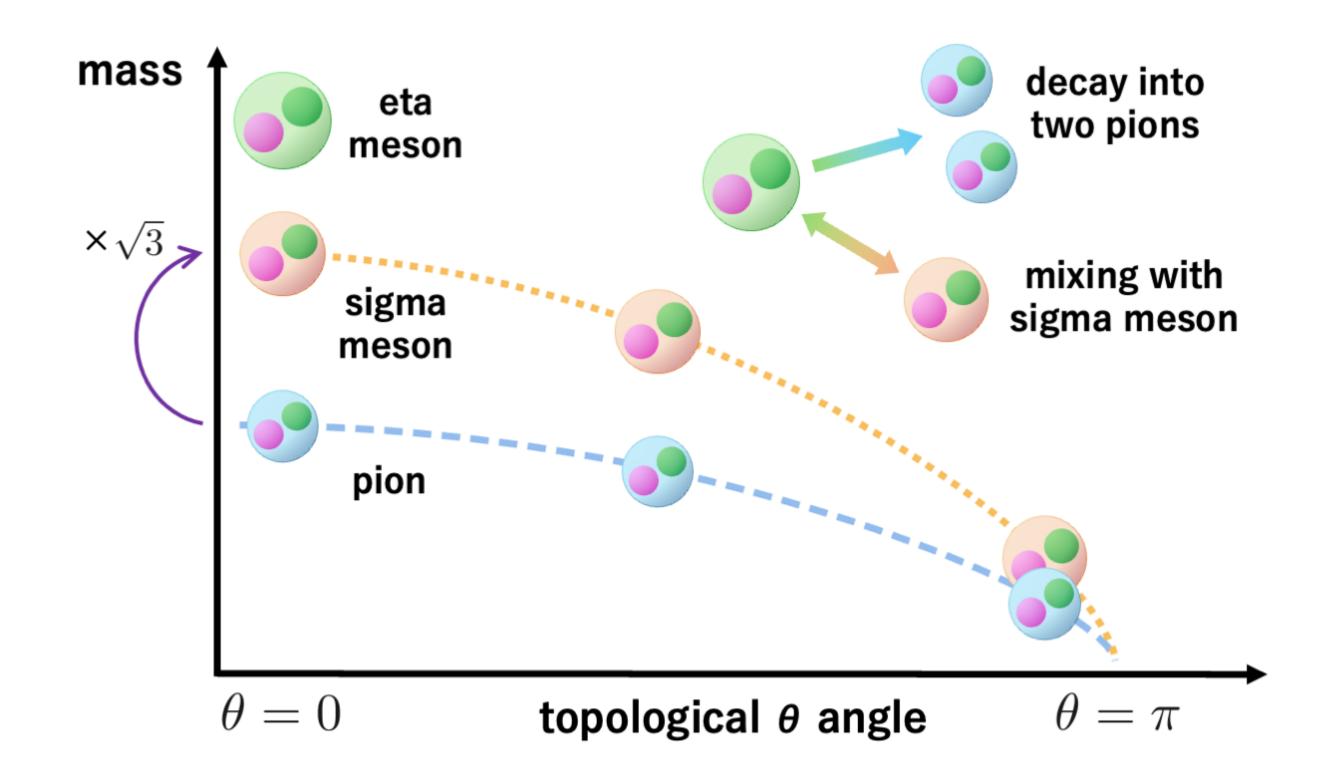


Short summary

- compute the mass spectrum of the 2-flavor Schwinger model by distinct methods
 - (1) correlation-function scheme
 - (2) one-point-function scheme
 - (3) dispersion-relation scheme

- θ-dependent spectra by these methods are consistent with each other and with analytic prediction
 - cf.) bosonization analysis [Coleman (1976)] [Dashen et al. (1975)]

[JHEP11 (2023) 231] [JHEP09 (2024) 155]



Outline

- 1. 2-flavor Schwinger model and calculation strategy
- 2. One-point-function scheme
- 3. Dispersion-relation scheme
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Schwinger model with two fermions

<u>Schwinger model = Quantum ElectroDynamics in 1+1d</u>

simplest nontrivial gauge theory sharing some features with QCD

$$\mathcal{L} = -\frac{1}{4g^2} F_{\mu\nu} F^{\mu\nu} + \frac{\theta}{4\pi} \epsilon_{\mu\nu} F^{\mu\nu} + \sum_{f=1}^{N_f} \left[i \bar{\psi}_f \gamma^\mu \left(\partial_\mu + i A_\mu \right) \psi_f - m \bar{\psi}_f \psi_f \right] \qquad \text{sign problem if } \theta \neq 0$$

- quantum numbers:
 - isospin J, parity P, G-parity $G = Ce^{i\pi J_y}$
- P and G are broken at $\theta \neq 0$
 - —> η becomes unstable due to $\eta \rightarrow \pi \, \pi$ decay and η σ mixing

$$N_f=2$$
 —> three "mesons"
$$\pi_a=-i\bar{\psi}\gamma^5\tau_a\psi \ : \ J^{PG}=1^{-+}$$

$$\sigma=\bar{\psi}\psi \ : \ J^{PG}=0^{++}$$

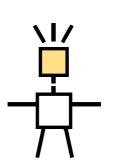
$$\eta = -i\bar{\psi}\gamma^5\psi \quad : \quad J^{PG} = 0^{--}$$

Calculation strategy

setup: staggered fermion with open boundary

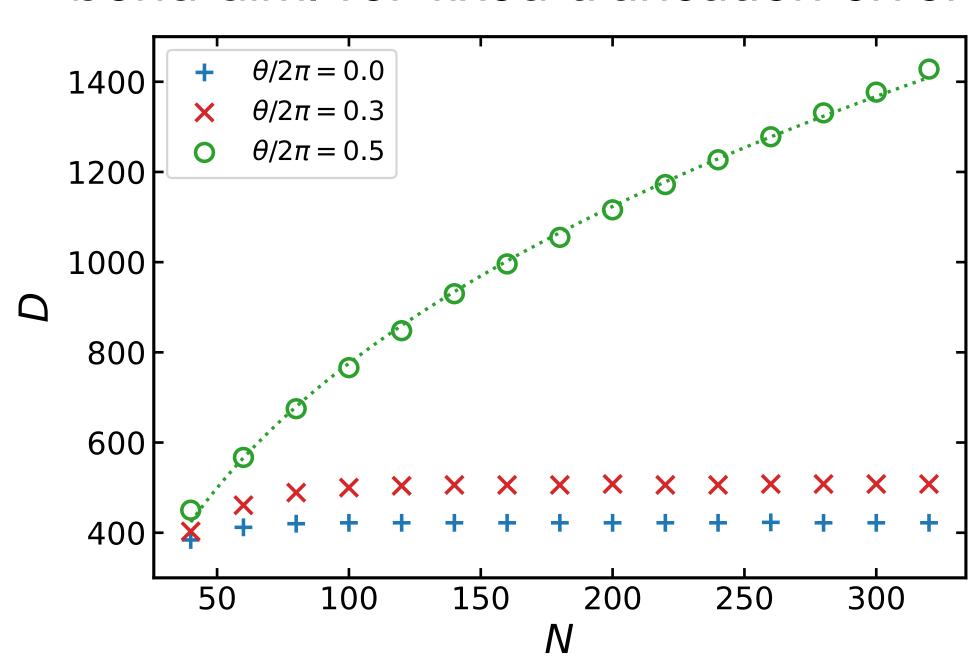
$$H = \frac{g^2 a}{2} \sum_{n=0}^{N-2} \left(L_n + \frac{\theta}{2\pi} \right)^2 + \sum_{f=1}^{N_f} \left[\frac{-i}{2a} \sum_{n=0}^{N-2} \left(\chi_{f,n}^{\dagger} U_n \chi_{f,n+1} - \chi_{f,n+1}^{\dagger} U_n^{\dagger} \chi_{f,n} \right) + m_{\text{lat}} \sum_{n=0}^{N-1} (-1)^n \chi_{f,n}^{\dagger}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

- rewrite to the spin Hamiltonian by Jordan-Wigner transformation after solving Gauss law and gauge fixing
- obtain the ground state as MPS by density-matrix renormalization group (DMRG)



[Kogut & Susskind (1975)] [Dempsey et al. (2022)]

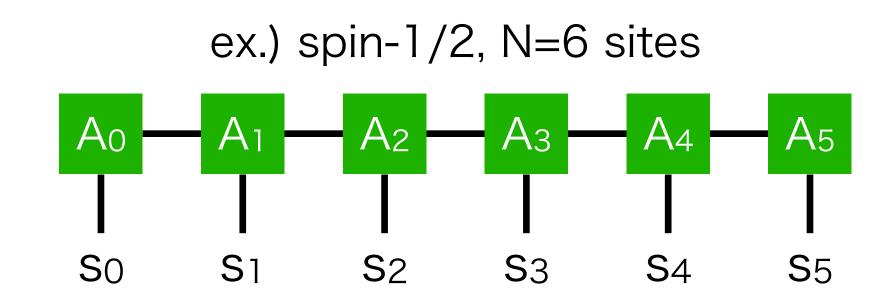
bond dim. for fixed truncation error



Approximation of states by MPS

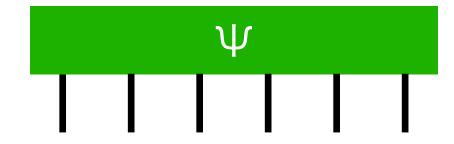
Matrix Product State (MPS)

