Introduction to Lattice QCD (part2)

Etsuko Itou (YITP, Kyoto U./RIKEN iTHEMS)

YITP long-term workshop
Hadrons and Hadron Interactions in QCD 2024 (HHIQCD2024)@ YITP, Kyoto U., 2024/10/16

Contents

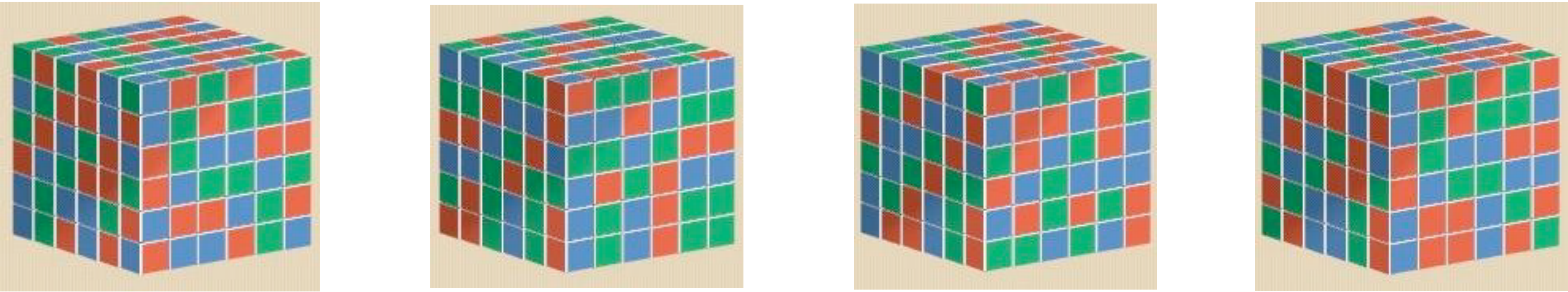
4. Hadron mass spectrum

Calculation strategy of Lattice QCD

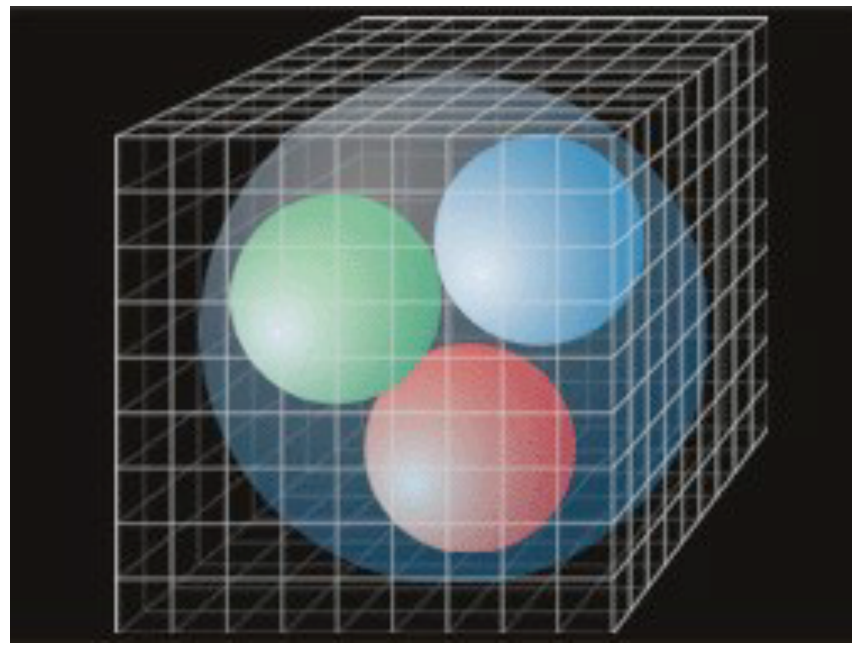
- We want to calculate the value: $\langle \mathcal{O} \rangle = \frac{1}{Z}\int D\phi \mathcal{O} e^{-S[\phi]}$

- Step1：Generate configuration samples

- Step2：Measure the value of observable for each conf.



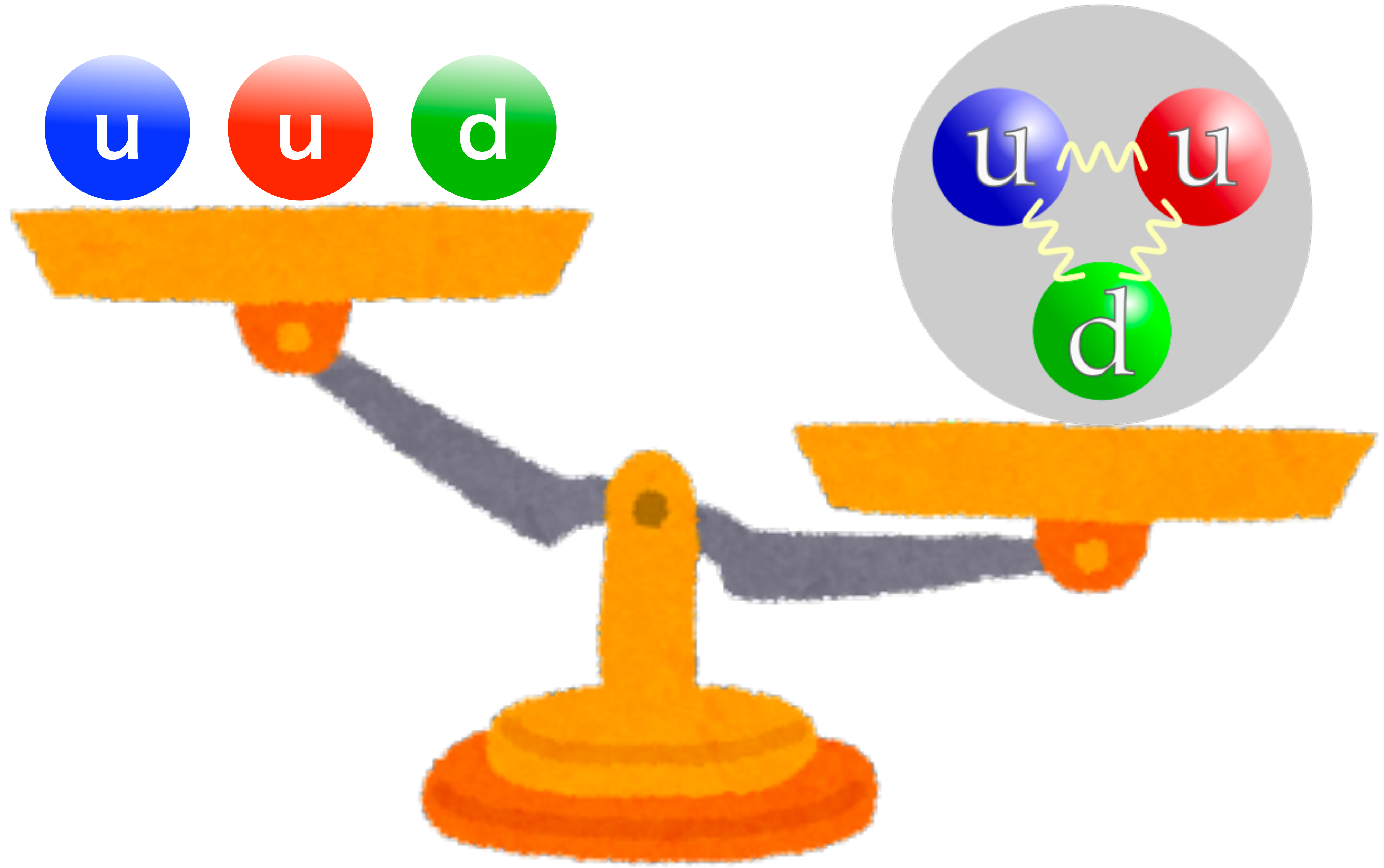
$\mathcal{O}_1$ $\mathcal{O}_2$ $\mathcal{O}_3$ $\mathcal{O}_N$



$$\langle O \rangle = \lim_{N\to\infty} \frac{1}{N}\sum_{i}^{N} O_i$$

Hadron spectrum

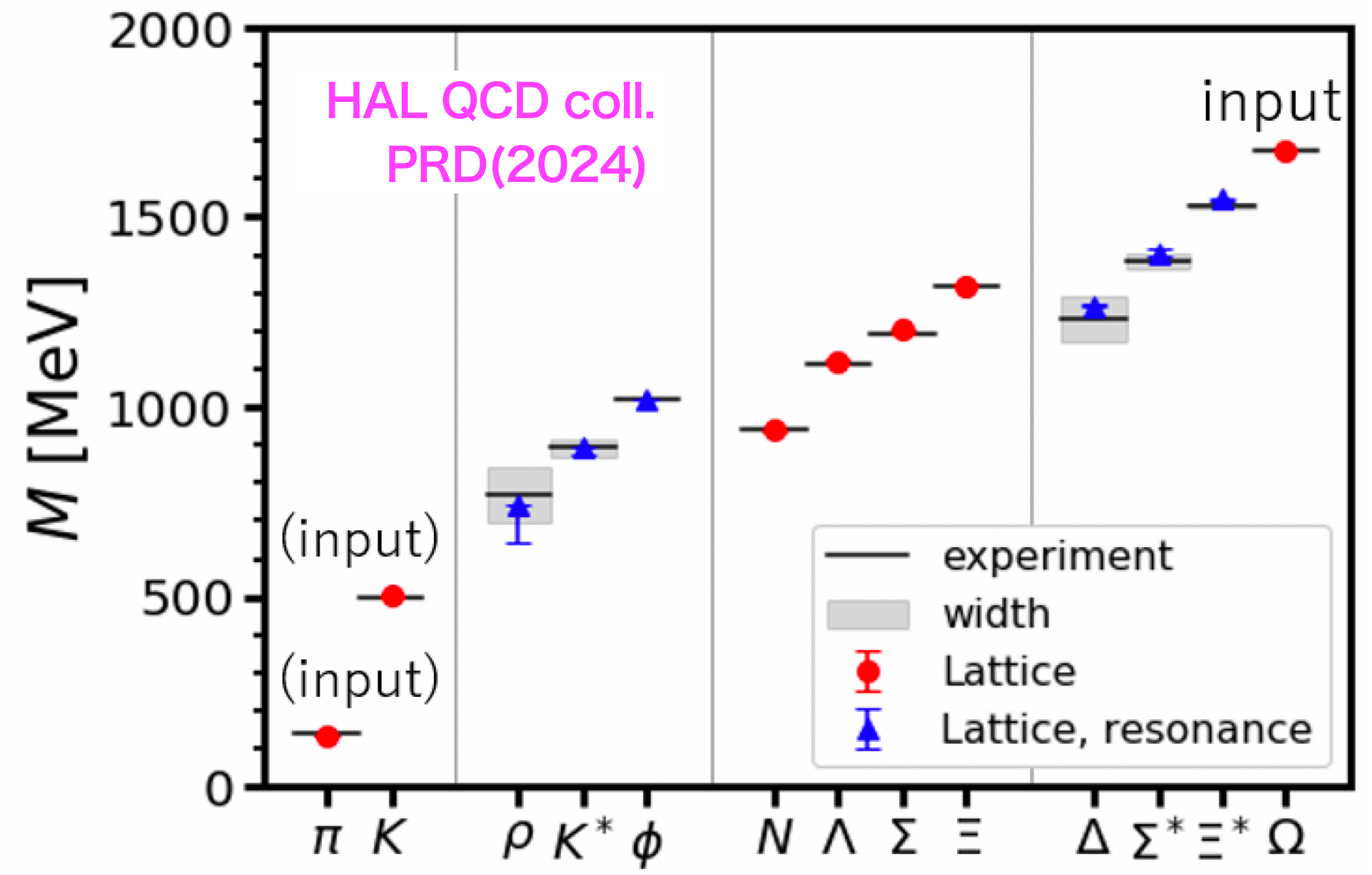
$$\mathscr{L} = -\frac{1}{4}F^a_{\mu\nu}F^a_{\mu\nu} + \bar{\psi}(i\gamma_\mu D_\mu + m)\psi$$



u,d quark mass ~ 2-5MeV
proton mass ~ 938MeV

- Hadron mass is very heavier than the sum of quark mass
- Input parameters are in QCD action
  lattice bare coupling g_0 ($\leftrightarrow a$)
  bare quark masses
- To give a theoretical prediction, taking into account of interaction effects correctly

Agreement between QCD predictions and experiments



- Input parameters are in QCD action
  lattice bare coupling g_0 ($\leftrightarrow a$)
  bare quark masses
  (Left panel: $m^0_{u,d}, m^0_s$)
- Only 3 inputs give more than 10 hadron masses, which are consistent with experimental data within a few % errors
- This is quantitative evidence that hadron micro-theory is QCD

2-pt fn. and mass of the low-lying mode

- The observable $\mathcal{O}$ to obtain the mass is the 2pt. fn. of the composite operator

  ($M = \bar{\psi}\gamma_5\psi,\ \bar{\psi}\gamma_i\psi,\ \bar{\psi}\psi$)

  $$C(\tau) = \sum_{\vec{x}} \langle M^\dagger(0,\vec{0})M(\tau,\vec{x})\rangle = \langle 0|M(0)e^{iPx}M(0)e^{-iPx}|0\rangle \text{ (Fourier transf.)}$$

  $$= \sum_k \int \frac{d^3p}{(2\pi)^3} \sum_{\vec{x}} \sum_n \langle 0|M^\dagger(0)|E_k(\vec{p})\rangle \frac{1}{2E_k(\vec{p})} \langle E_k(\vec{p})|M(0)|0\rangle \frac{1}{2E_k(\vec{p})} + \cdots$$

  $$= \sum_k \frac{|\langle 0|M(0)|E_k(\vec{p})\rangle|^2}{2m_k} e^{-m_k\tau} + \cdots,$$ ← the sum of $e^{-m_k\tau}$, k labels k-th excited state

  Here $E_k(\vec{p})$ denotes an one-particle state w/ momentum $\vec{p}$ and mass $m_k = E_k(\vec{0})$

- In large τ, the lowest mode ($k=0$) remains $C(\tau) = \dfrac{|\langle 0|M(0)|E_0\rangle|^2}{2m_0} e^{-m_0\tau} + \mathcal{O}(e^{-\Delta m_n\tau})$.

  In the case of $M = \bar{\psi}\gamma_5\psi$, the lowest mode is named "pion" then m_0 gives the pion mass

Hadron spectrum (calc. strategy)

- From the quarks, we would like to construct the 2-pt. fn. of hadron

- (Step 1) Calculate the quark propagator (using supercomputer)

$$D^{-1} = \bar{\psi}(x)^a_\alpha \ \psi(y)^b_\beta$$

- (Step 2) Measure the composite particle correlator expressed by the quark propagator (using supercomputer)

$$M(x) = \bar{\psi}\Gamma\psi(x), \Gamma = 1, \gamma_5, \gamma_\mu, \cdots$$

- (Step 3) Calculate mass from the behavior of long-time range of correlations (local PC is available)

(Step 1) Calculate the quark propagator

- The QCD action : $\mathscr{L} = -\frac{1}{4}F^a_{\mu\nu}F^a_{\mu\nu} + \bar{\psi}(i\gamma_\mu D_\mu + m)\psi$ quark bilinear form

- On the lattice, the lattice Dirac operator (Wilson fermion) is given by

$$D^{(W)}\psi(x) = \psi(x) - \kappa\sum_\mu [(1-\gamma_\mu)U_\mu(x)\psi(x+\hat{\mu}) + (1+\gamma_\mu)U^{-1}_\mu(x-\hat{\mu})\psi(x-\hat{\mu})]$$

$\kappa \propto 1/m^0$: hopping parameter

Symbolically, we denote it as $D^{(W)}(x,y)\psi(y)$ It is written by link variables.

From here, $D(x,y)$ denotes the lattice Dirac op. : $D(x,y) = (i\gamma_\mu D_\mu + m)$

- $D(x,y)$ has 2 color indecies and 2 spinor indices w/ contract $\bar{\psi}(x)^a_\alpha$ and $\psi(y)^b_\beta$

Quark propagator is $[D^{-1}(x,y)]^{a,b}_{\alpha,\beta} = \bar{\psi}(x)^a_\alpha \; \psi(y)^b_\beta$: It is a huge matrix.

the quark propagator

- In cont. limit, it expands to perturbatively

$D^{-1}(x, y) =$

- We'd like to calculate all possible diagrams (analytically impossible..)

How to calculate the quark propagator numerically

- If we consider $D(x,y)\phi(y) = \delta_{x,x_0}$, then $\phi(y) = D(x_0,y)^{-1}$ is the quark propagator

- Solve a huge linear equations $A \cdot x = b$

- Algorithm: conjugate gradient (CG) method

  Improvements: prepare a vector $\eta = Db$, then solve $x = (D^\dagger D)^{-1}\eta$

  Eigenvalue of $(D^\dagger D)$ is real, there is a fast algorithm to obtain its inverse matrix

- Comment: the size of matrix

  $[D^{-1}(x,y)]^{a,b}_{\alpha,\beta}$: spacetime vol. = N_s^4, color = 3 x 3(complex), spinor = 4 x 4

  [size of $[D^{-1}(x,y)]^{a,b}_{\alpha,\beta}$] = $(N_s^4 \times 3 \times 4)^2$

  In HAL QCD paper (2024), we take $N_s = 96$, the quark propagator is $10^9 \times 10^9$ matrix ! !