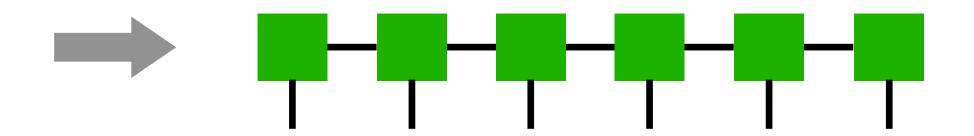
$$|\Psi\rangle = \sum_{\{s_i\}} \operatorname{Tr} \left[A_0(s_0) A_1(s_1) \cdots \right] |s_0 s_1 \cdots\rangle$$



- . $A_i(s_i)$: $D_{i-1} \times D_i$ matrix with a spin index $s_i \in \{\uparrow, \downarrow\}$ (D_i : bond dimension)
- . Any state can be written as MPS by repeating SVD, but $D_i = O(2^{N/2})$ in general.

$$|\Psi\rangle = \sum_{\{s_i\}} \Psi(s_0, s_1, \cdots) |s_0 s_1 \cdots\rangle$$





. Even with a cutoff $D_i \leq \text{const}$, MPS efficiently approximates low-energy states of 1+1d gapped systems of any size N. \rightarrow numerical cost = $O(ND^3)$

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Two-point correlation function?

- In lattice QCD, correlation functions are measured with spatial integral
 - —> zero-momentum projection: $\sum_{x} \langle \mathcal{O}(0,0)\mathcal{O}(x,\tau) \rangle \sim e^{-M\tau}$
- Equal-time correlator in Hamiltonian formalism:

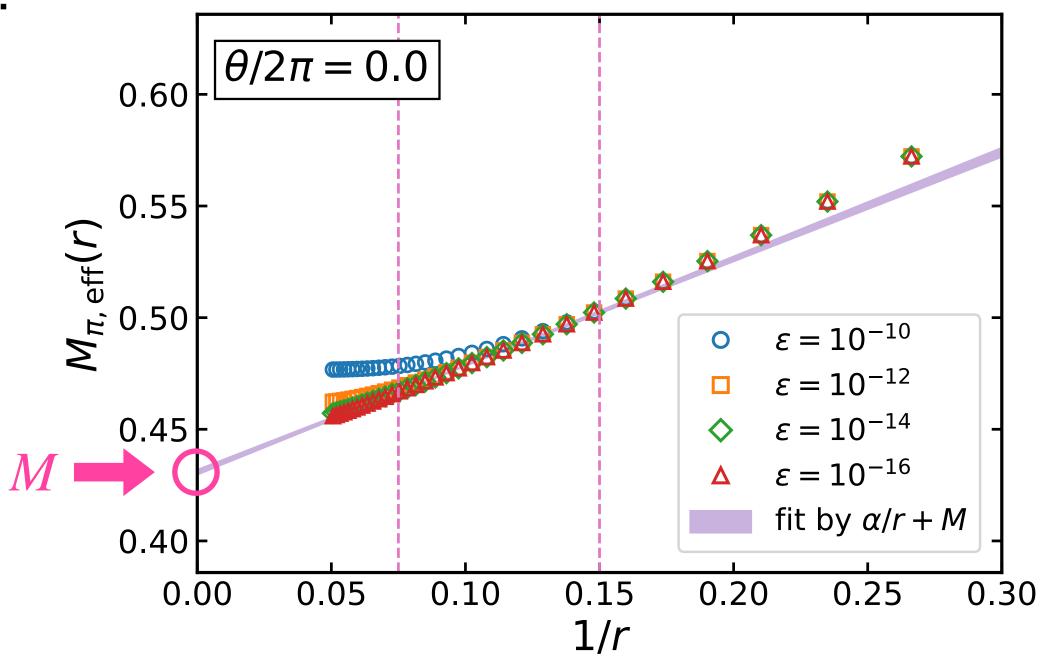
$$C(r) = \langle \mathcal{O}(0,0) \mathcal{O}(r,0) \rangle \sim \frac{1}{r^{\alpha}} e^{-Mr}$$

—> effective mass:
$$M_{\text{eff}}(r) = -\frac{d}{dr} \log C(r) \sim \frac{\alpha}{r} + M$$

• Bond dim. must be large enough to see 1/r behavior

significant truncation effect

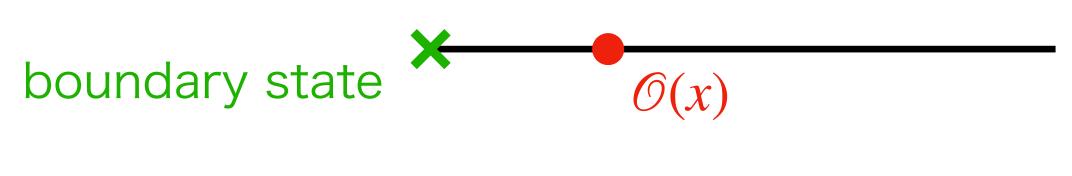
effective mass of π meson



One-point-function scheme

Regarding the boundary (defect) as the source of mesons, obtain the masses from the one-point functions

- . 1pt. function $\langle \mathcal{O}(x) \rangle_{\rm obc}$ measures the correlation with the boundary state |bdry>
- . |bdry> has translational invariance in time direction
 - --> zero-momentum projection --> exponential decay

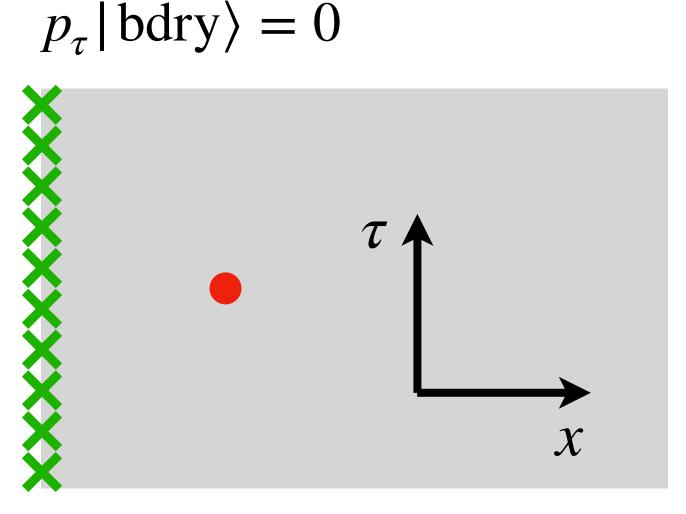


$$\langle \mathcal{O}(x) \rangle_{\text{obc}} \sim \langle \text{bdry} | e^{-Hx} \mathcal{O} | 0 \rangle_{\text{bulk}} \sim e^{-Mx}$$

TN truncation effect is much smaller



Euclidean space

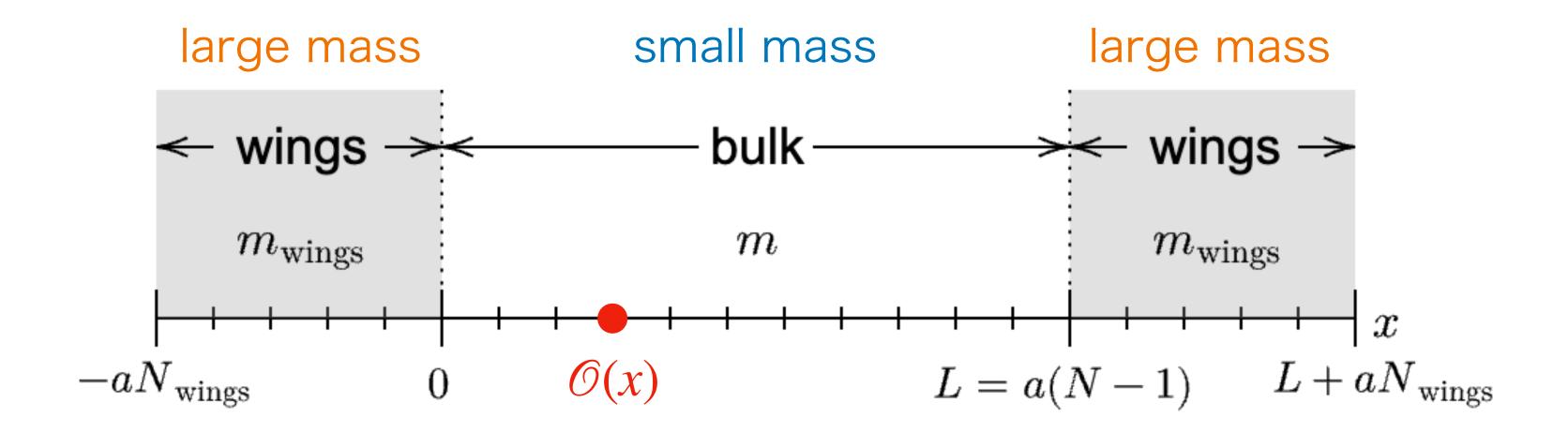


cf.) wall source method

Some technical improvement

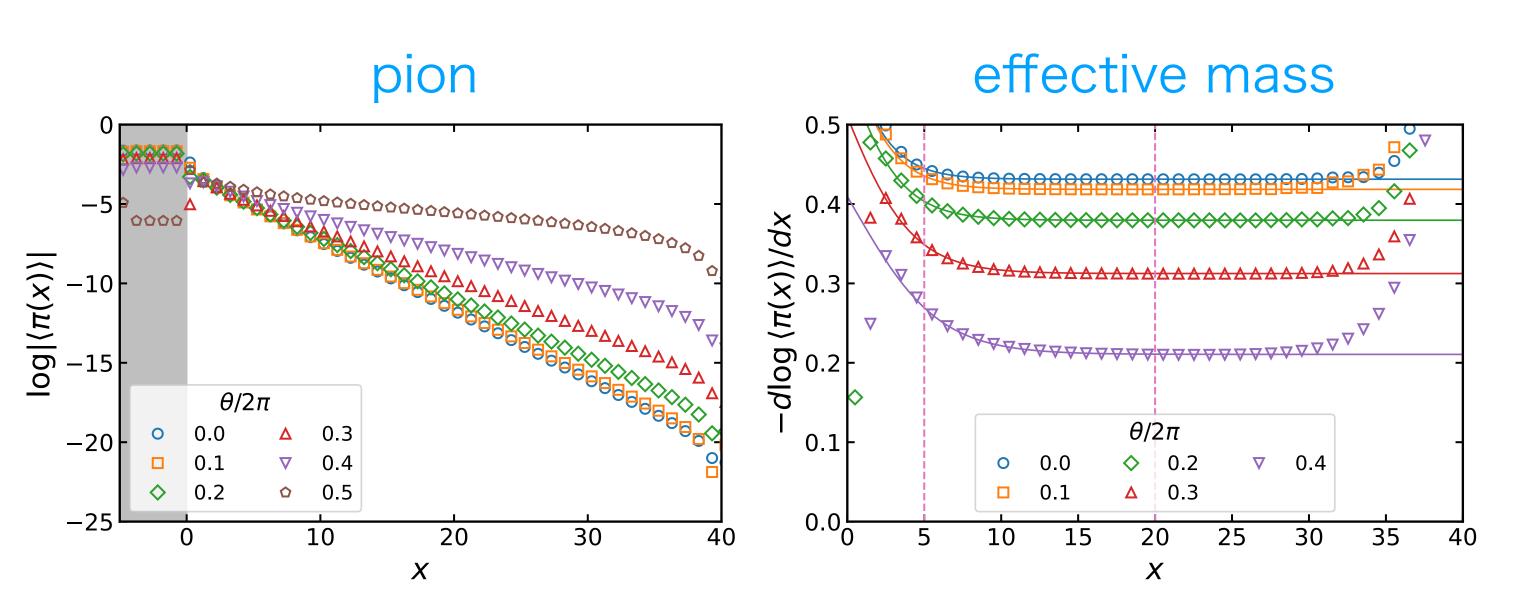
The boundary state (bdry | is specified by "the wings" attached to the lattice, which have the same quantum number as the target meson

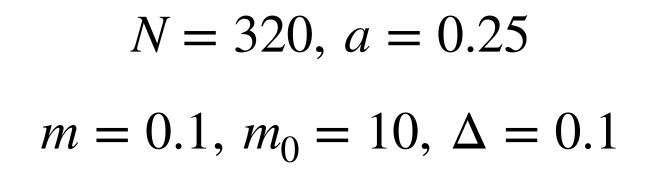
e.g.) Dirichlet b.c.
$$m_{\rm wings}\gg m$$
 isospin-breaking b.c. $m_{\rm wings}=m_0\exp(\pm i\Delta\gamma^5)$



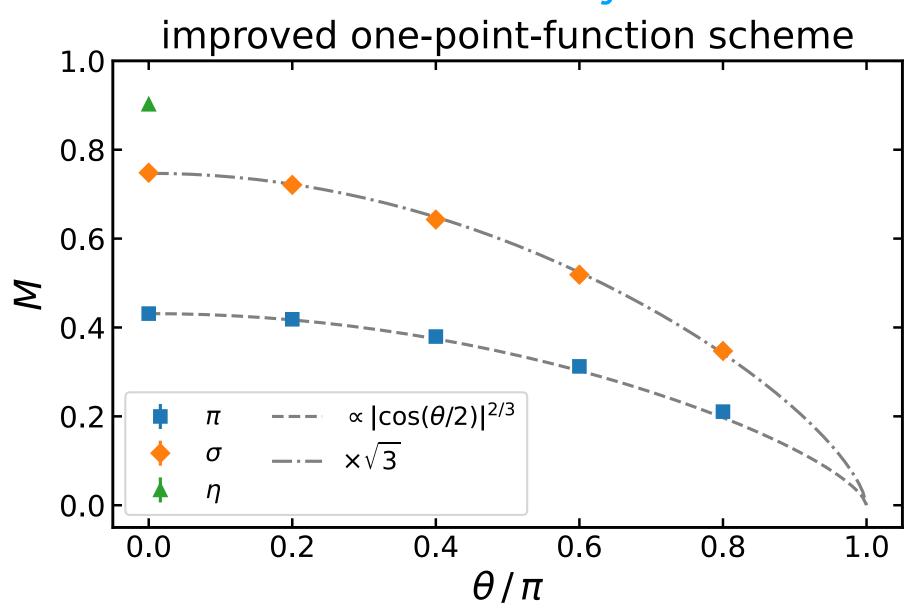
Spectrum by the one-point function

- Dirichlet b.c. for the singlets / isospin-breaking b.c. for the triplets
- . Assuming $\langle \mathcal{O}(x) \rangle \sim Ae^{-Mx} + Be^{-(M+\Delta M)x}$, the effective mass should be $\sim M + \frac{\Delta M}{1 + Ce^{\Delta Mx}}$





summary



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Dispersion-relation scheme

Obtain the dispersion relation $E = \sqrt{K^2 + M^2}$ directly from the excited states (momentum excitations of the mesons)

- . ℓ -th excited state $|\Psi_{\ell}\rangle$
 - = the lowest energy eigenstate satisfying $\langle \Psi_{\ell'} | \Psi_{\ell} \rangle = 0$ for $\ell' = 0, 1, \dots, \ell-1$
- obtained by DMRG, adding the projection term to H

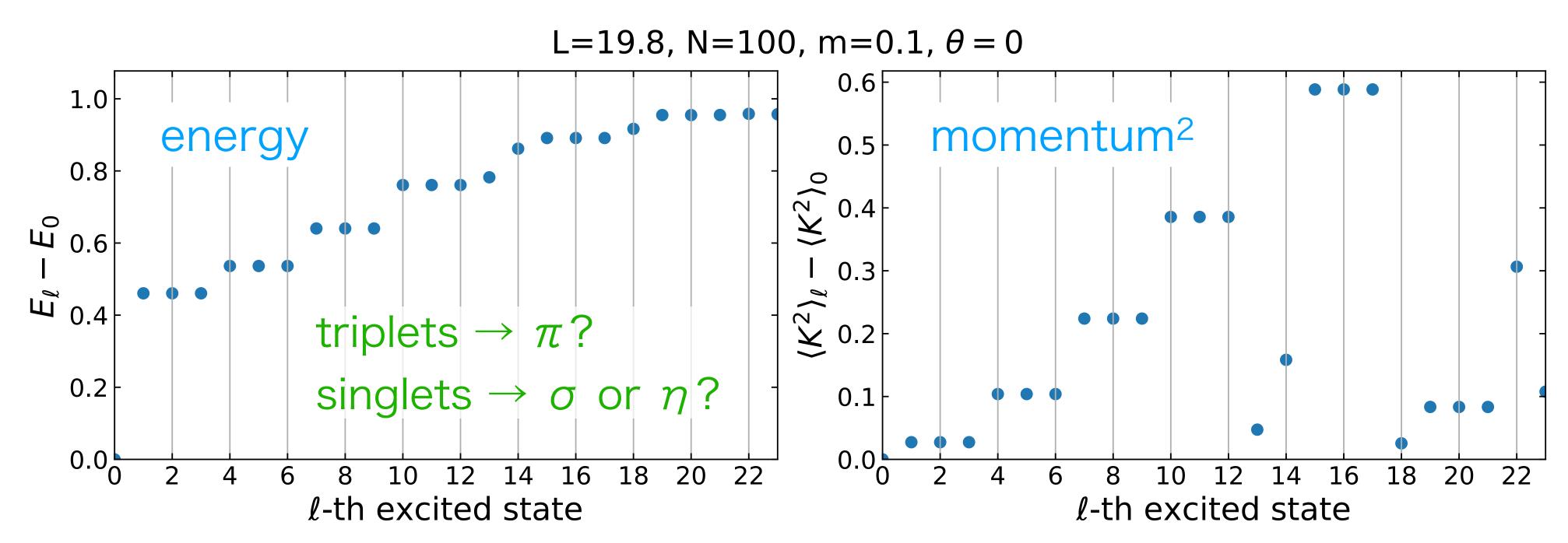
[Stoudenmire & White (2012)] [Banuls et al. (2013)]