(Step 2) Construct the composite state correlator from the quark propagator

- $C(\tau) = \sum_{\vec{x}} \langle M^\dagger(0,\vec{0}) M(\tau,\vec{x}) \rangle = \sum_{\vec{x}} \langle (\bar{\psi}\Gamma\psi(0,\vec{0}))^\dagger \; \bar{\psi}\Gamma\psi(\tau,\vec{x}) \rangle$

$$= \int d^3x \mathrm{Tr}\left[\Gamma_{\alpha\beta}\, D^{-1}(x,0)^{bd}_{\beta\gamma}\, (\Gamma^\dagger)_{\gamma\rho}\, D^{-1}(0,x)^{ca}_{\rho\sigma}\, \delta^{ab}\, \delta^{cd}\right] = \left\langle \mathrm{Tr}\left[\Gamma\, D^{-1}(x,0)\, \Gamma^\dagger\, D^{-1}(0,x)\right] \right\rangle$$

Multiply the matrix and take the trace

- If the pseudo-scalar ,$\Gamma = \gamma_5$, the Dirac op. is γ_5-hermiticity (hermiticity in Euclidean spacetime) $\gamma_5 D^\dagger \gamma_5 = D$ then

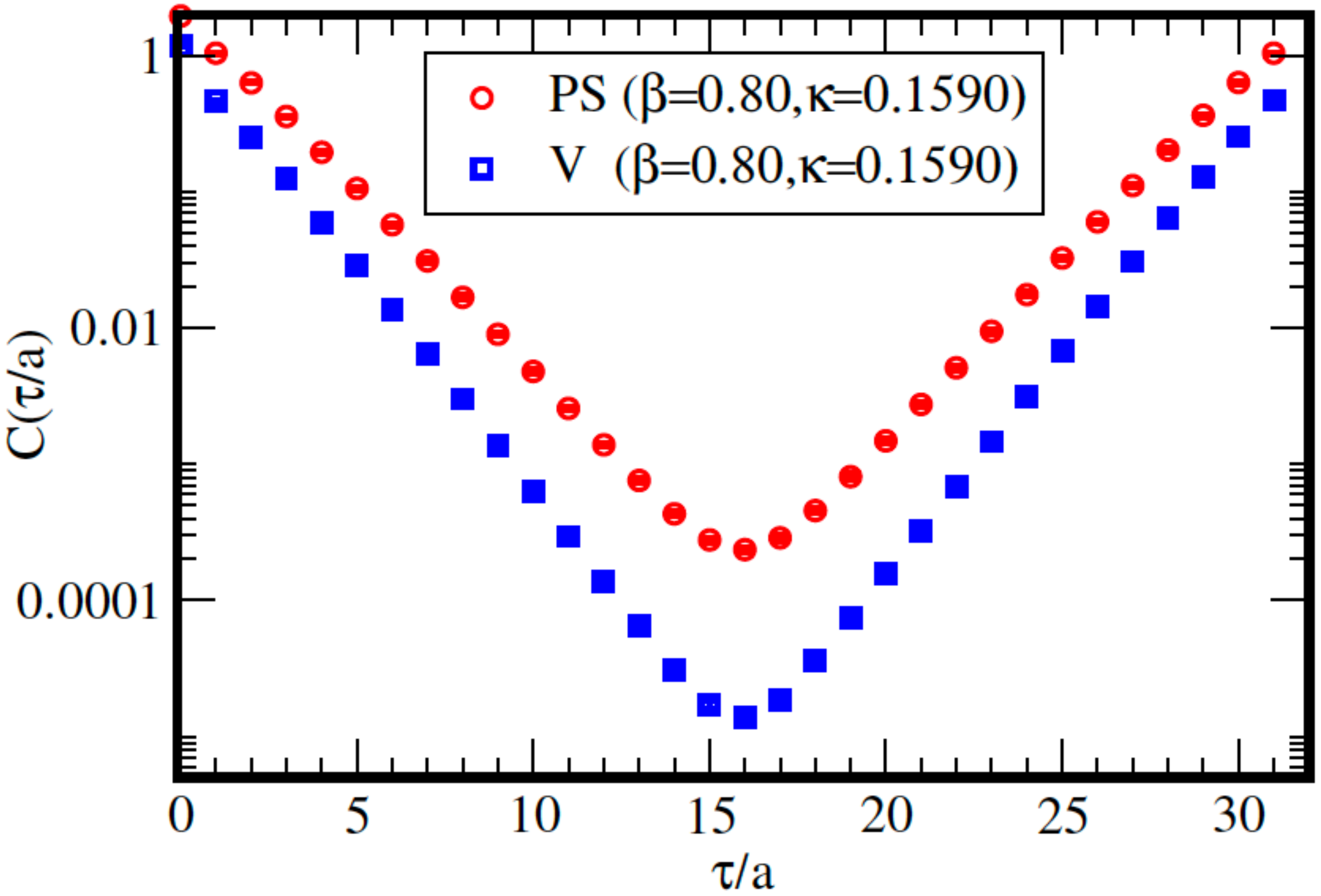
$$C_{PS}(\tau) = \left\langle \mathrm{Tr}\left[(D^{-1})^\dagger(0,x)\, D^{-1}(0,x)\right] \right\rangle$$

Using the Schwartz inequality, for any Γ (such that $\Gamma^2 = 1$)

$$\mathrm{Tr}\Gamma\, D^{-1}(x,0)\, \Gamma\, D^{-1}(0,x) = \mathrm{Tr}\Gamma\gamma_5 (D^{-1})^\dagger(0,x) \gamma_5 \Gamma D^{-1}(0,x) \leq \mathrm{Tr}(D^{-1})^\dagger(0,x) D^{-1}(0,x)$$

QCD inequality and the lightest meson

- $C_{(\bar{\psi}\Gamma\psi)}(\tau) \leq C_{PS}(\tau)$ for any Γ (such that $\Gamma^2 = 1$) in whole τ



Pseudo-scalar op.: $M = \bar{\psi}\gamma_5\psi$

vector meson op.: $M = \bar{\psi}\gamma_1\psi$

$C_V(\tau) \leq C_{PS}(\tau)$ and never cross

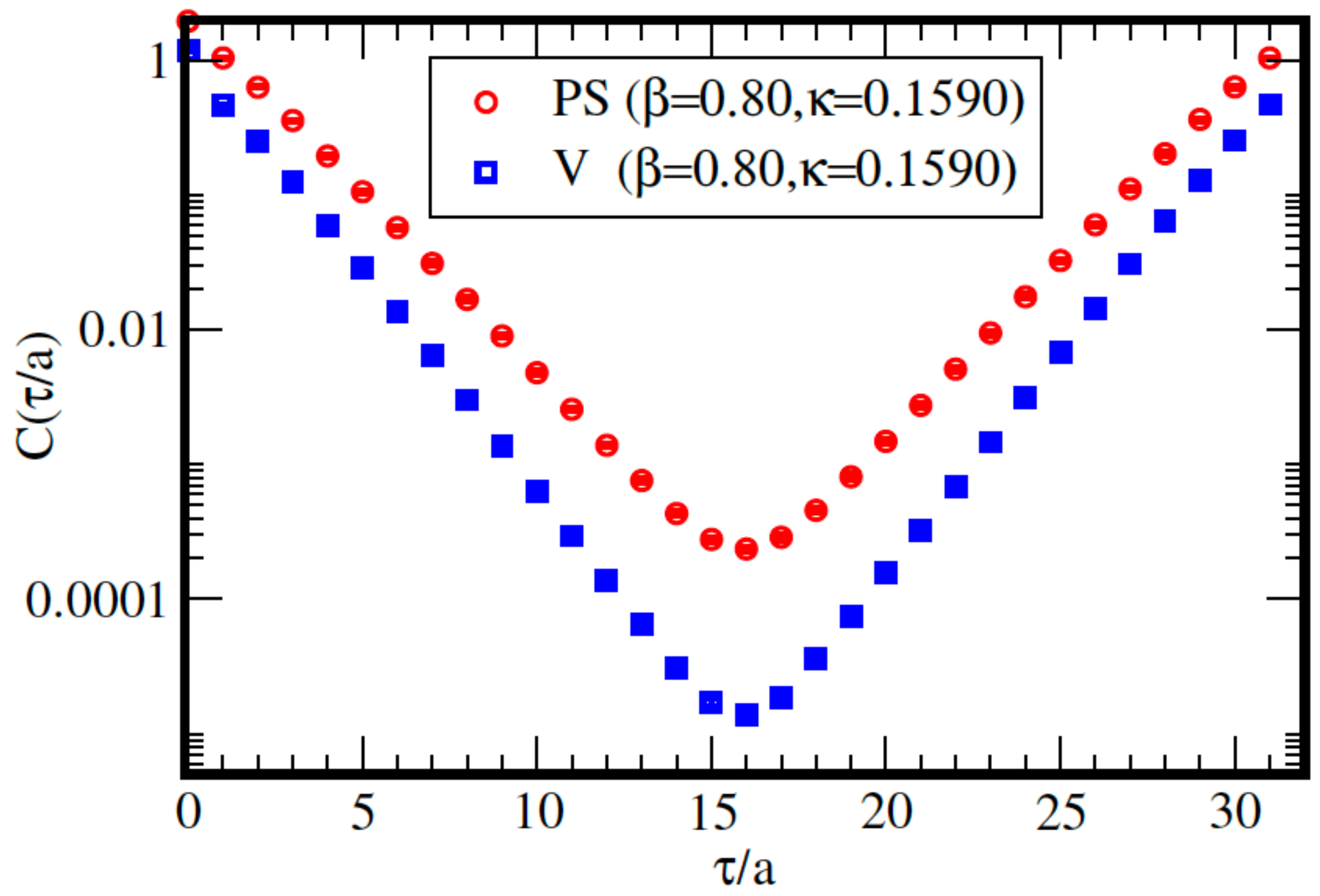
The slopes in $C_{PS}(\tau) \approx e^{-m_\pi \tau}$ are gentler than those in $C_V(\tau) \approx e^{-m_\rho \tau}$.

$m_\pi \leq m_{(\bar{\psi}\Gamma\psi)}$ for any mesons

Periodicity of the lattice

- In lattice simulations, we usually impose periodic b.c.
  Then the meson correlation fn. has a cosh shape:

  $$C(\tau) \sim e^{-m\tau} + e^{-m(N_\tau - \tau)} \sim \cosh(m(\tau - N_\tau/2))$$



- Note: This is not the case with regard to baryons
  For instance the nucleon (N), the positive and negative mass eigenstates of parity ($N^{\pm}$) have different masses ($m_{N^+} \neq m_{N^-}$)

  Then the slope of forward and backward correlation fn. $N^{\pm}$ shows asymmetry against τ

QCD inequality and the lightest meson

- $C_{(\bar{\psi}\Gamma\psi)}(\tau) \leq C_{PS}(\tau)$ for any Γ (such that $\Gamma^2 = 1$) => pion is the lightest meson

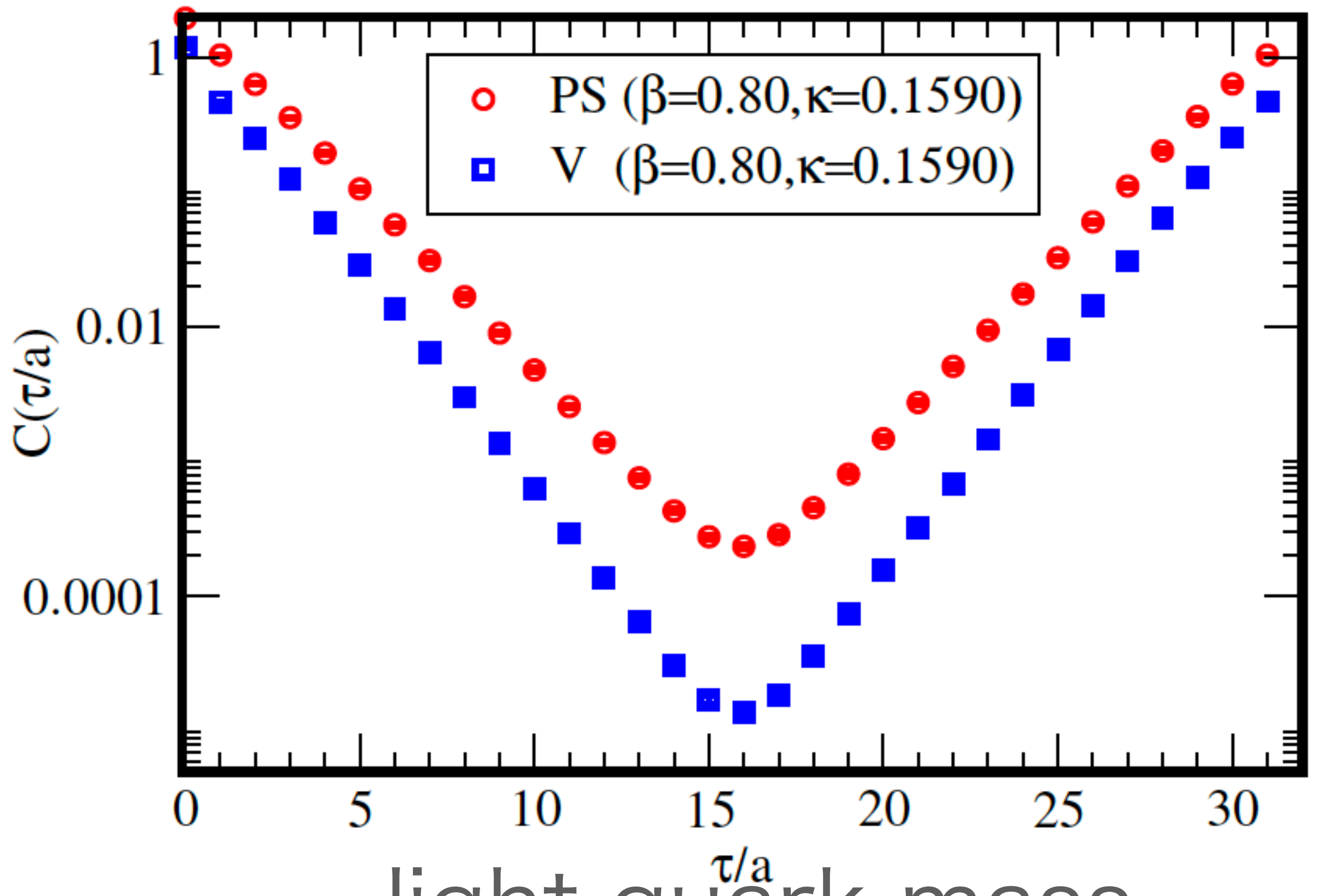
- Here, we assume
  (1) the Dirac op. has the γ_5-hermiticity
  (2) no disconnected contribution to the 2-pt. fn.

- (1) is broken if the finite-density term is included
  $\gamma_5 D^\dagger(\mu)\gamma_5 = D(-\mu)$ not $\gamma_5 D^\dagger(\mu)\gamma_5 = D(\mu)$

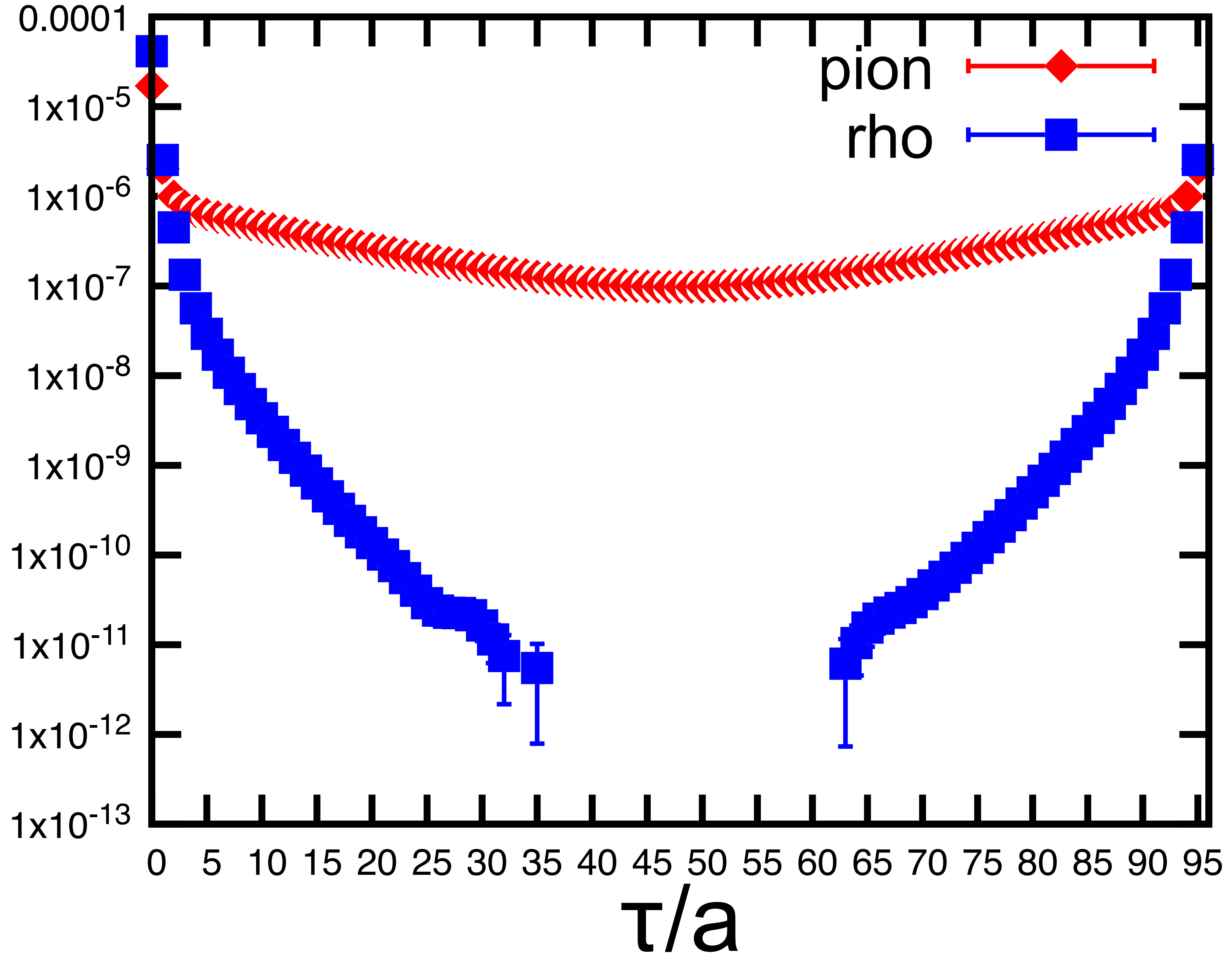
- (2) is broken if iso-singlet scalar meson

Quark mass dependence of correlation fns.

heavy quark mass



light quark mass



- Top panel: $m_\pi/m_\rho \sim 0.8$ (heavy quark mass)

  Bottom panel: $m_\pi/m_\rho \sim 0.2$ (light quark mass)

  (physical point)

  By changing lattice bare mass (κ),

  this ratio is a result of.