$$H_{\ell} = H + W \sum_{\ell'=0}^{\ell-1} |\Psi_{\ell'}\rangle \langle \Psi_{\ell'}| \longrightarrow \text{cost function: } \langle \Psi_{\ell}|H|\Psi_{\ell}\rangle + W \sum_{\ell'=0}^{\ell-1} \left|\langle \Psi_{\ell'}|\Psi_{\ell}\rangle\right|^2 \qquad W > 0$$

measure the energy E and the total momentum $K = \sum_f \int dx \, \psi_f^\dagger (i\partial_x - A_1) \psi_f$

Energy spectrum at $\theta = 0$

- . energy gap: $\Delta E_{\ell} = E_{\ell} E_0$
- . momentum square: $\Delta K_{\ell}^2 = \langle K^2 \rangle_{\ell} \langle K^2 \rangle_0$
- .identify the states by measuring quantum numbers: \mathbf{J}^2 , J_z , $G=Ce^{i\pi J_y}$



Quantum numbers

isospin:
$$J_a = \frac{1}{2} \int dx \ \psi^{\dagger} \tau^a \psi$$
 $[H, \mathbf{J}^2] = [H, J_z] = 0$

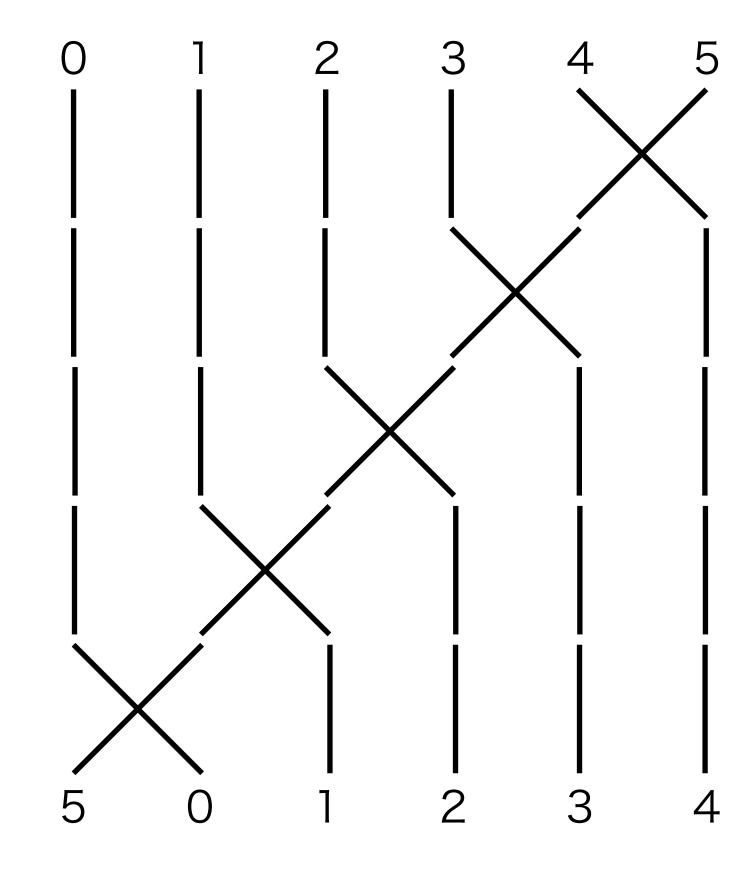
- charge conjugation:
 - = exchange particles/anti-particles
 - = exchange even/odd sites and flip each spin
 - = 1-site translation and σ^x operator

$$C := \prod_{f=1}^{N_f} \left(\prod_{n=0}^{N-1} \sigma_{f,n}^{x} \right) \left(\prod_{n=0}^{N-2} (SWAP)_{f;N-2-n,N-1-n} \right)$$

 $[H, C] \neq 0$ due to the boundary

. G-parity: $G = C \exp(i\pi J_y)$

1-site translation



$$\sum_{k}^{j} \left(\text{SWAP} \right)_{f;j,k} = \frac{1}{2} \left(\mathbf{1}_{f,j} \mathbf{1}_{f,k} + \sum_{a} \sigma_{f,j}^{a} \sigma_{f,k}^{a} \right)$$

Result of quantum numbers

results at $\theta = 0$

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

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

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

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

singlets

ℓ	$oxed{J^2}$	J_z	G	P
0	0.00000003	-0.00000000	0.27984227	3.896×10^{-7}
13	0.00000003	0.00000000	0.27865844	1.273×10^{-7}
14	0.00000003	0.00000000	0.27508176	-2.765×10^{-8}
18	0.00000028	0.00000006	-0.27390909	-6.372×10^{-7}
22	0.00001537	0.00000115	0.26678987	7.990×10^{-8}
23	0.00003607	-0.00000482	-0.27664779	5.715×10^{-7}

ℓ	$oldsymbol{J}^2$	J_z	G	P
1	2.00000004	0.99999997	0.27872443	-6.819×10^{-8}
2	2.00000012	-0.00000000	0.27872416	-6.819×10^{-8}
3	2.00000004	-0.99999996	0.27872443	-6.819×10^{-8}
4	2.00000007	0.99999999	0.27736066	7.850×10^{-8}
5	2.00000006	0.00000000	0.27736104	7.850×10^{-8}
6	2.00000009	-0.99999998	0.27736066	7.850×10^{-8}
7	2.00000010	1.00000000	0.27536687	-8.838×10^{-8}
8	2.00000002	0.00000000	0.27536702	-8.837×10^{-8}
9	2.00000007	-0.99999998	0.27536687	-8.838×10^{-8}
10	2.00000007	0.99999998	0.27356274	9.856×10^{-8}
11	2.00000005	0.00000001	0.27356277	9.856×10^{-8}
12	2.00000007	-0.99999999	0.27356274	9.856×10^{-8}
15	1.99999942	0.99999966	0.27173470	-1.077×10^{-7}
16	2.00000052	0.00000000	0.27173482	-1.077×10^{-7}
17	2.00000015	-1.00000003	0.27173470	-1.077×10^{-7}
19	2.00009067	1.00004377	0.27717104	-3.022×10^{-8}
20	2.00002578	-0.00000004	0.27717020	-3.023×10^{-8}
21	2.00003465	-1.00001622	0.27717104	-3.023×10^{-8}

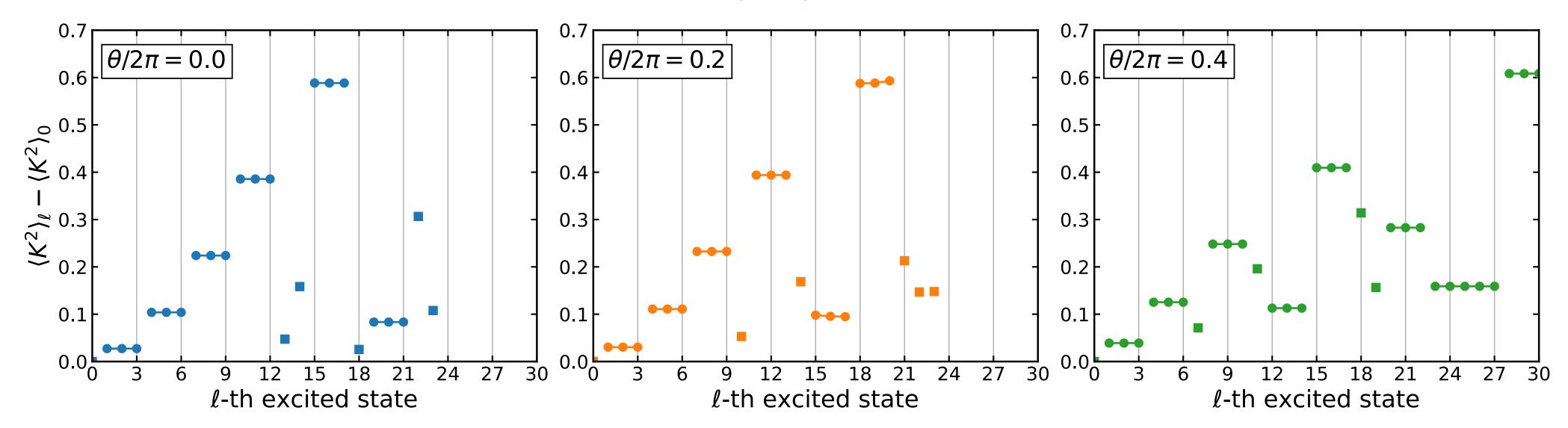
Extension to $\theta \neq 0$

- G-parity is no longer the quantum number —> η disappears
- singlet projection to obtain σ with reasonable computational cost

$$H_{\ell} = H + W \sum_{\ell'=0}^{\ell-1} |\Psi_{\ell'}\rangle\langle\Psi_{\ell'}| + W_{J}J^{2}$$

cf.) quantum-number preserving DMRG

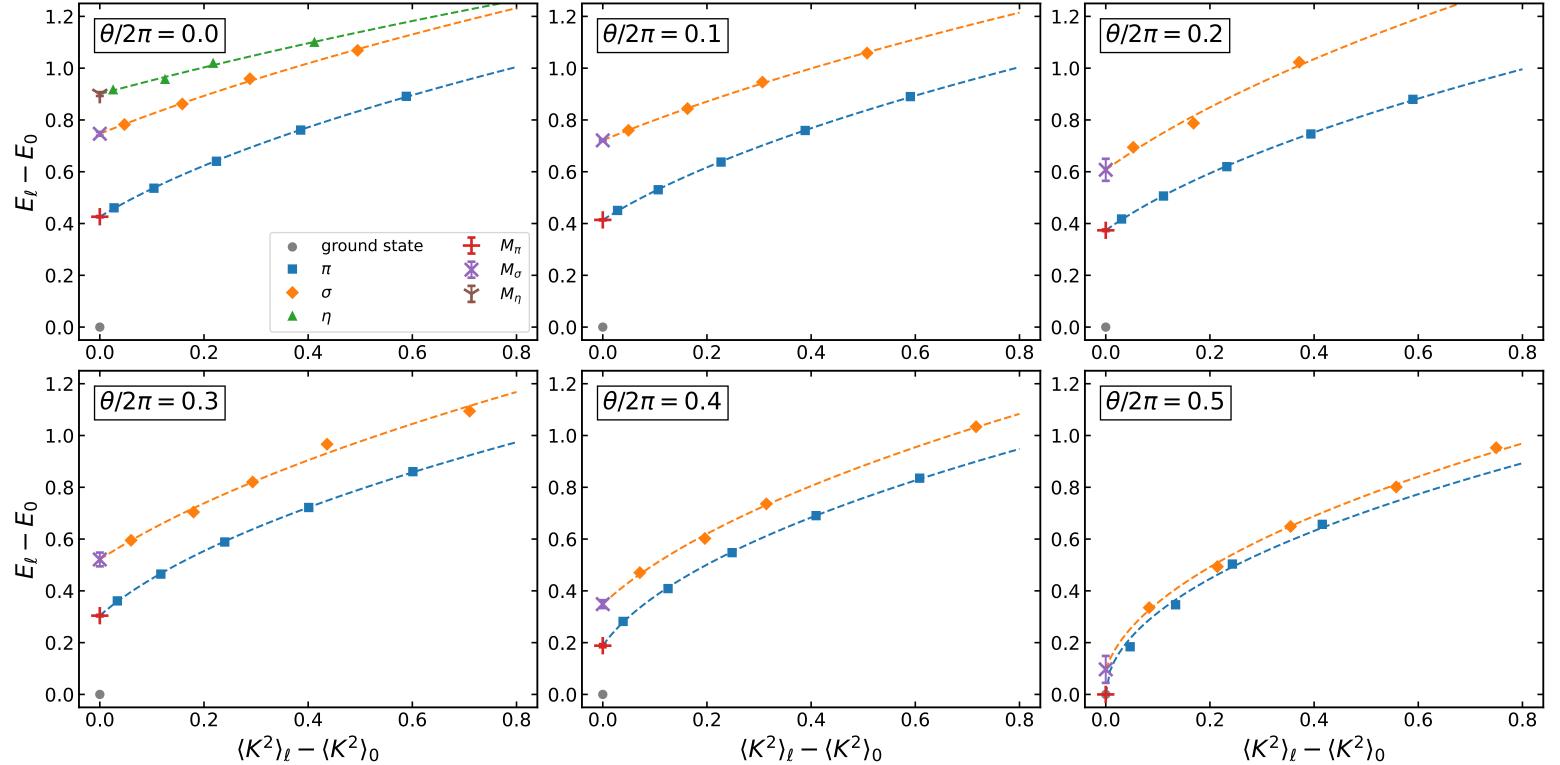
momentum²



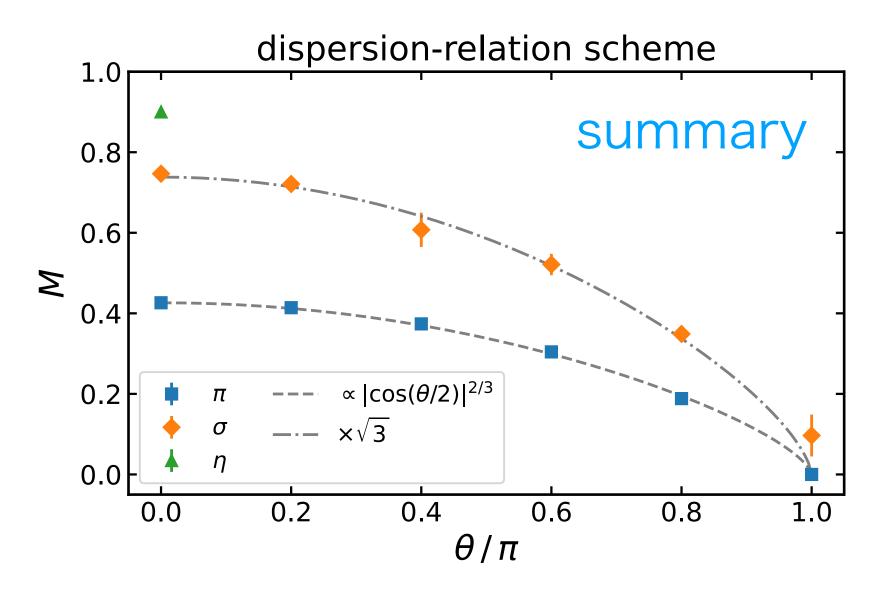
Result of dispersion relation

. plot ΔE_{ℓ} against ΔK_{ℓ}^2 and fit the data by $\Delta E = \sqrt{b^2 \Delta K^2 + M^2}$ for each meson





Around $\theta/2\pi=0.2$, σ is contaminated by a remnant of η due to the mixing



Outline

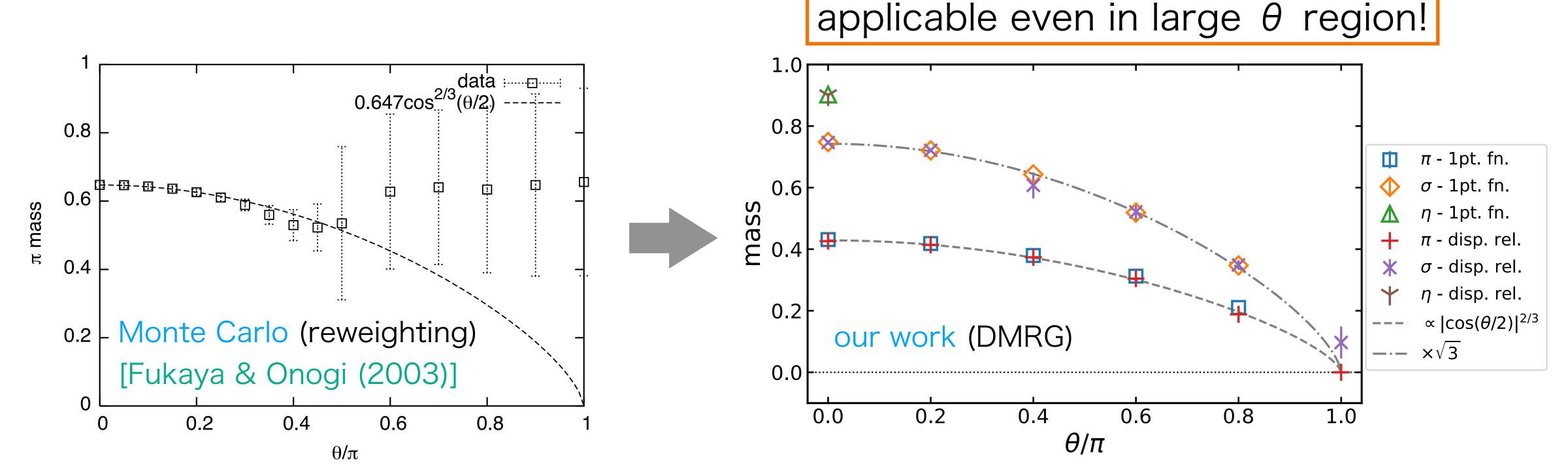
- 1. 2-flavor Schwinger model and calculation strategy
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Summary

- The two schemes give consistent results and look promising
- consistent with predictions by the bosonization [Coleman (1976)] [Dashen et al. (1975)]

$$M_{\pi}(\theta) \propto |\cos(\theta/2)|^{2/3}$$
 $M_{\sigma}(\theta)/M_{\pi}(\theta) = \sqrt{3}$



Discussion and prospect

Large volume limit and continuum limit

[Schwägerl et al. (2025)]

- 2+1 dimensions
- Analyses using the wave functions for the scattering problem
- Real-time evolution to study the decay of unstable mesons
 - TN method: Time-Dependent Variational Principle?