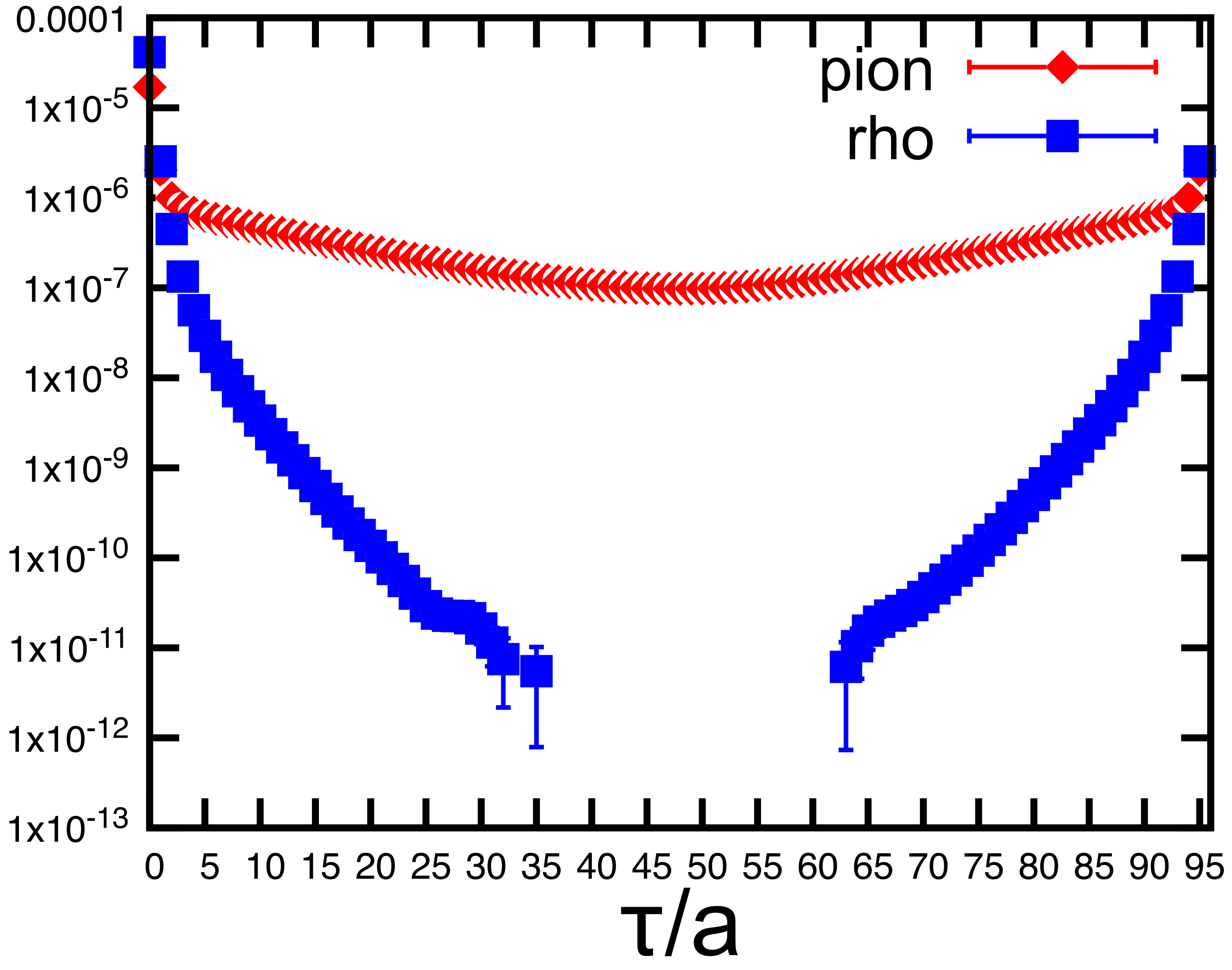
- In lighter quark mass, ρ can decay to 2 pion.

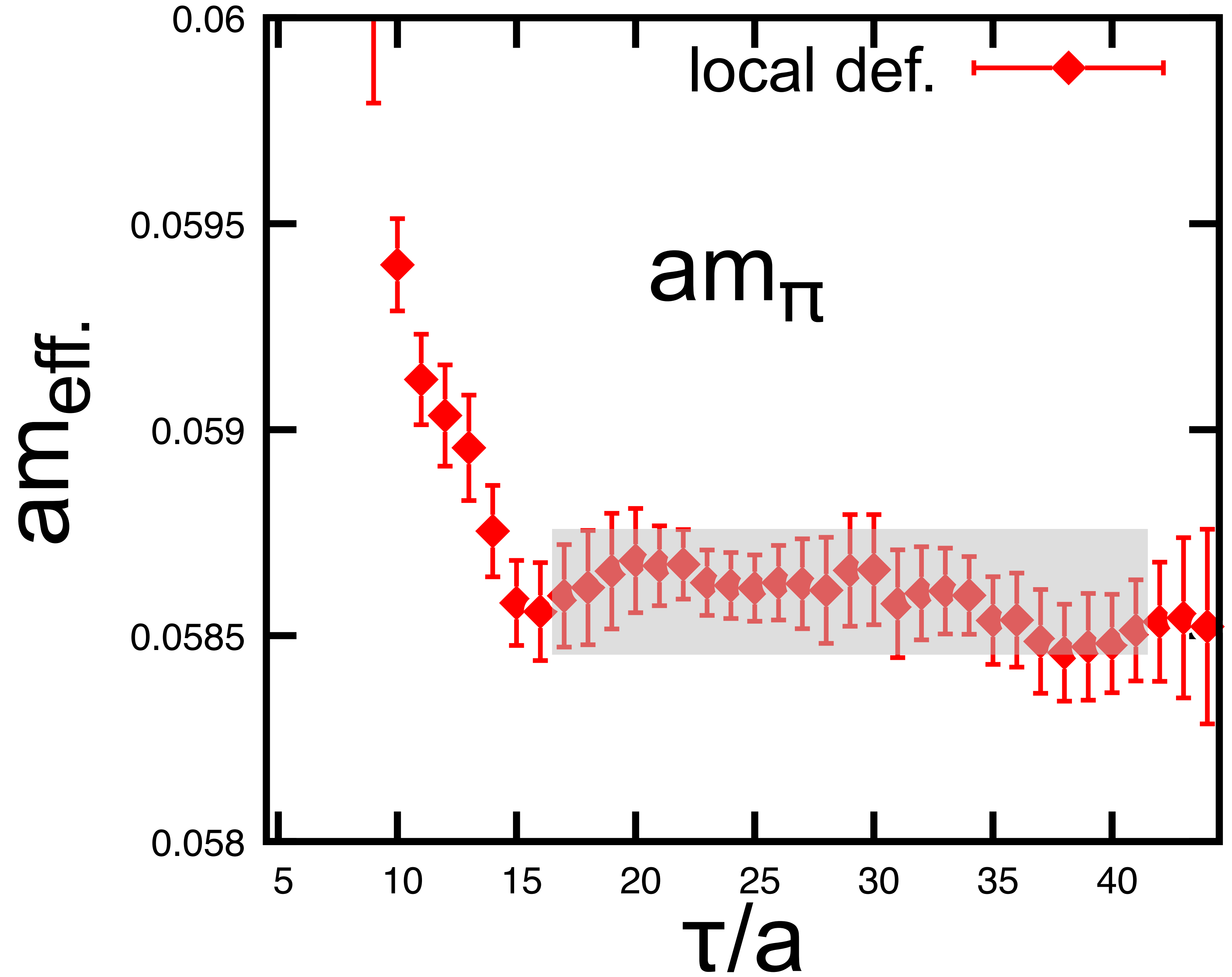
  ρ cannot propagator long time.

  The signal of the correlation fn. becomes noisy in long τ regime.

  Hard to obtain precise data for heavier hadron mass

(Step 3) Calculate mass from the long-time range of correlations

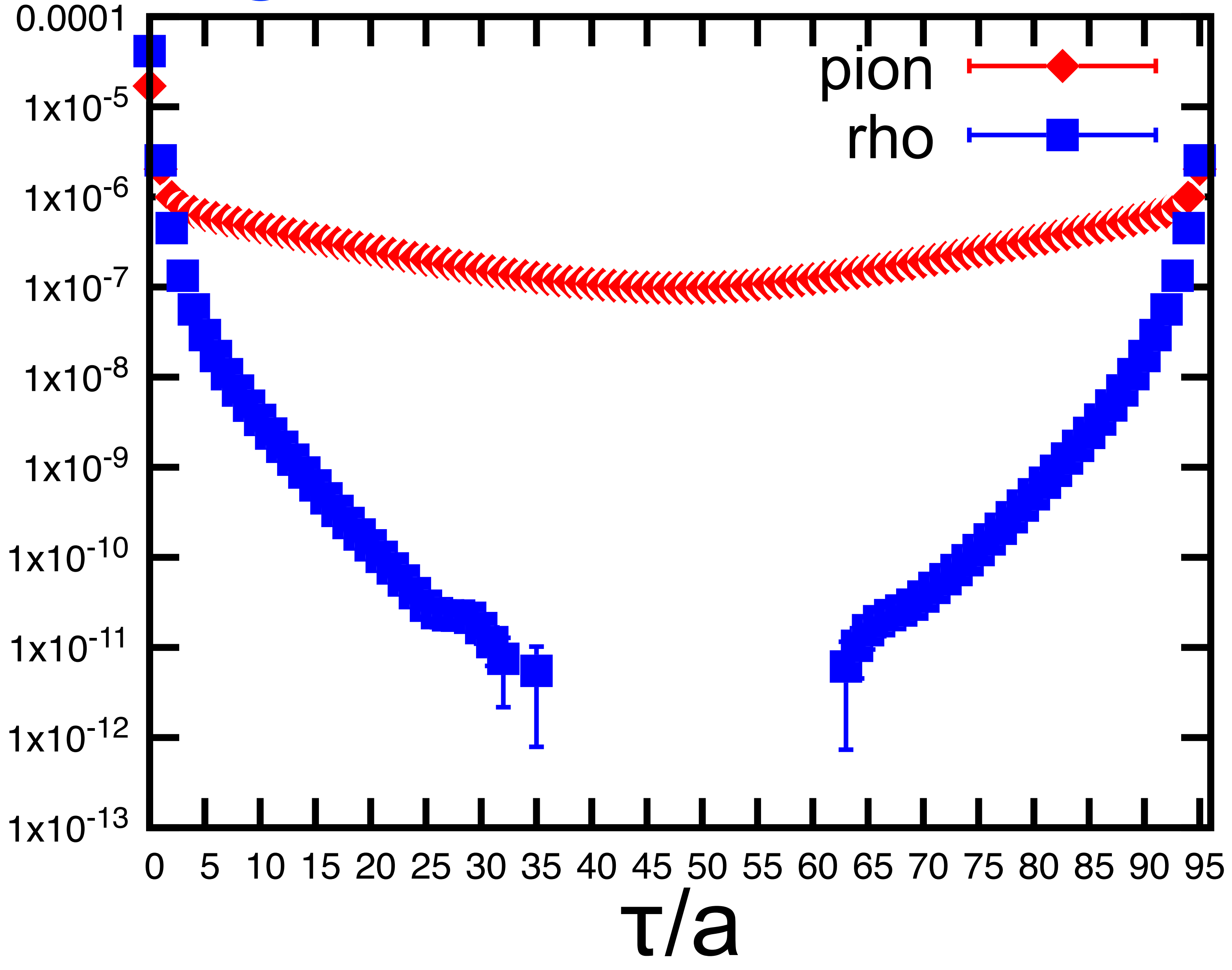


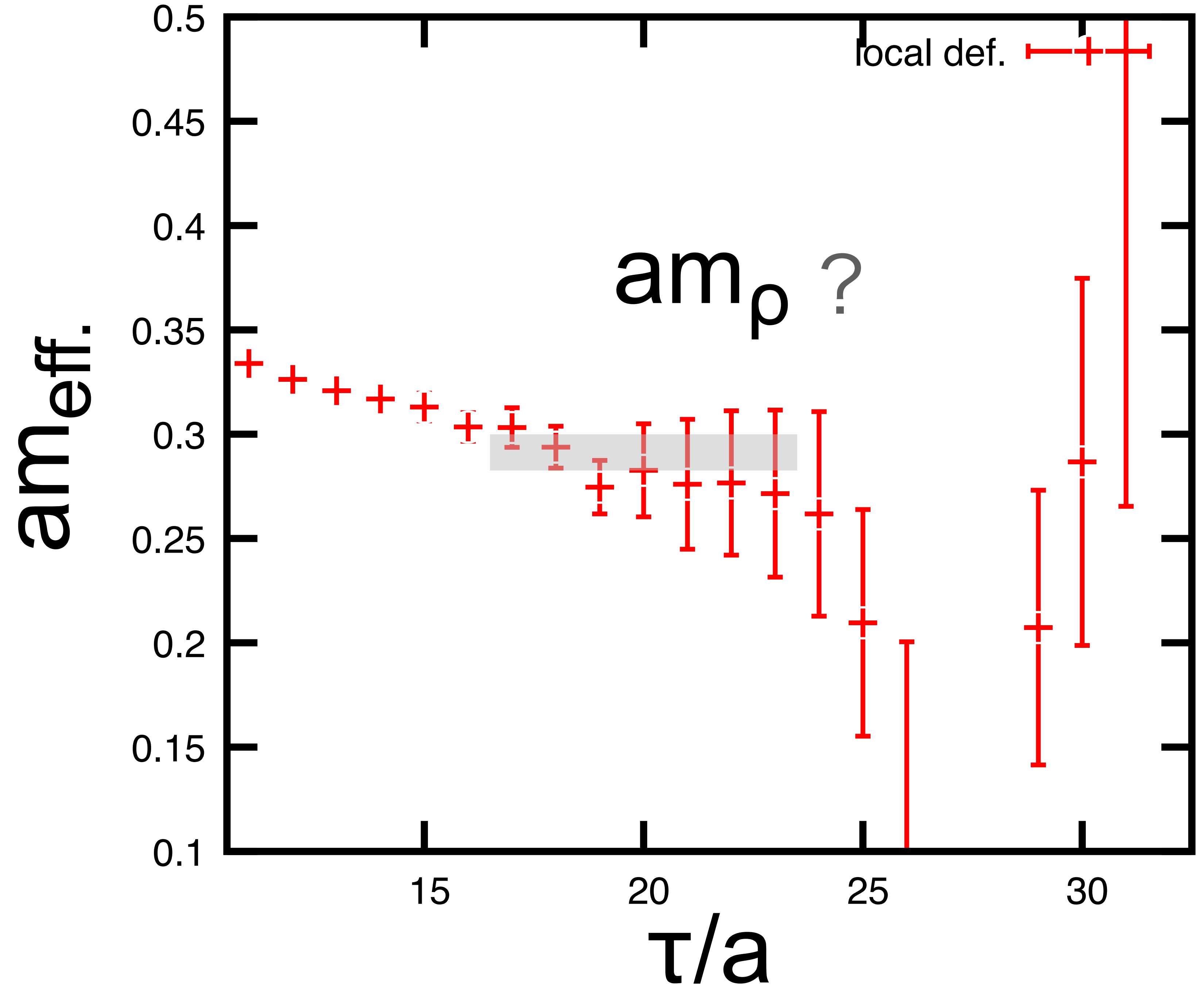


1. Fit the data in the appropriate τ region with $f(\tau) = c_0 + c_1 e^{-c_2 \tau}$ the best-fit value of $c_2 = m$

2. Calc. effective mass $m_{eff}(\tau) = -\log[C(\tau+1)/C(\tau)]$ In long τ, it should converge with the lowest state mass Find a plateau of m_{eff}

Heavy (unstable) meson case





- Calc. effective mass

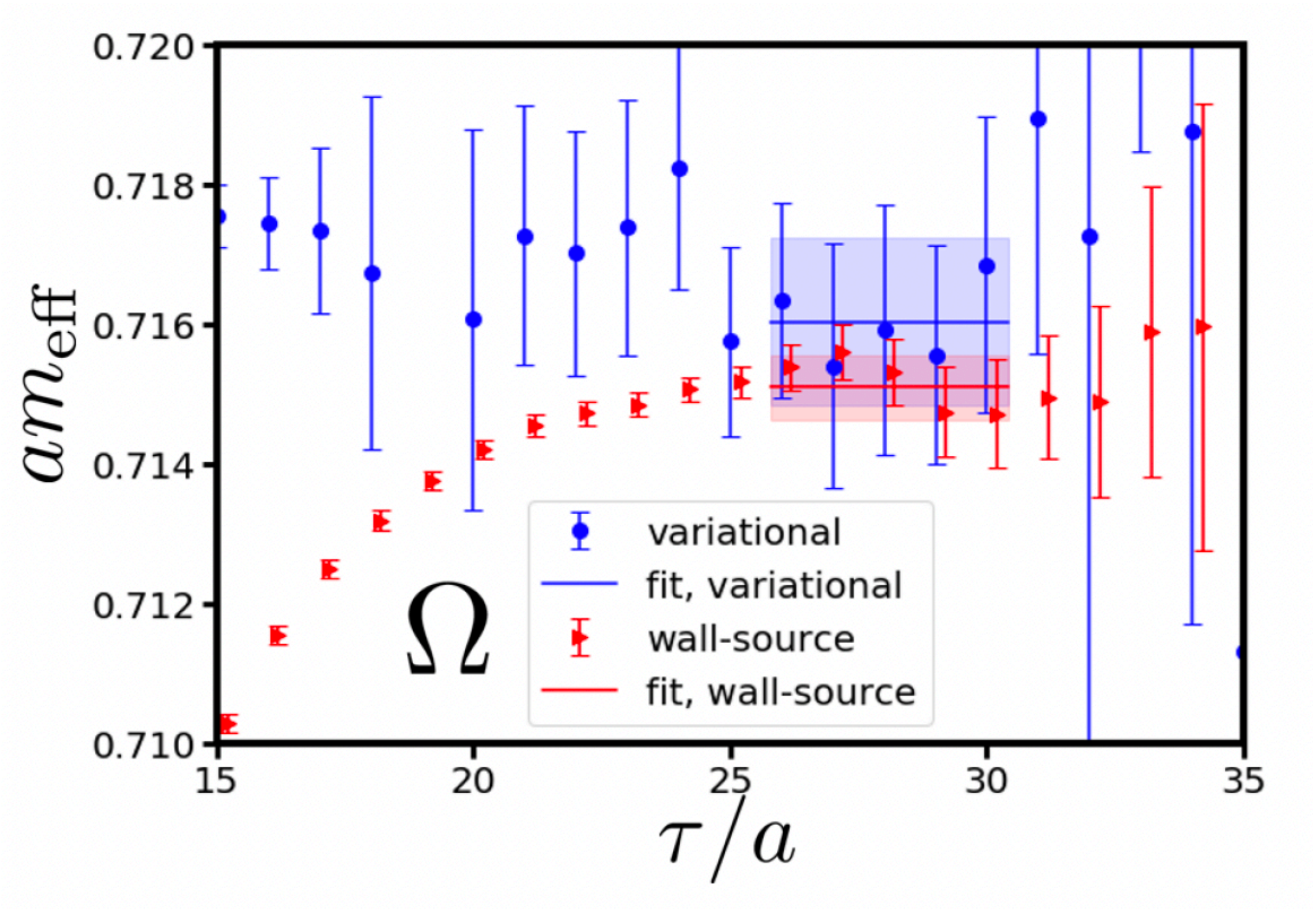
  $$m_{eff}(\tau) = -\log[C(\tau+1)/C(\tau)]$$