[Haegeman et al. (2011)] [Yang & White (2020)]

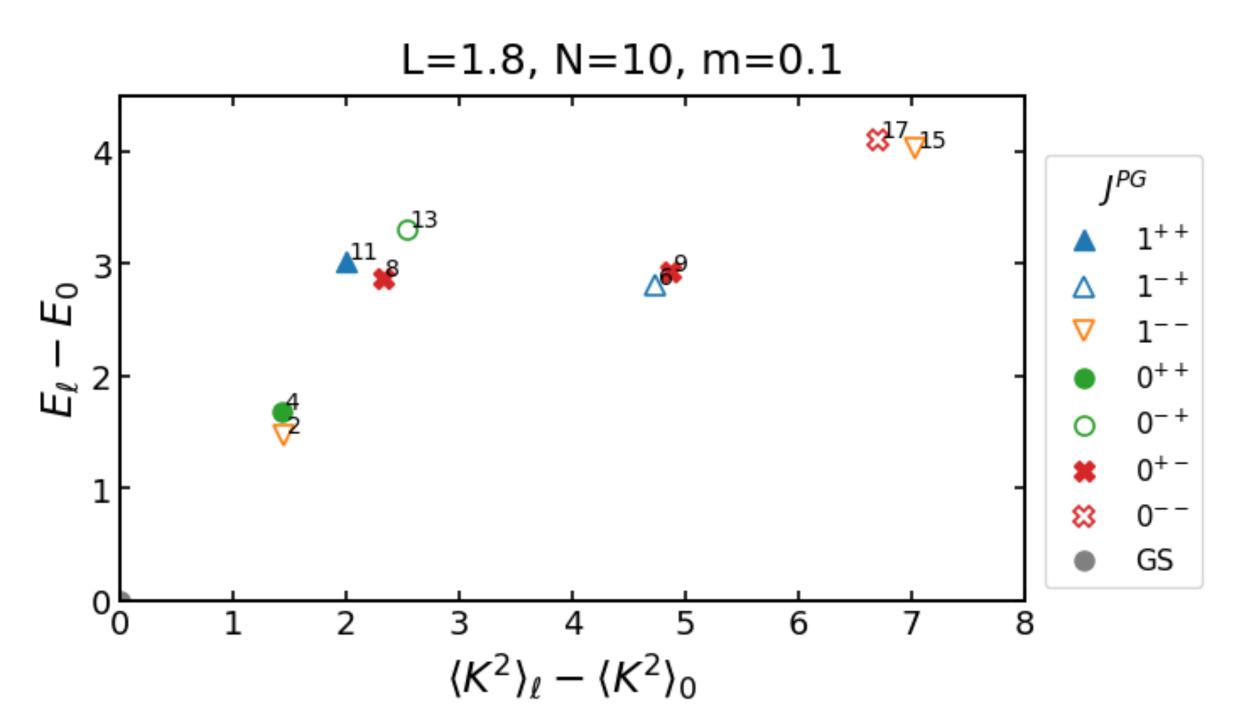
TN-QC hybrid method: encoding TN states into quantum circuits?

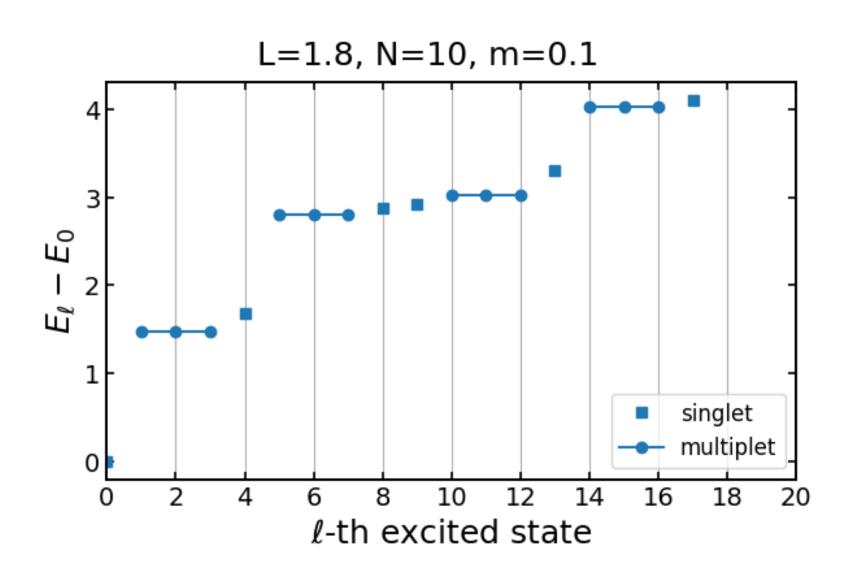
[Shirakawa et al. (2021)]

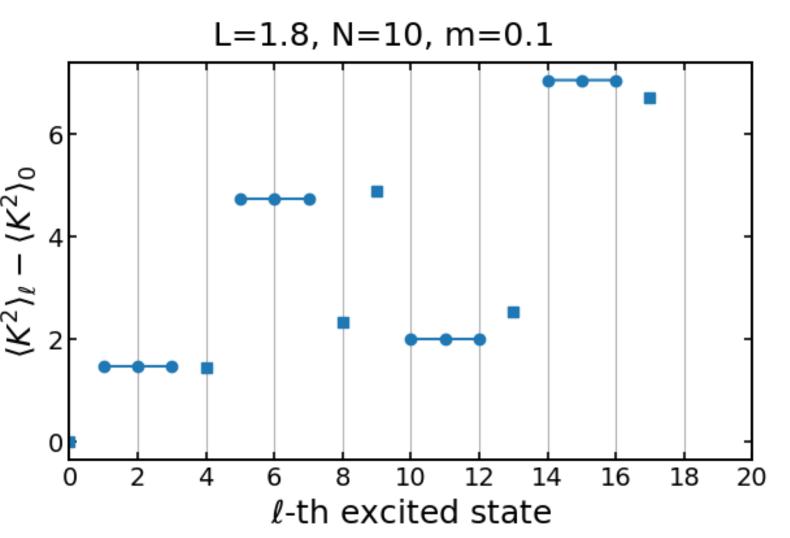
• Full Quantum algorithm to find excited states?

Small N: N = 10, a = 0.2 (20 qubits)

- The lowest excitations
 are not consistent with pion triplets 1⁻⁺
- . L = a(N-1) = 1.8 is smaller than $1/M_{\pi} \sim 2.4$



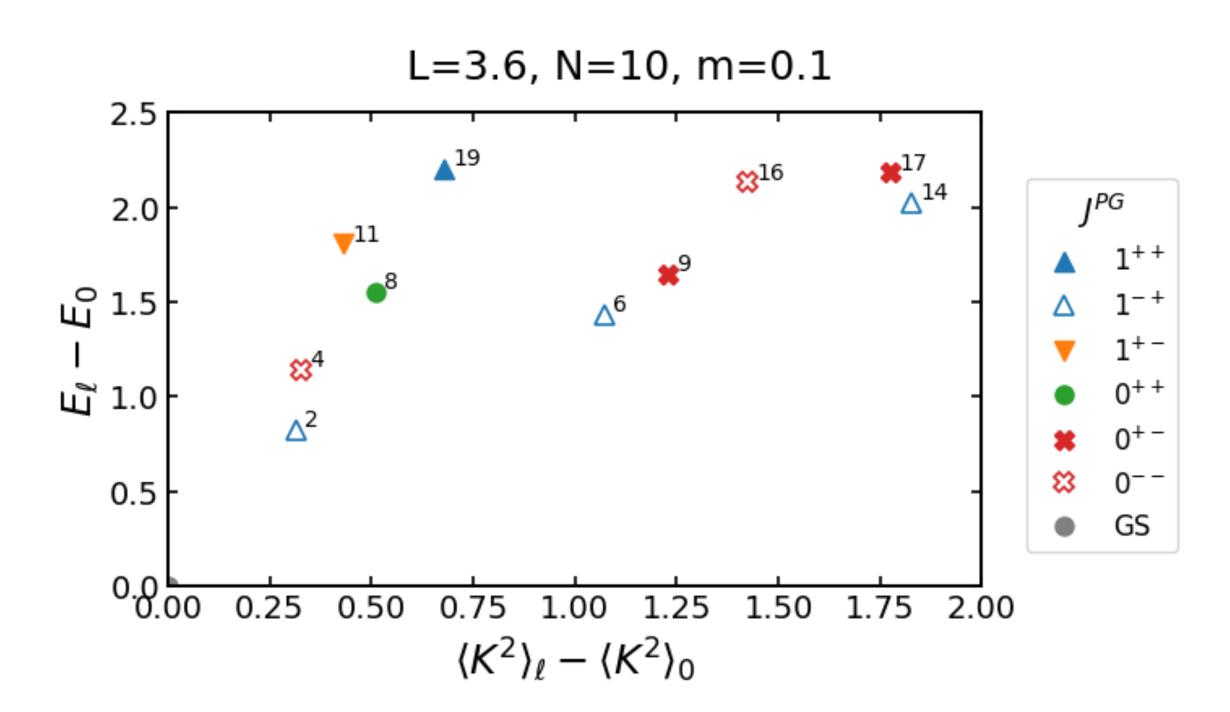


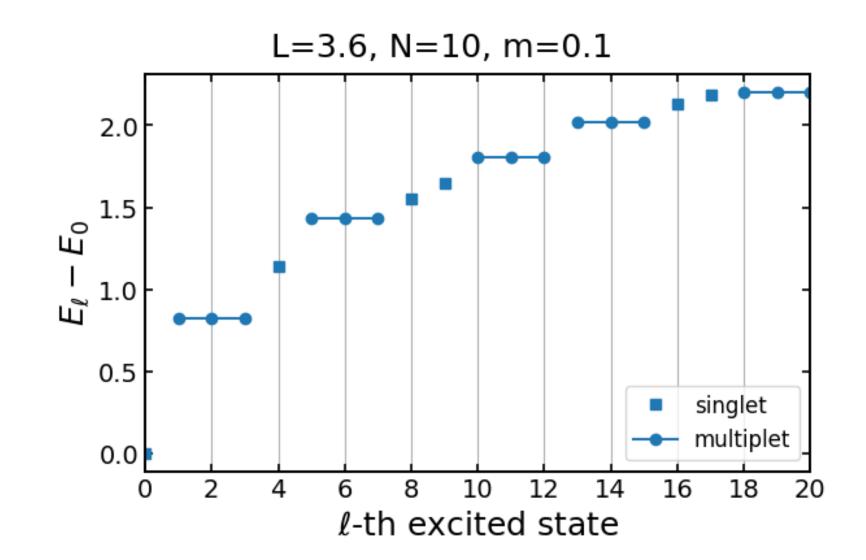


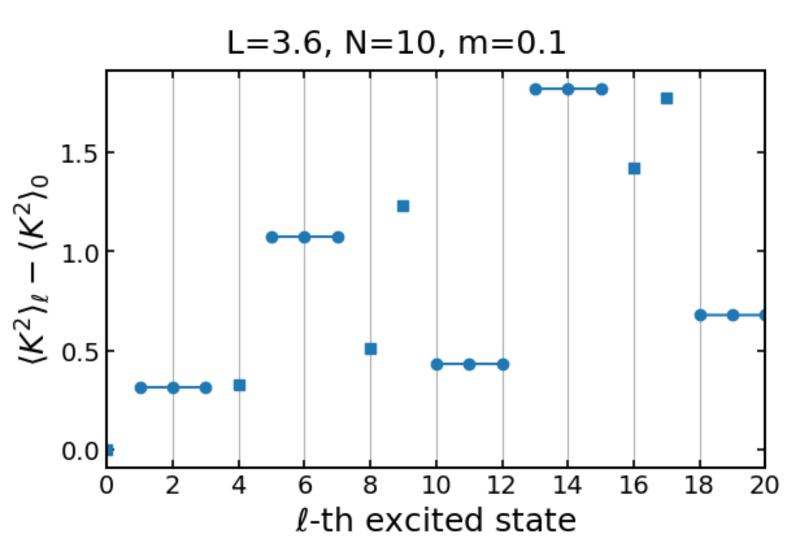
Small N: N = 10, a = 0.4 (20 qubits)

The lowest excitations
 become consistent with pion triplets 1⁻⁺

$$L = a(N-1) = 3.6 > 1/M_{\pi} \sim 2.4$$





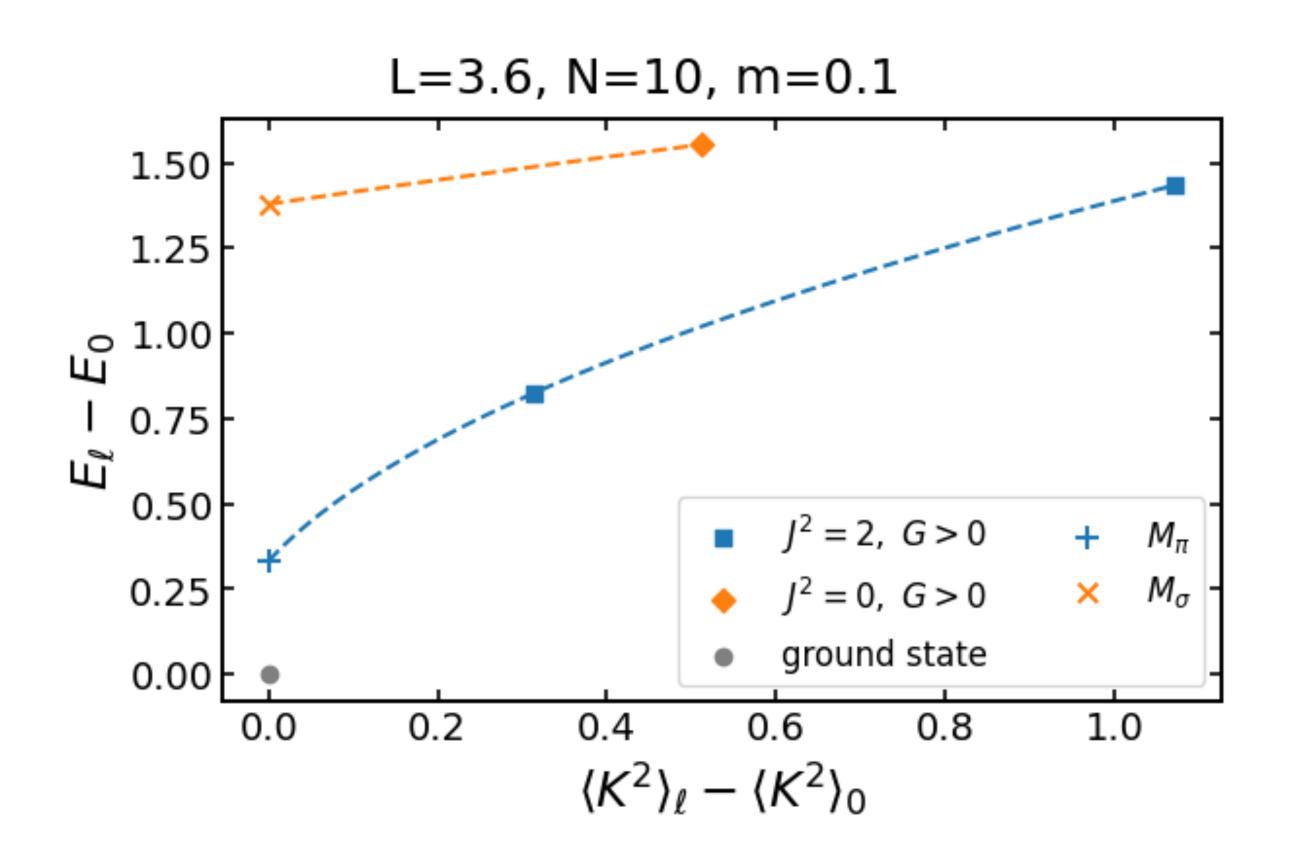


Dispersion relation for L=3.6

- $\ell = (1,2,3), (5,6,7)$ —> pions?
- $\ell = 8$ —> sigma meson?
- . solutions of $E = \sqrt{b^2 K^2 + M^2}$