  In long τ, it should converge with the lowest state mass

  Find a plateau of m_{eff}

- It is difficult to find a plateau for heavy (unstable) case

Choice of source term



wall source: $q_{s,a}(x_0) = \sum_{\vec{x_0}} q_a(\vec{x_0}, 0)$

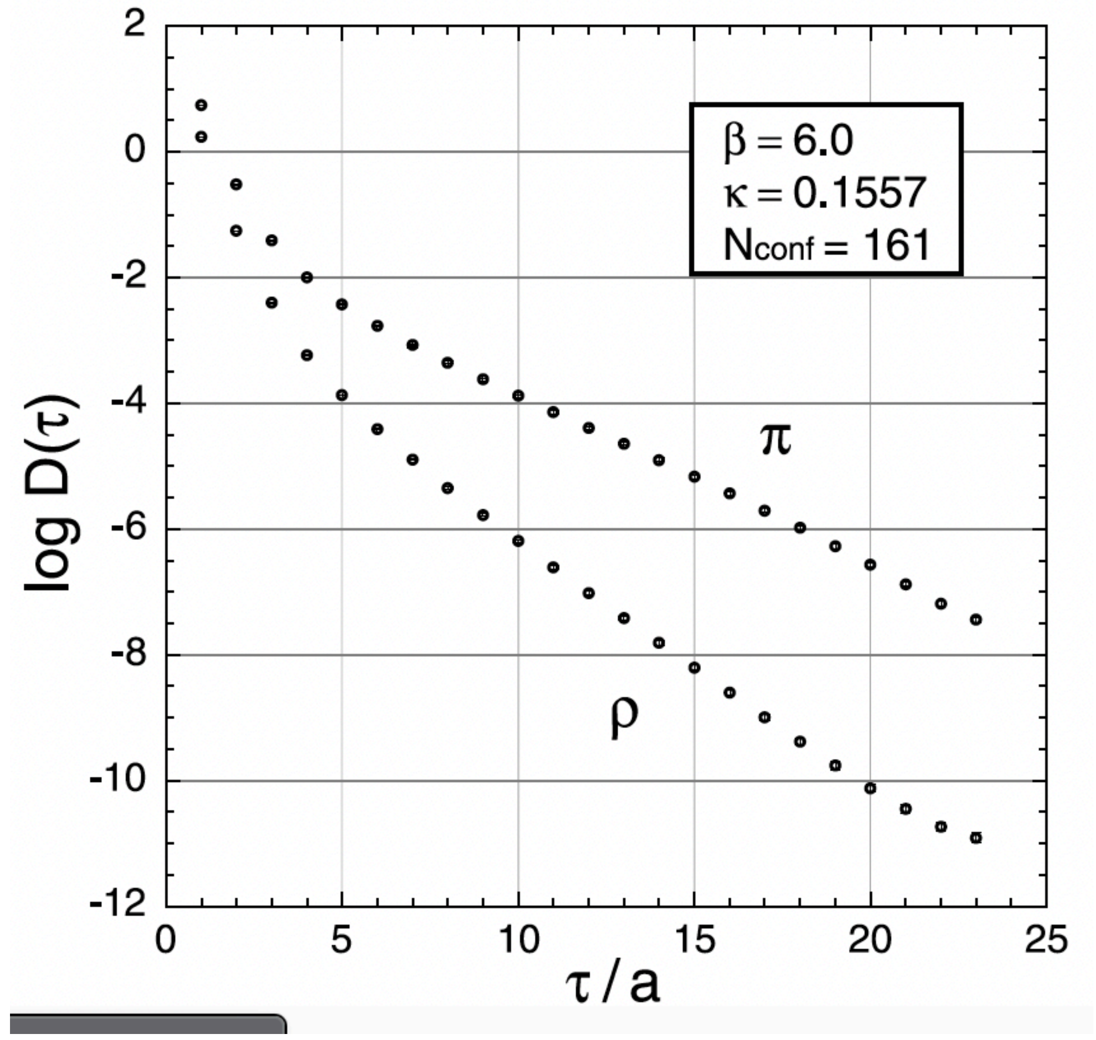
smeared source: $q_{s,a}(x_0) = \sum_{\vec{x_0}} f_q(|\vec{x_0} - \vec{y}|)\; q_a(\vec{y}, 0)$

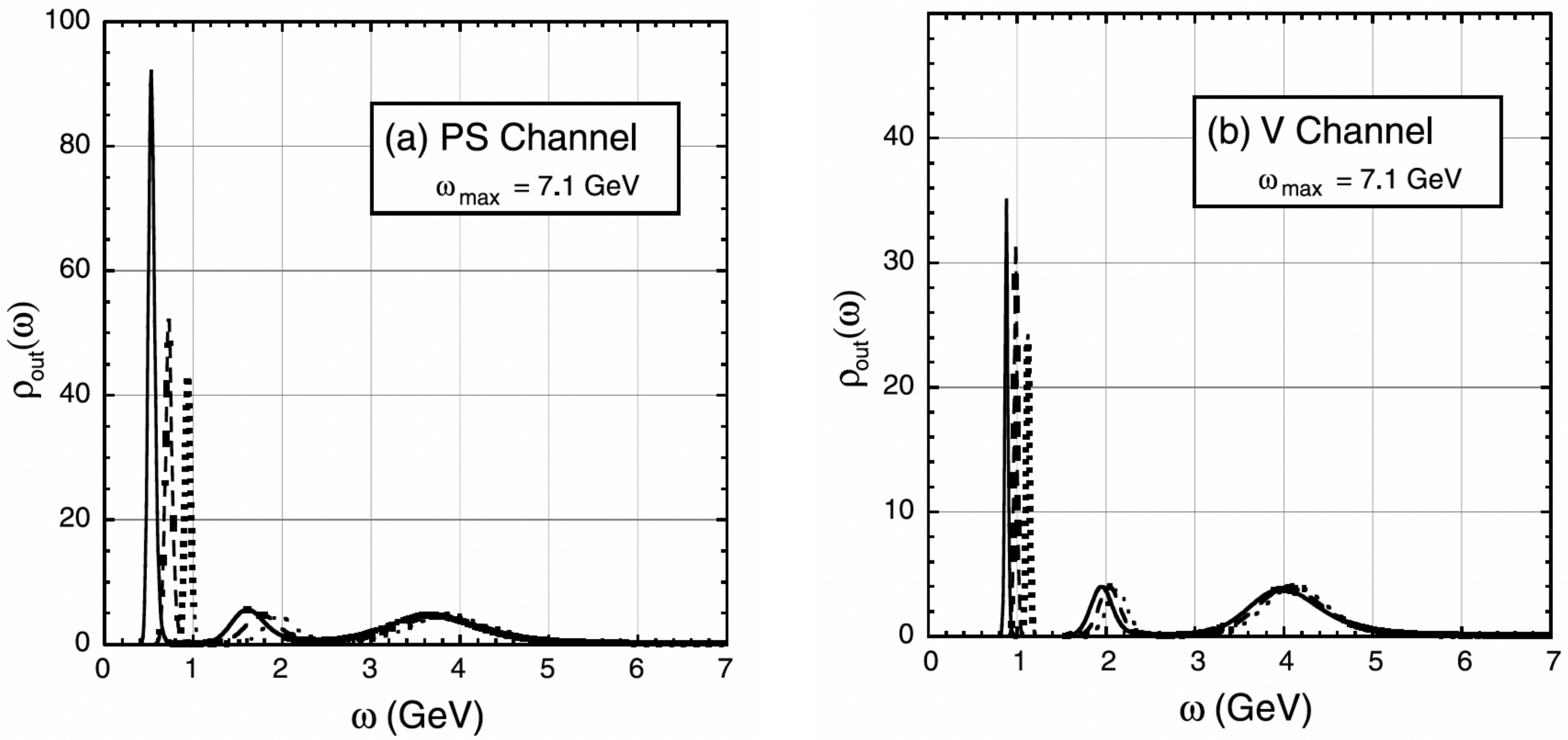
(smeared quark op. in $|\vec{x_0} - \vec{y}|$ regime)

- To obtain the quark propagator, we solve
  $D(x,y)\phi(y) = \delta_{x,x_0}$
- We introduce source op.
  $D(x,y)\phi(y) = \delta_{x,x_0} q_s(x_0)$ at $x = x_0$
- Changing source op. changes the operator mixing around $x = x_0$

  But it does not change the long distance behavior
- Changing source op. gives a cross check of the contamination of excited state/boundary effect

Other analysis of the correlation fn.

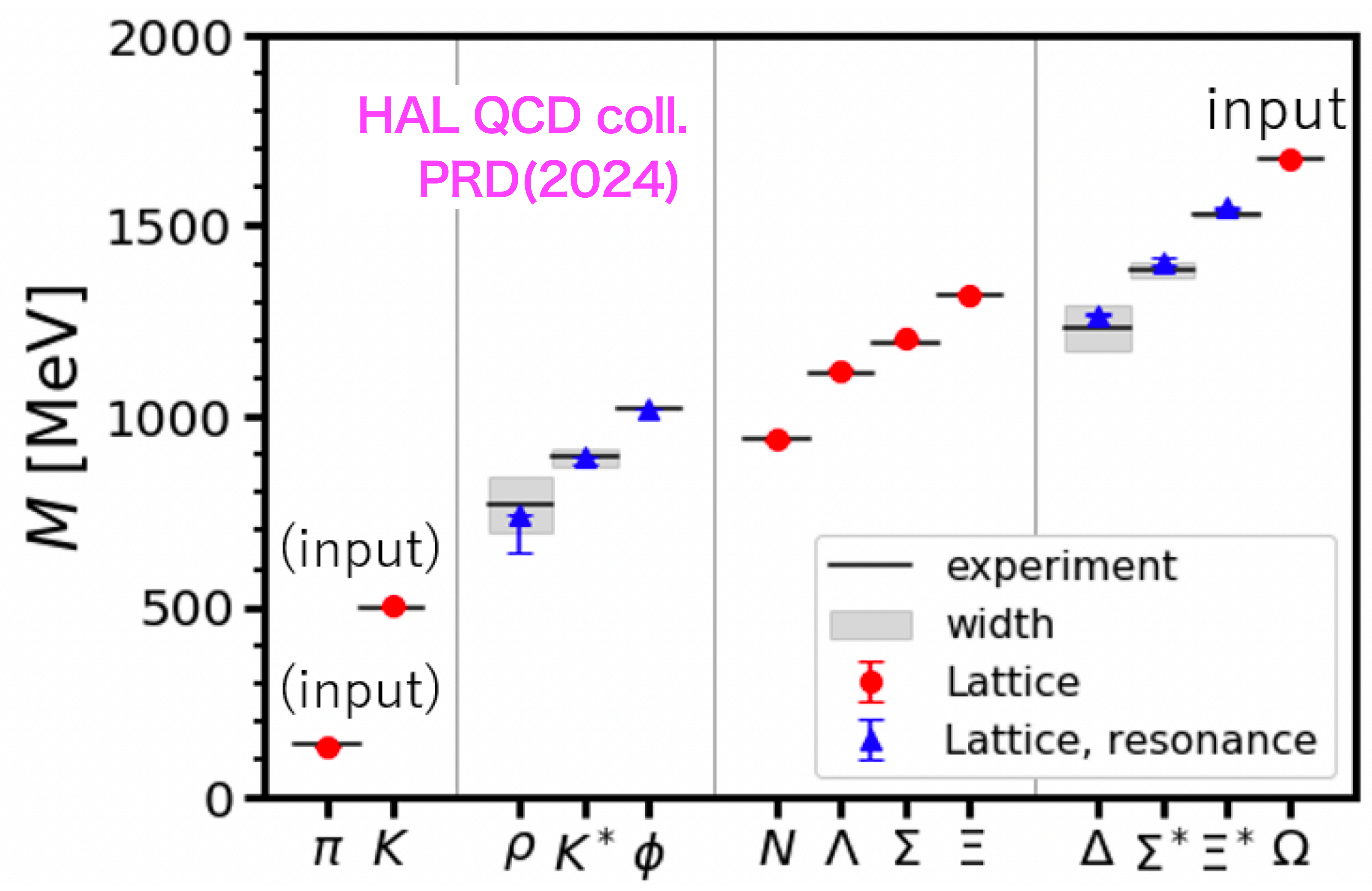




M.Asakawa, T.Hatsuda, Y.Nakahara,
Prog.Part.Nucl.Phys. 46 (2001) 459-508

- Can we obtain the spectrum function? -> Yes!
- $C(\tau) = \int_{-\infty}^{+\infty} d\omega K(\tau,\omega)\rho(\omega),\ K(\tau,\omega) = \frac{\cosh\left(\omega(\frac{N_\tau}{2} - \tau)\right)}{\sinh(\frac{\omega N_\tau}{2})}$
- Note: on the lattice, # of data points of $C(\tau)$ is finite, it makes difficult to obtain $\rho(\omega)$ (it becomes ill-posed inverse problem)
- Maximal entropy method
  Sparse modeling method
  Machine leaning... are proposed
- Obtaining $\rho(\omega)$ is very useful for the other quantities (viscosity, PDF...)

Physical scale setting



- all quantities are dimension-less

- 3 input parameters

  g_0 ($\to a$), $\kappa_{u,d}$ (m^0_{ud}) , κ_s (m^0_s)

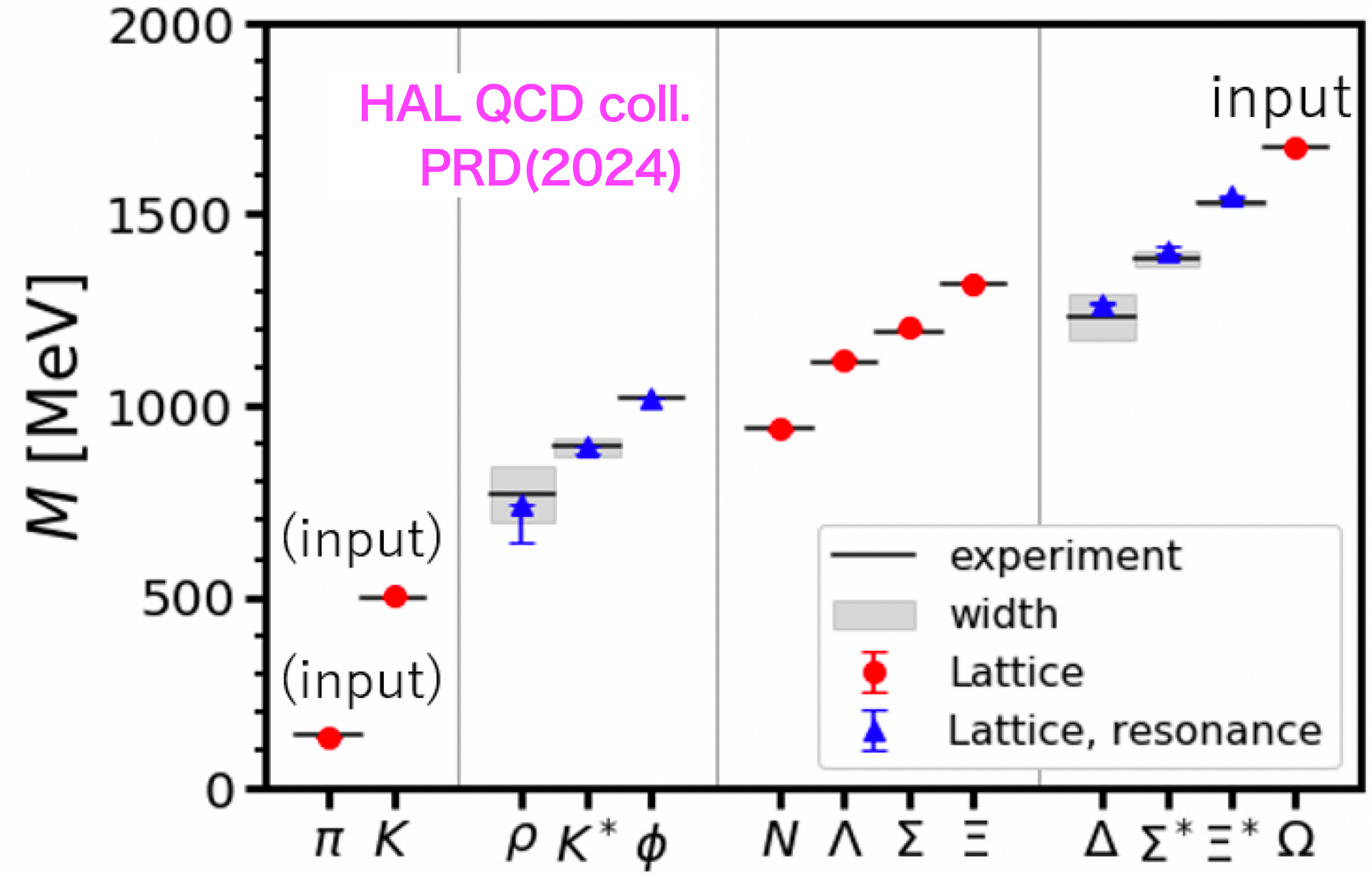
- In HAL QCD paper, we calc.

  am_Ω -> fix the scale $a \approx 2.3\text{GeV}^{-1}$

  am_π -> fix $\kappa_{u,d}$, ($\kappa_{u,d}$=0.126117)

  am_K -> fix κ_s, (κ_s=0.124902)

Summary of mass spectrum calculation



- Calculate hadron correlation fn., which is written by quark propagator
- Seeing long propagation time, we can extract the mass of low-lying state for composite state
  pseudo-scalar meson -> pion
  vector meson -> rho
- The mass of excited states/unstable particles can be obtained using the same strategy

6. Advanced topics for mass spectrum

QCD inequality and the lightest meson

- $C_{(\bar{\psi}\Gamma\psi)}(\tau) \leq C_{PS}(\tau)$ for any Γ (such that $\Gamma^2 = 1$)

- Here, we assume

  (1) the Dirac op. has γ_5-hermiticity $\gamma_5 D^{\dagger}(\mu)\gamma_5 = D(\mu)$

  (2) no disconnected contribution to the 2-pt. fn.

- (1) is broken if the finite-density term is included

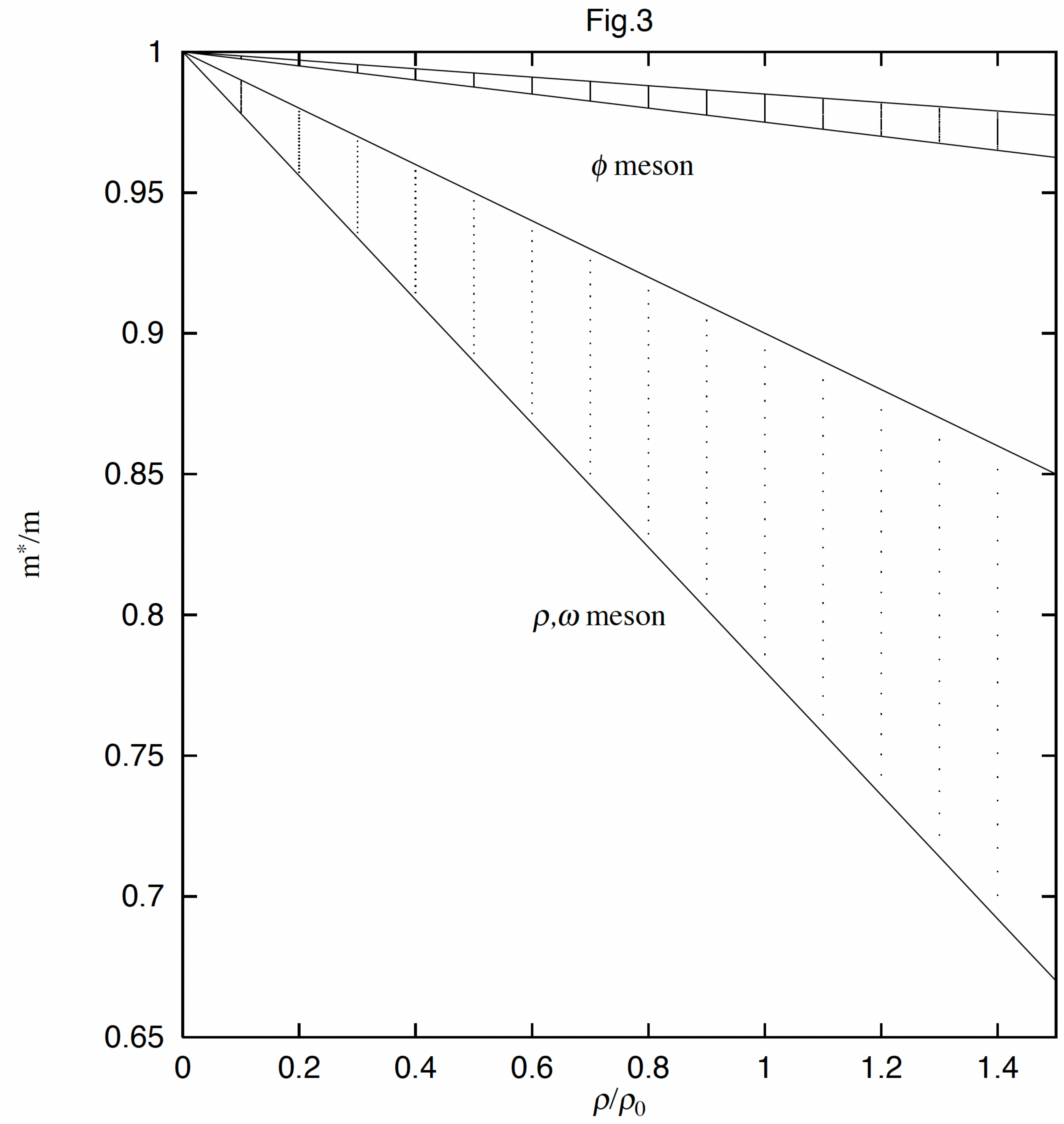
  $$\gamma_5 D^{\dagger}(\mu)\gamma_5 = D(-\mu)$$

- (2) is broken if iso-singlet scalar meson

In density regime, what is the lightest meson?

$m^*(\rho)/m(\rho_0)$ ratio as a fn of density (ρ)

ρ_0 : standard nuclear density



T. Hatsuda, H. Shiomi and H. Kuwabara
Prog. Theor. Phys. 95(1996)1009

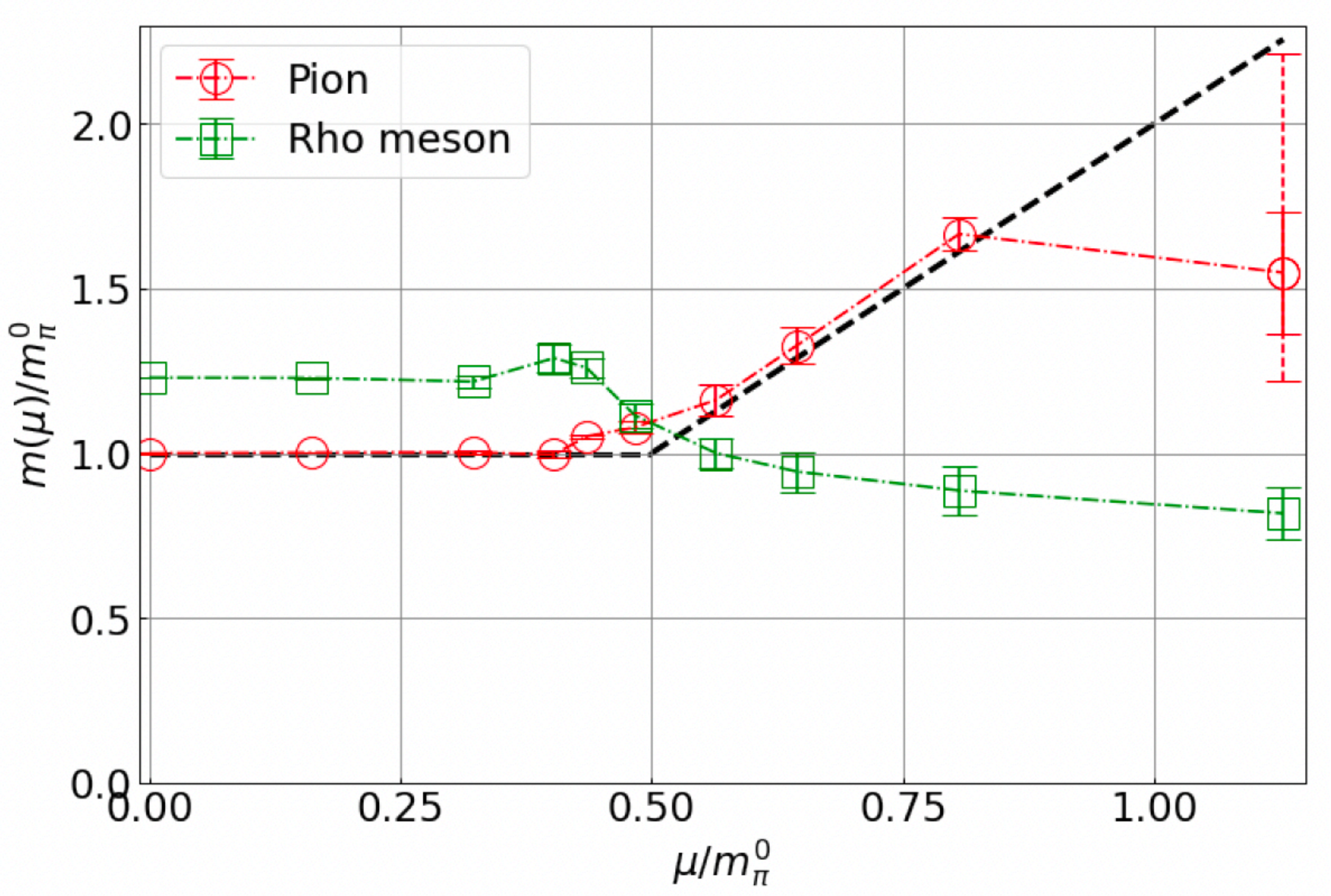
- In high-density regime, it is believed that chiral symmetry becomes restored
- According to several analytical studies, vector mesons gets lighter and lighter as density increases

Hatsuda-Lee(1992)

- Some experimental data also indicate mass shift of vector meson

cf.) J-PARC E16 experiment

Lattice simulation results for dense 2color QCD



K.Murakami, D.Suenaga, K.Iida, EI,
PoS LATTICE2022 (2023) 154

- Lattice simulation of dense QCD is extremely difficult because of the sign problem
- There are ab initio calculations in gauge theory that avoid the sign problem and are similar to QCD (2color QCD)
- It is shown that rho is lighter than pion in high-density regime
- Related topics of density QCD will be discussed during the 4th week of this workshop

Sign problem and new directions

- What is the sign problem？

  It comes from non-positivity of euclidean action in path-integeral formula using Monte Carlo simulation: $\langle \mathcal{O} \rangle = \frac{1}{Z}\int D\phi \mathcal{O} e^{-S[\phi]}$

  In importance sampling method, $e^{-S[\phi]}$ is the Boltzmann weight to generate emsambles

  Should be real and positive, but adding the density term (or θ term) the $S[\phi]$ takes complex value.

  The sign problem proves to be NP-hard. If the system size increases, the cost increases faster than poly.

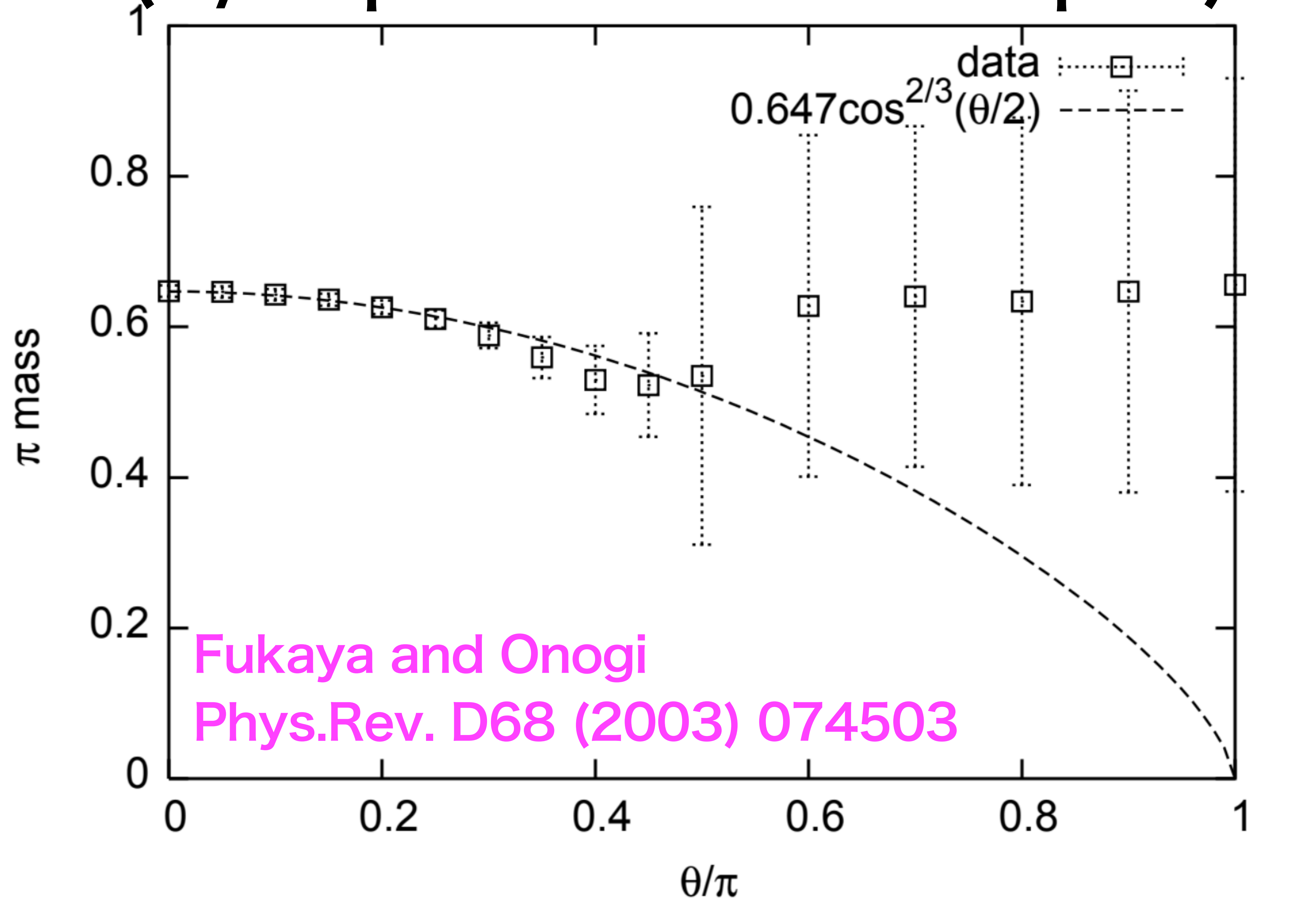
  (Troyer and Wiese: Phys. Rev. Lett. 94, 170201, 2005)

- To avoid this, a new direction of ab initio calculation based on the Hamiltonian formalism has recently proposed (5th week of this workshop)

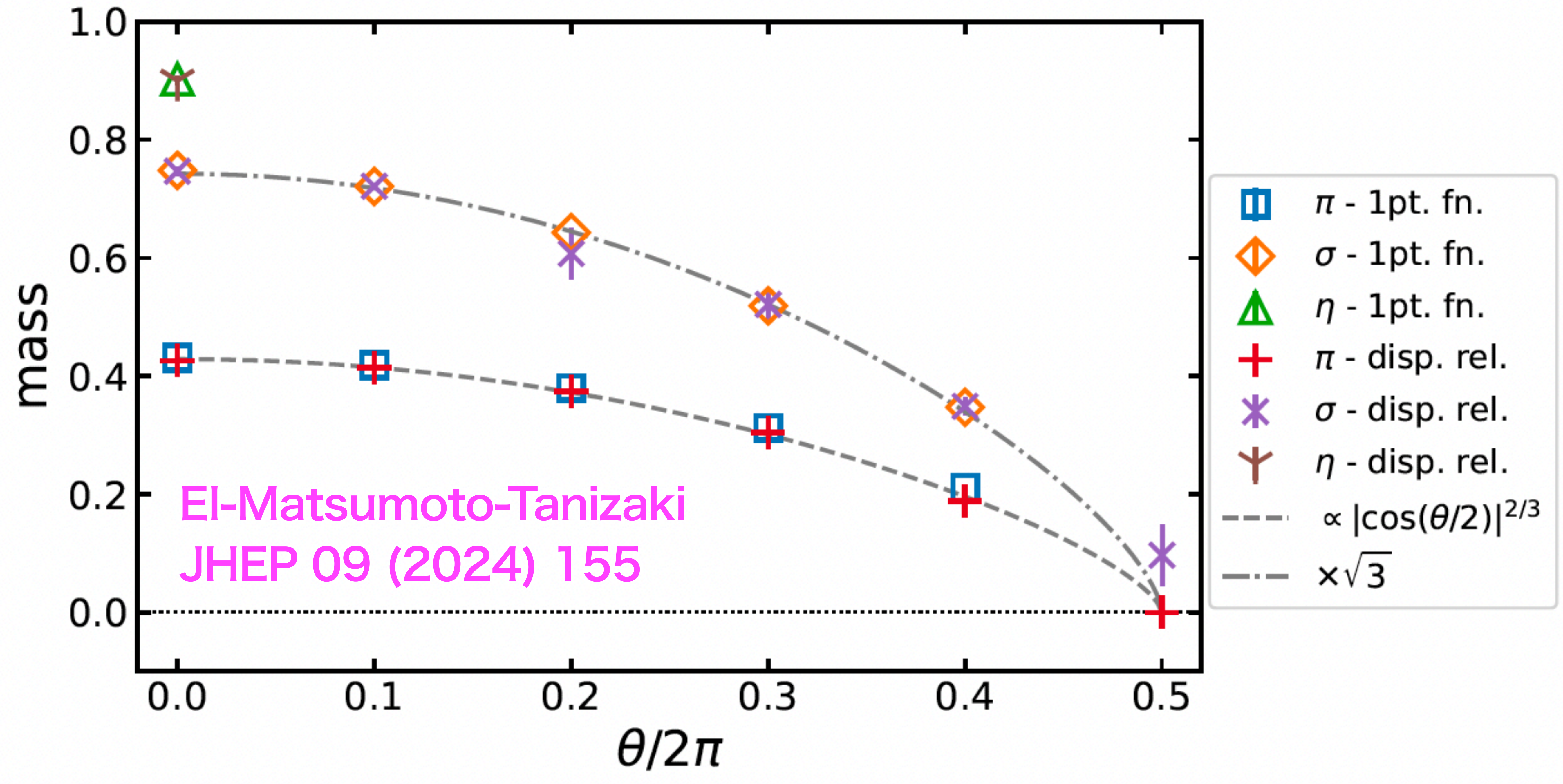
$\theta \neq 0$ regime (sign problem emerges in MC)