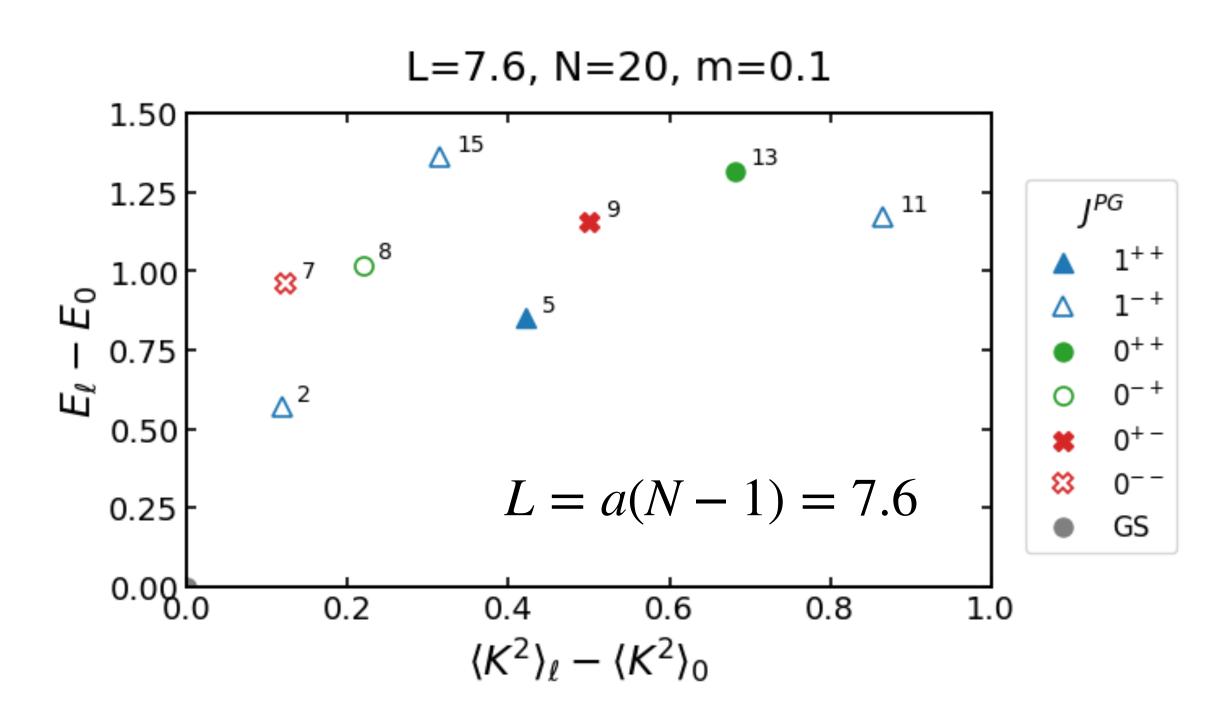
$$M_{\pi} = 0.332, b = 1.35$$

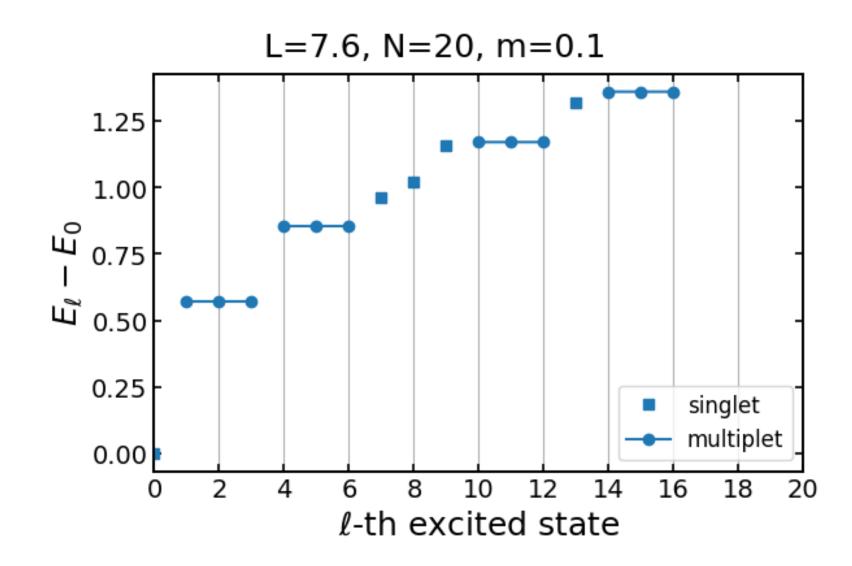
$$M_{\sigma} = 1.38, b := 1$$

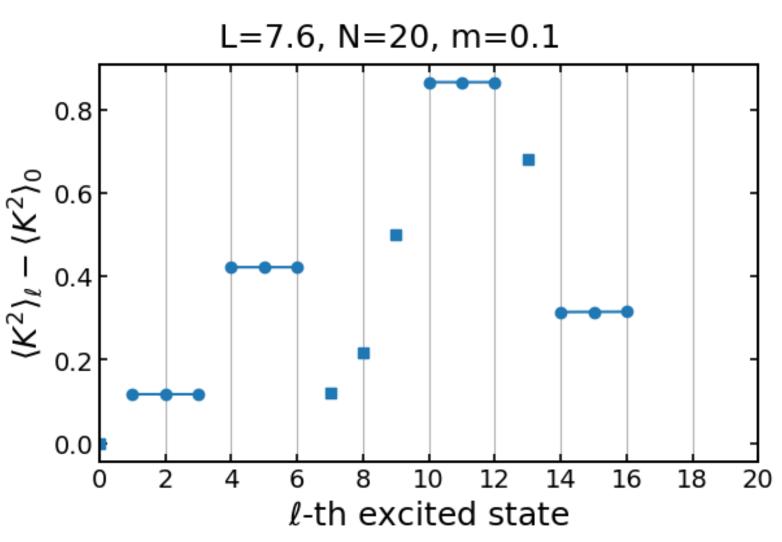


Middle N: N = 20, a = 0.4 (40 qubits)

- The behavior of the pions approaches the case of N = 100!
- sigma and eta mesons start to appear







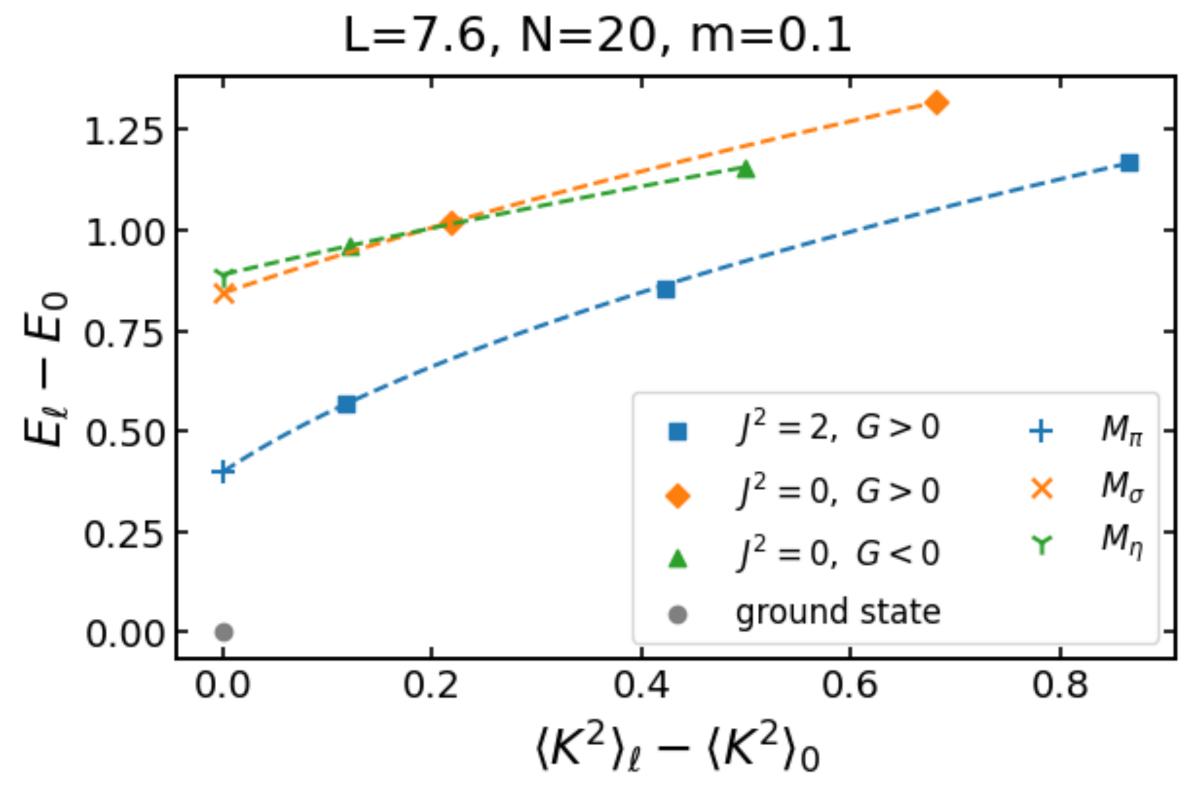
Dispersion relation for L=7.6

- $\ell = (1,2,3), (4,5,6), (10,11,12)$ —> pions?
- $\ell = 8,13$ —> sigma meson?
- $\ell = 7.9$ —> eta meson?
- . fitting/solutions of $E = \sqrt{b^2 K^2 + M^2}$

$$M_{\pi} = 0.40(2), b = 1.18(2)$$

$$M_{\sigma} = 0.843, b = 1.23$$

$$M_{\eta} = 0.889, b = 1.05$$



consistent with $M_{\pi} = 0.426(2)$ for N=100

Thank you for listening.