Nf=2 1+1dim. QED (Schwinger model)

Monte Carlo based on Lagrangian (w/ improvement techniques)



Tensor network based on Hamiltonian



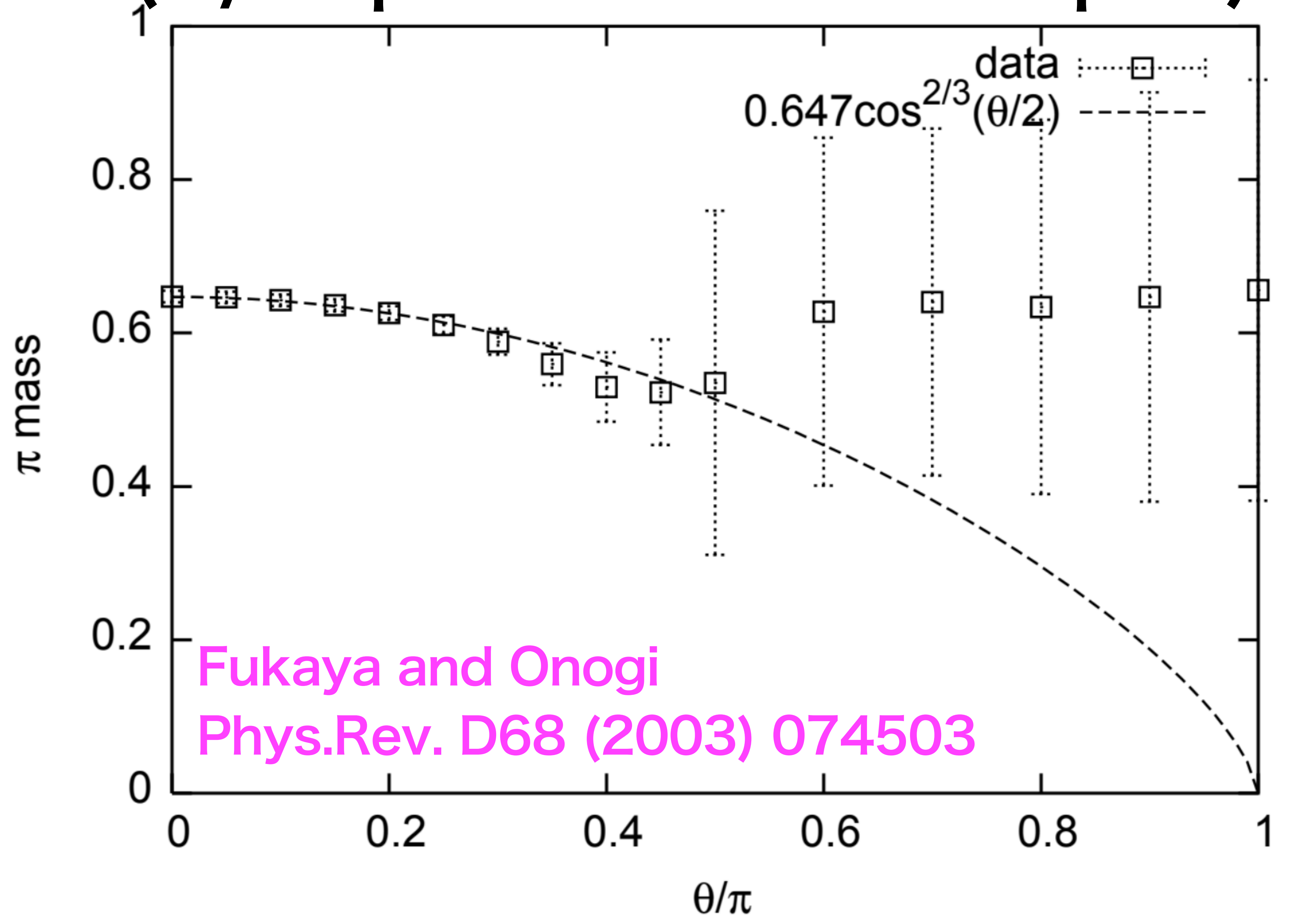
- In large θ, the signal is very noisy because of the sign problem
- Difficult to find a heavy η-meson and σ-meson

- Straightforwardly apply to $\theta = \pi$ regime (even near CFT)
- Results are consistent with theoretical predictions

$\theta \neq 0$ regime (sign problem emerges in MC)

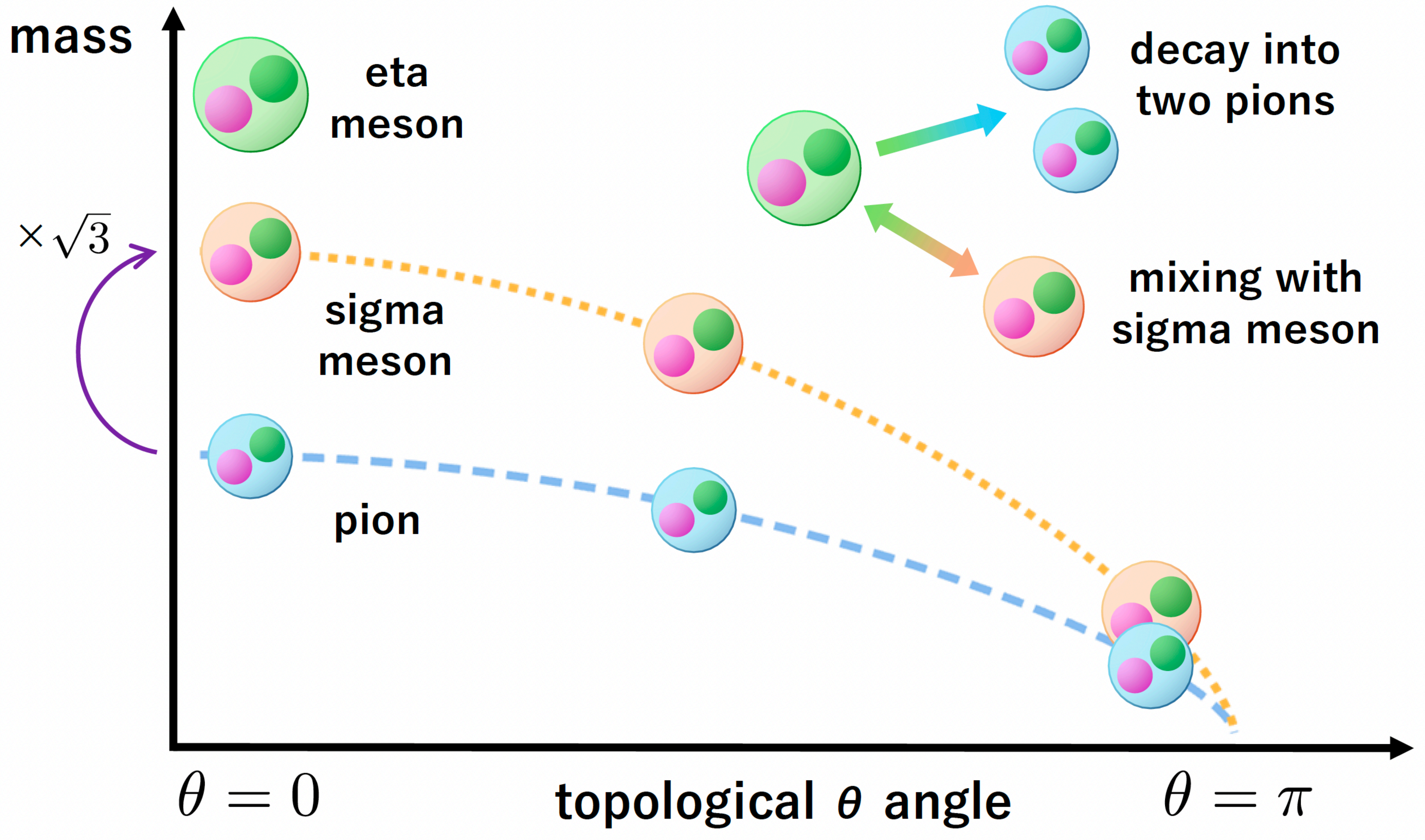
Nf=2 1+1dim. QED (Schwinger model)

Monte Carlo based on Lagrangian (w/ improvement techniques)



- In large θ, the signal is very noisy because of the sign problem
- Difficult to find a heavy η-meson and σ-meson

Tensor network based on Hamiltonian

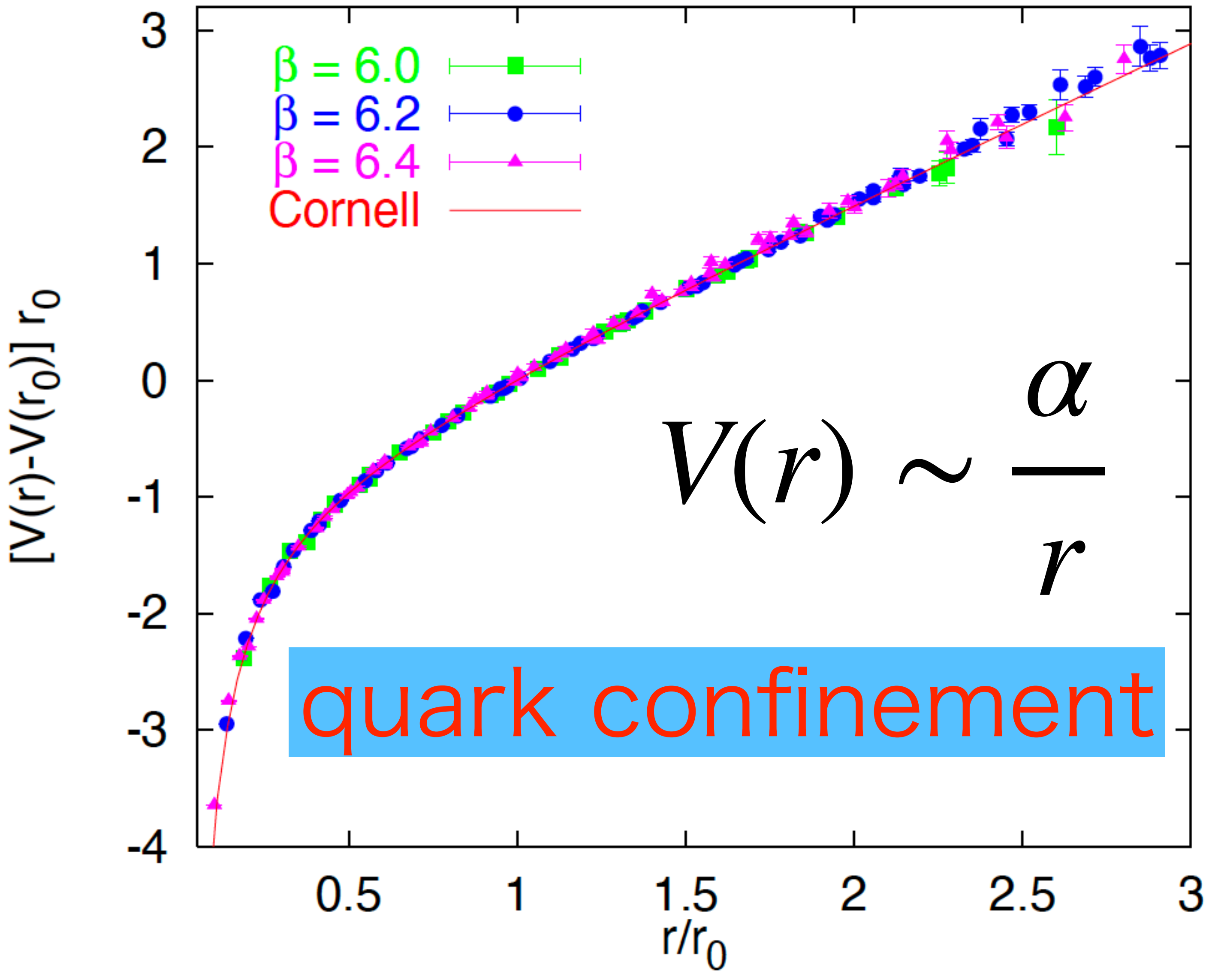


- Straightforwardly apply to $\theta = \pi$ regime (even near CFT)
- Results are consistent with theoretical predictions

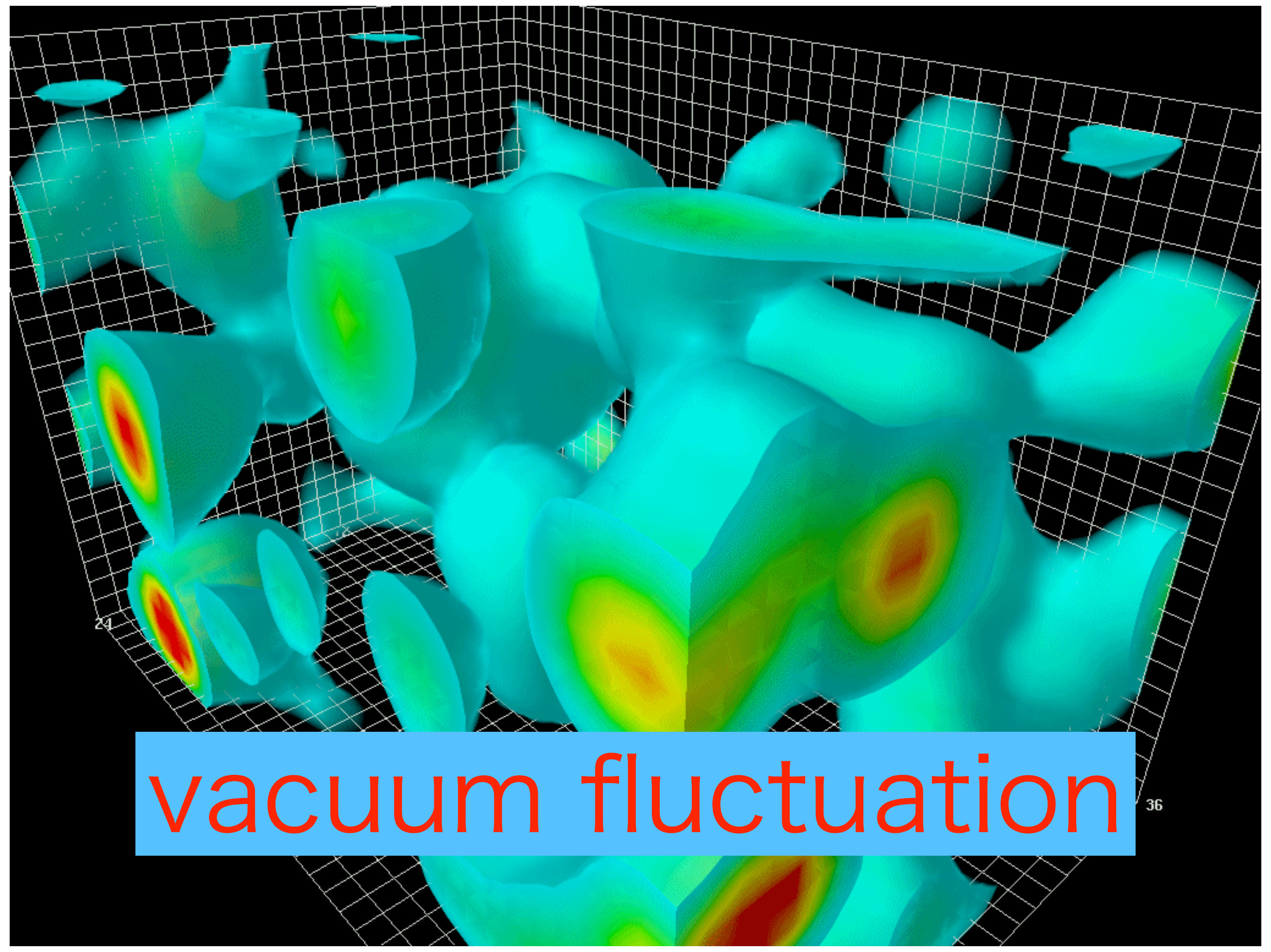
Other quantities

Successes of Lattice MC QCD

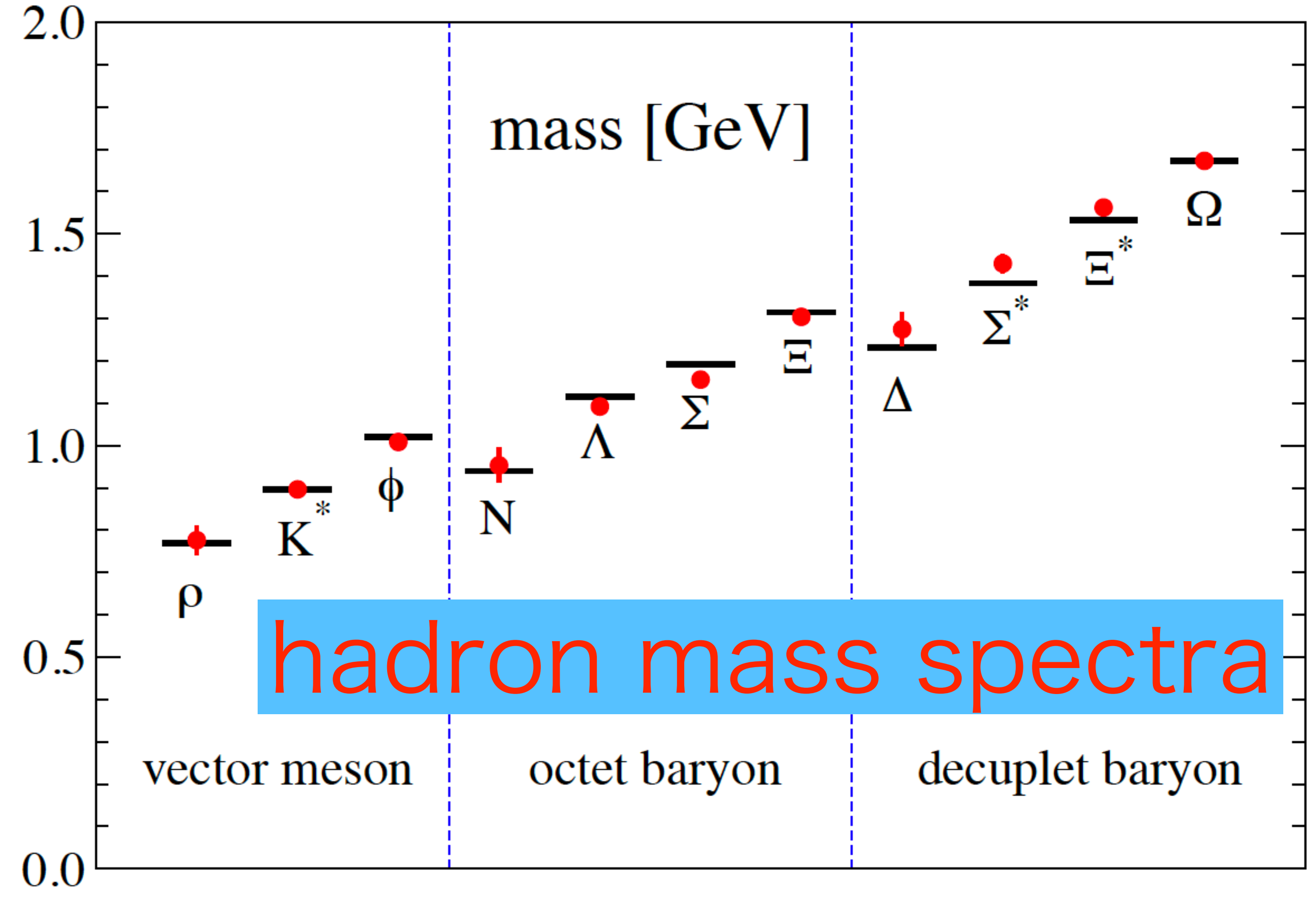
G.Bali, Phys.Rept.343:1 (2000)

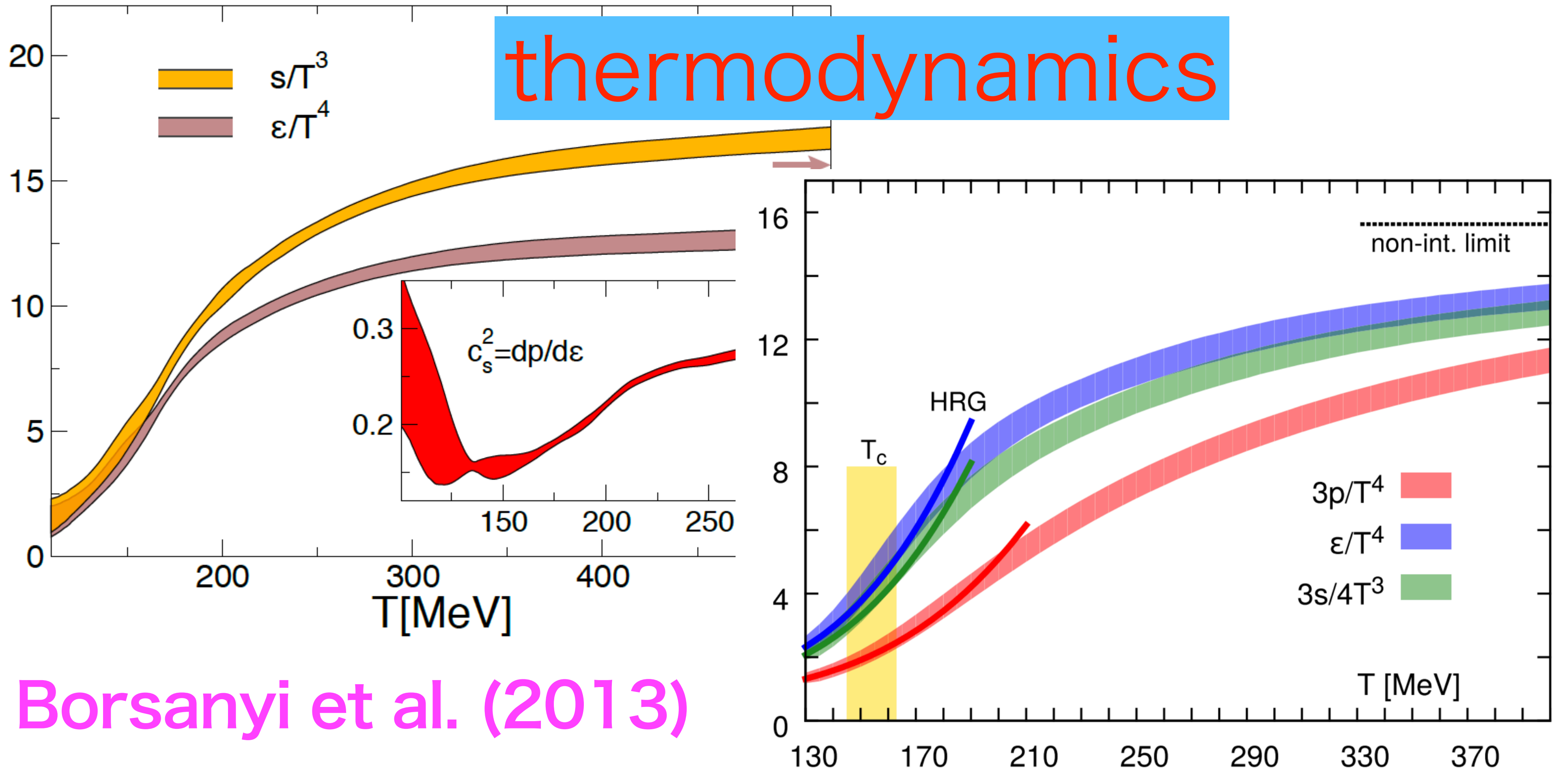


©Derek B. Leinweber



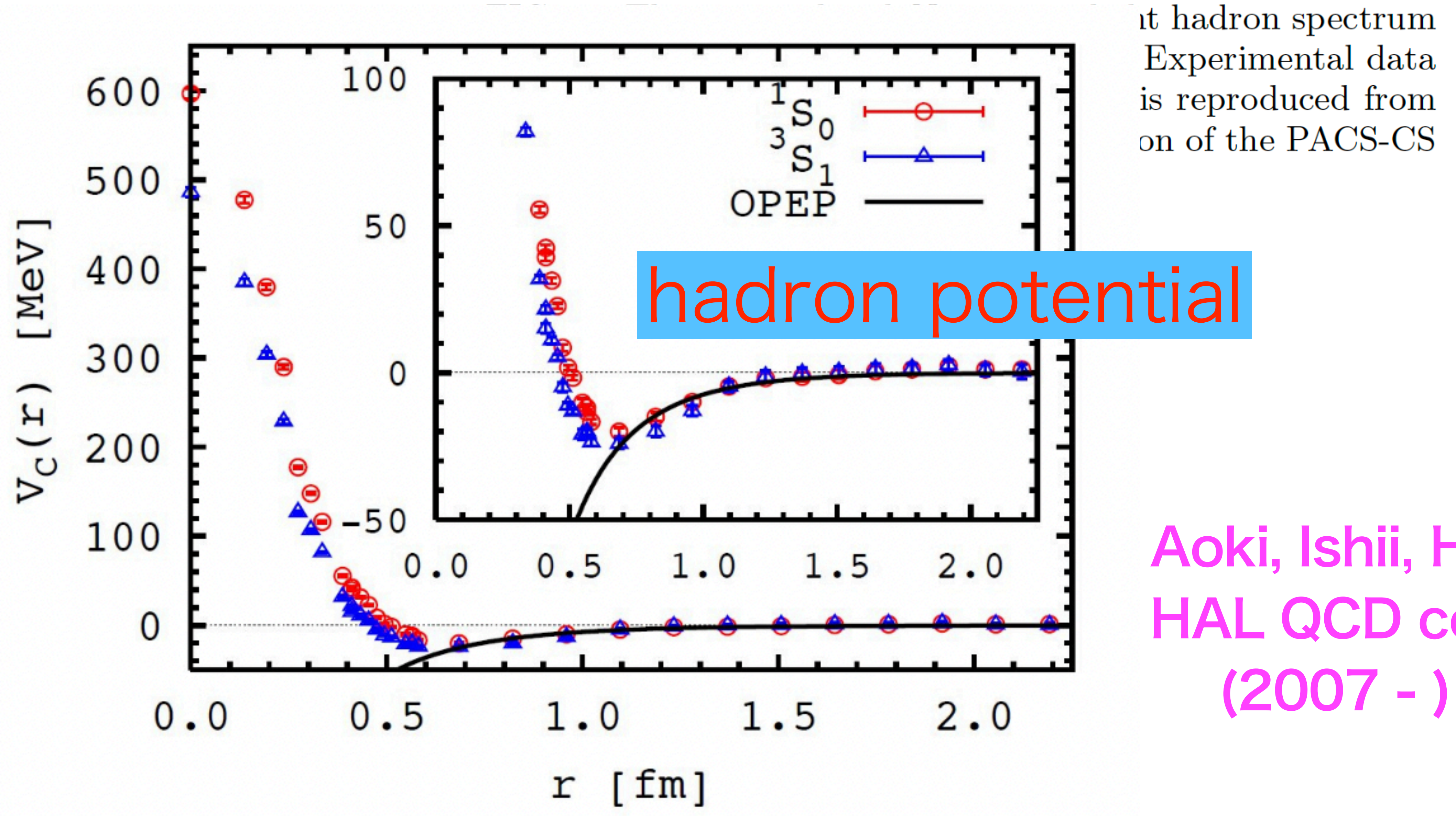
Z.Fodor and C.Hoelbling
arXiv:1203.4789





Borsanyi et al. (2013)

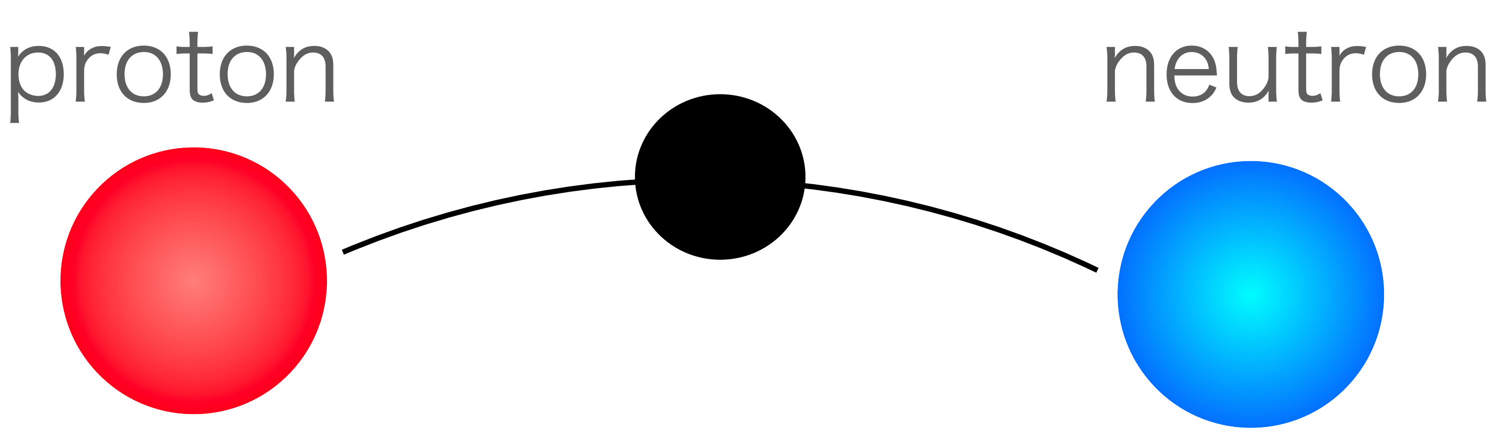
HotQCD (2014)

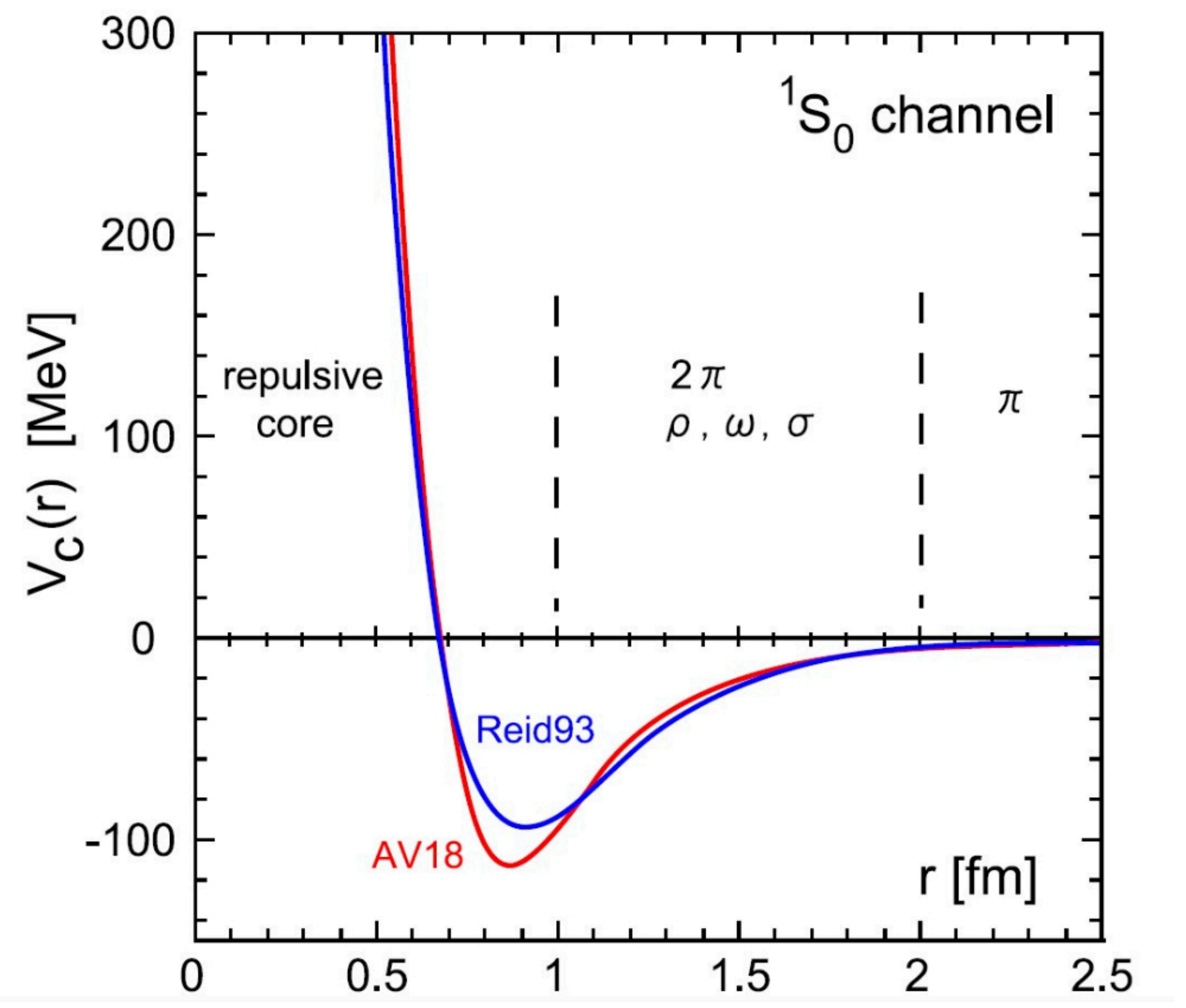


Aoki, Ishii, Hatsuda
HAL QCD coll.
(2007 -)

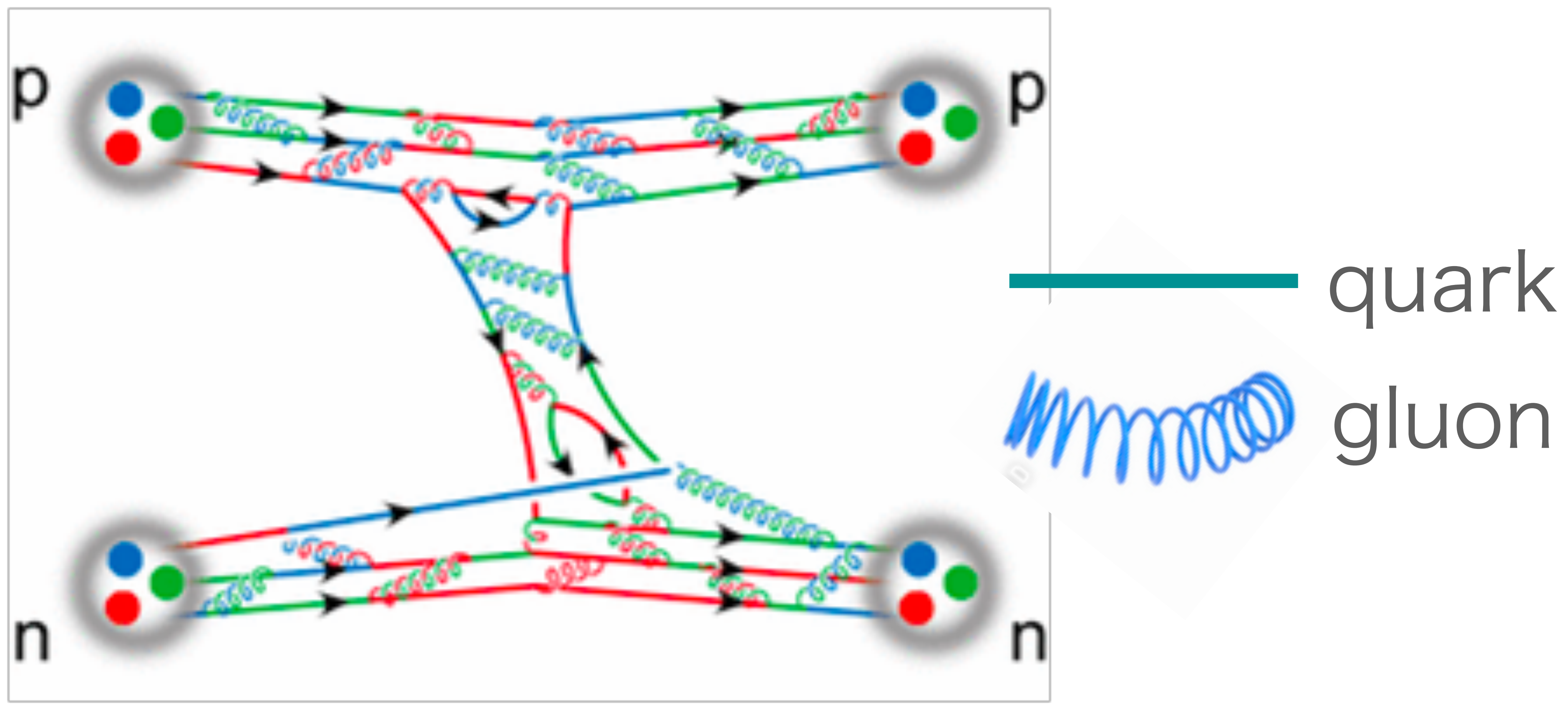
Hadron interaction potential is also calculated by Lattice

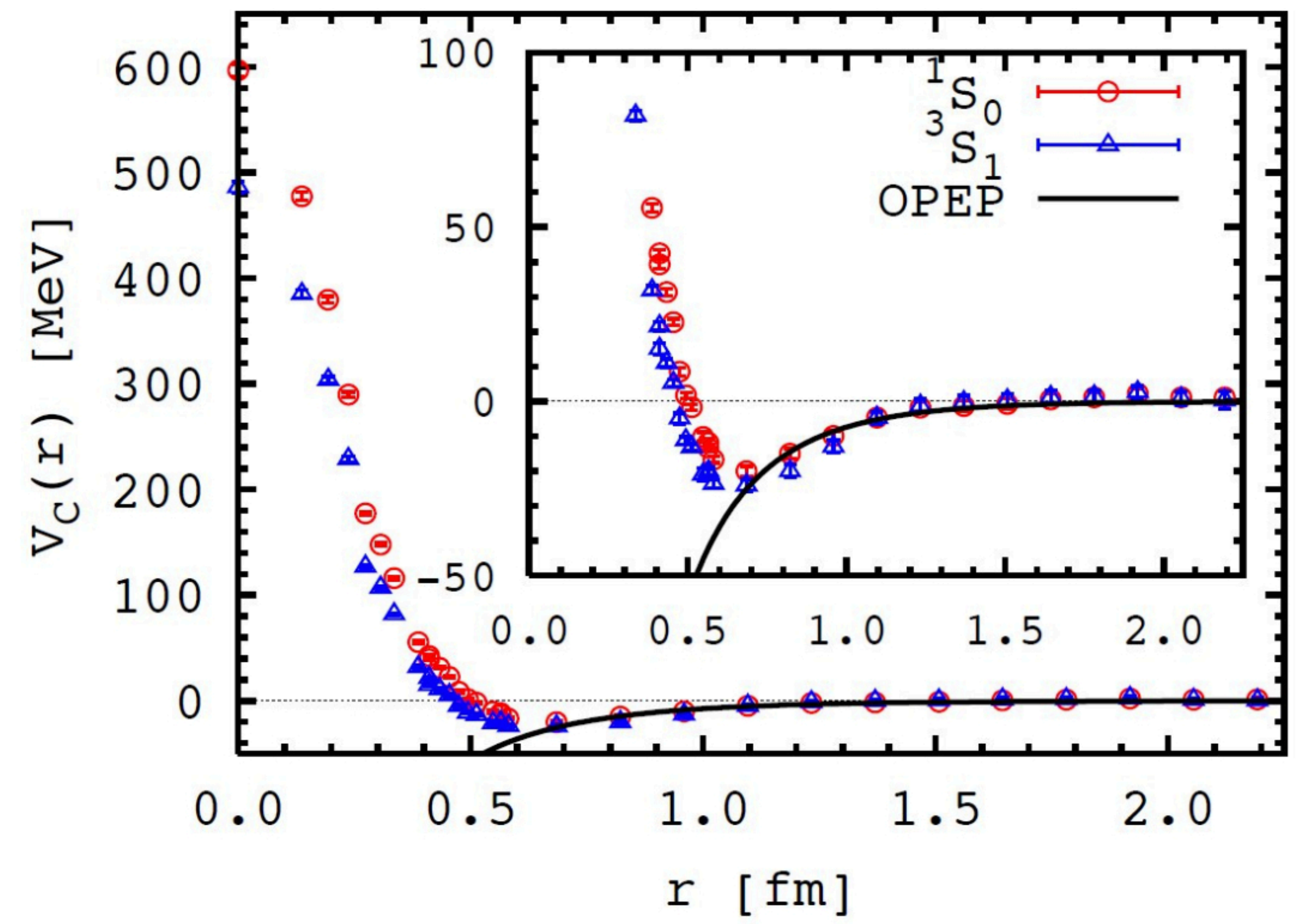
Yukawa interaction





Microscopical picture described by quarks





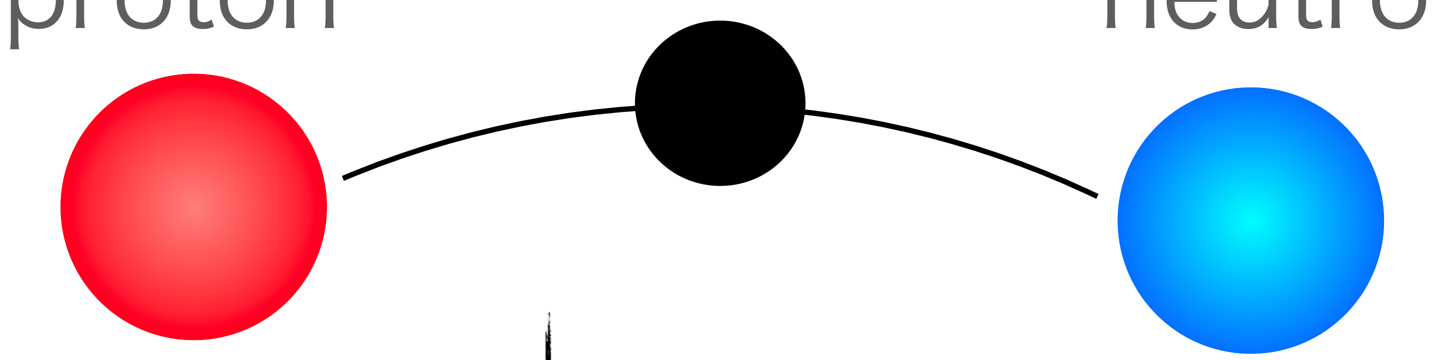
Hadron interaction potential is also calculated by Lattice

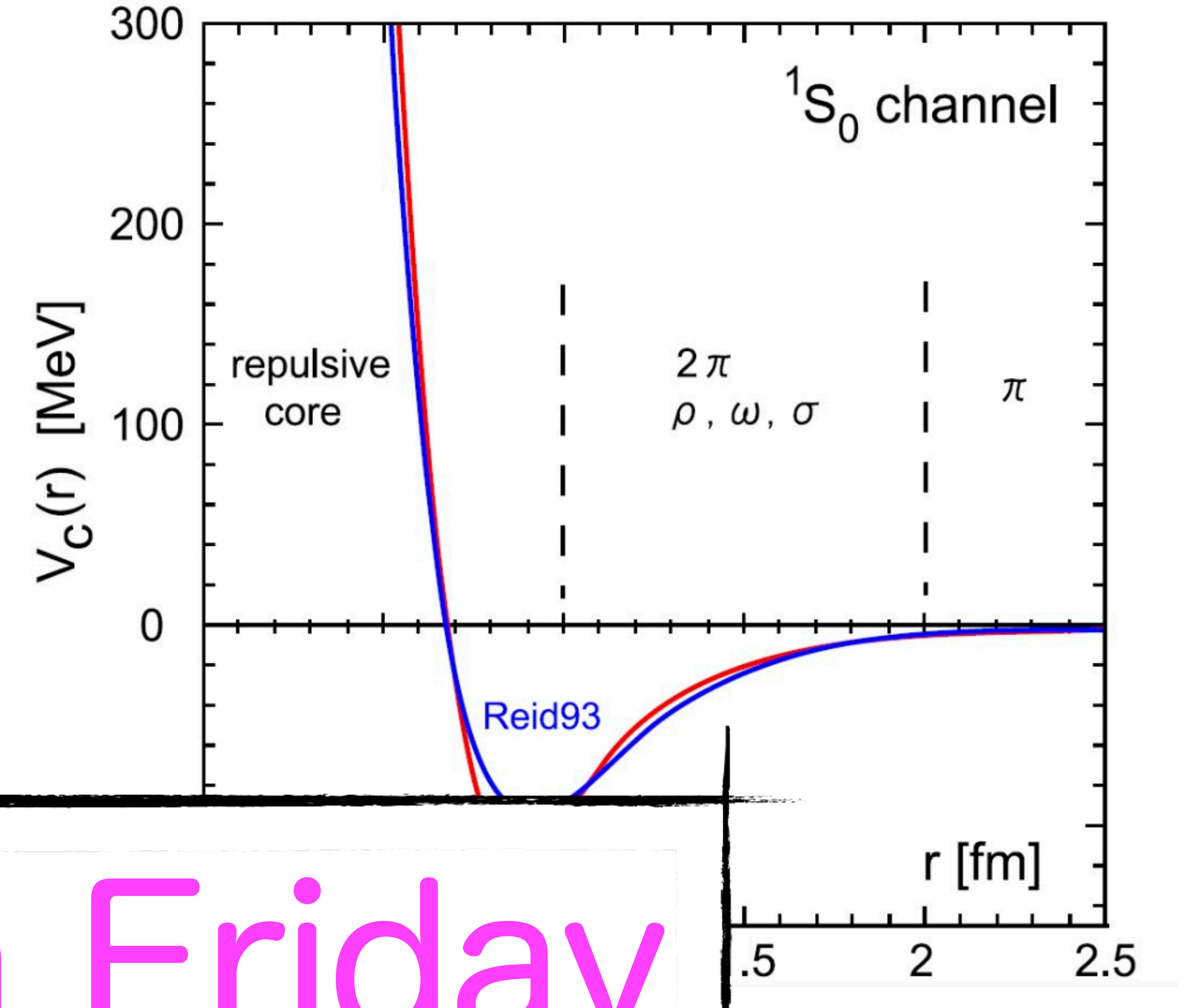
Yukawa interaction

pion (meson)

proton

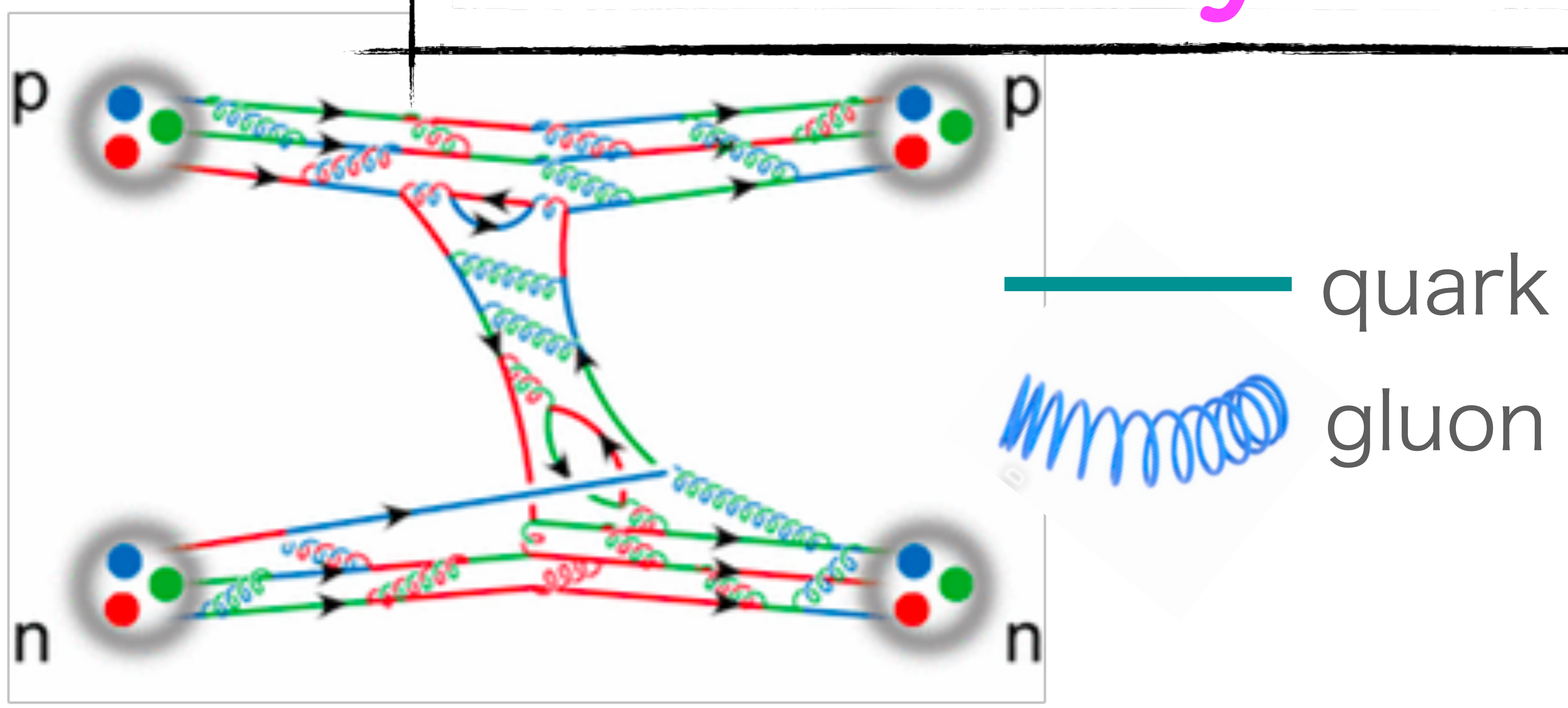
neutron

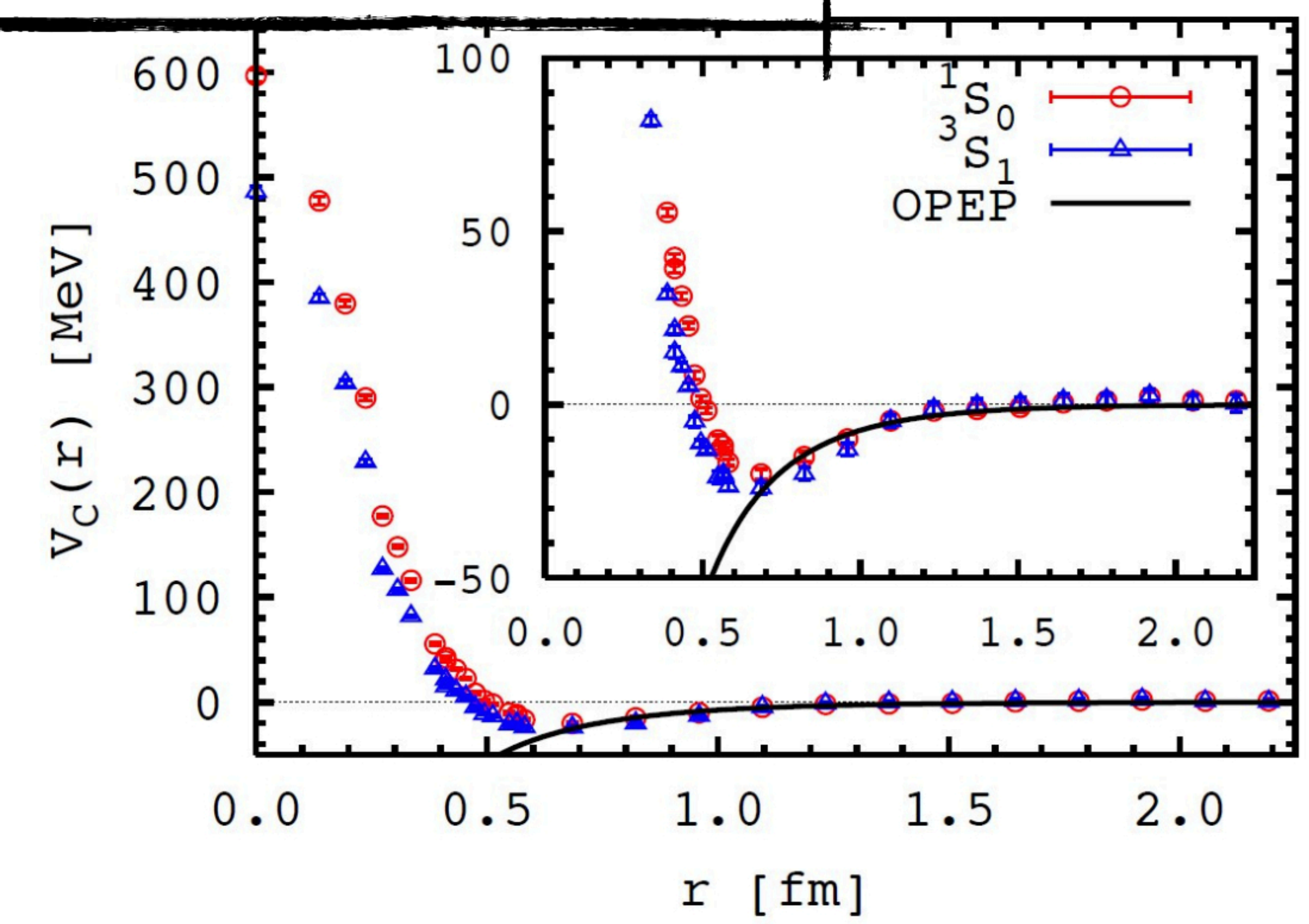




Lecture by T. Doi on Friday

Microscopical p





7. Summary

Summary

- Lattice regularization is only known the gauge invariant and nonperturbative formula.

- From lattice model calculation, we can obtain $\langle \mathcal{O} \rangle$ of actual QCD, thanks to the asymptotic freedom of non-abelian gauge theories

- In simulations, we do not perform an actual path-integral.
  Estimate the value of $\langle \mathcal{O} \rangle$ using Monte Carlo (importance sampling) method
  Now, we have some exact algorithms to perform its calculation

- Physical quantities even for hadron (composite particle) can be calculated from quarks and gluons theory