Izu workshop
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A study of $\Theta^+(udud\bar{s})$ in Lattice QCD with Optimal Domain-Wall Fermion

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Outline:

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2. Three Interpolating Operators for $(udud\bar{s})$
3. Computation of Quark Propagators
4. Mass Spectrum of 3×3 Correlation Matrix
5. Concluding Remarks

References:

TWC & Hsieh, hep-ph/0403020 v2

Introduction

Before Jan'03, any hadron can be interpreted as a bound state of 3 quarks (baryon) or 2 quarks (meson).
However, in Jan'03, the exotic baryon $\Theta^+(1540)$ (with the quantum numbers of K^+n) was observed by LEPS collaboration at SPring-8.
Later it was confirmed by some expt. groups.

The remarkable features of $\Theta^+(1540)$:
(i) $S = +1$ implies min. quark content $udud\bar{s}$.
(ii) decay width < 15 MeV, but its mass is 105 MeV above KN threshold.

However, there are quite a number of expt. which so far have not observed $\Theta^+(1540)$ or any pentaquarks !

In Oct'03, NA49 group at CERN has observed another exotic baryon $\Xi^{--}_{3/2}(1862)$ (with the quantum numbers of $\Xi^-\pi^-$, and $\Gamma < 18$ MeV), and two iso-partners, $\Xi^{-}_{3/2}$ and $\Xi^{0}_{3/2}$. Their quark contents are $dsds\bar{u}, dsus\bar{u}, dsus\bar{d}$.

In Mar'04, H1 collaboration at HERA has observed a narrow resonance $\Theta_c(3099)$ (with the quantum numbers of $D^{*-}p$, and $\Gamma < 15$ MeV). Its minimal quark content is $udud\bar{c}$. It is the first exotic baryon with $\bar{c}$, implying the existence of other exotic baryons with heavy quarks.

However, $\Xi^{--}_{3/2}$ or Θ_c has not been seen by other experiments.

Historically, the exp. search for $\Theta^+(1540)$ was motivated by the predictions of the chiral-soliton model [Diakonov,Petrov,Polyakov,'97], an outgrowth of the Skyrme model.

Even though the chiral solition model seems to provide very close predictions for the mass and the width of $\Theta^+(1540)$, obviously, it cannot reproduce all aspects of QCD.

Theoretically, the central question is whether the spectrum of QCD possesses 5Q baryons, with the correct quantum numbers, masses, and decay widths.

At present, the most viable approach to solve QCD nonperturbatively from first principles is lattice QCD.

In practice, one uses an interpolating op. which has a significant overlap with the pentaquark baryon states. Then compute time-correlation function of this operator, and from which to extract the mass of its even/odd parity state.

The diquark-diquark-antiquark [Jaffe & Wilzcek,'03] picture has been useful in constructing the inter. op. (source) for pentaquark baryons.

The eff. int. bet. two light quarks via 1-gluon exch.

$$H_{eff} \sim -(\vec{\lambda}_1 \cdot \vec{\lambda}_2)(\vec{\sigma}_1 \cdot \vec{\sigma}_2) = 4P^f_{12} + \frac{4}{3}P^s_{12} + 2P^c_{12} - \frac{2}{3}$$

where $\vec{\sigma}_i$ and $\vec{\lambda}_i$ are spin and color op. of the quark, and P^f_{12}, P^s_{12} and P^c_{12} are flavor, spin and color exchange op.

$$\begin{aligned} P^f_{12} &= (2+3\vec{\beta}_1 \cdot \vec{\beta}_2)/6 \\ P^s_{12} &= (1+\vec{\sigma}_1 \cdot \vec{\sigma}_2)/2 \\ P^c_{12} &= (2+3\vec{\lambda}_1 \cdot \vec{\lambda}_2)/6 \\ P^f_{12}P^s_{12}P^c_{12} &= -1 \end{aligned}$$

flavor	spin	color	δE
6_s	1_a	6_s	4
6_s	3_s	$\bar{3}_a$	8/3
$\bar{3}_a$	3_s	6_s	$-4/3$
$\bar{3}_a$	1_a	$\bar{3}_a$	-8

Salient features of diquark correl. seem to persist even at the hardronic scale where QCD is strongly coupled.

In Jaffe-Wilzcek model, diquark transforms like spin singlet (1_s), color anti-triplet ($\bar{3}_c$), and flavor anti-triplet $\bar{3}_f = \{ud, ds, us\}$.

Then pentaquark baryons with light quarks emerge as the color singlet in

$$(\bar{3}_c \times \bar{3}_c) \times \bar{3}_c = 1_c + 8_c + 8_c + \overline{10_c}$$

and flavor multiplets in

$$(\bar{3}_f \times \bar{3}_f) \times \bar{3}_f = (1_f + 8_f) + 8_f + \overline{10}_f$$

If the light antiquark is replaced with heavy $\bar{c}$ or $\bar{b}$, then the flavor multiplets are reduced to the triplet (3_f) and the antisextet ($\bar{6}_f$).

For lattice QCD, one has options to use a local or smeared source for any baryon, provided its correlation function has a significant overlap with the baryon state.

First, to construct local diquark op. $[ud]$ as

$$[\mathbf{u}^T \Gamma \mathbf{d}]_{xa} \equiv \epsilon_{abc}(\mathbf{u}_{x\alpha b}\Gamma_{\alpha\beta}\mathbf{d}_{x\beta c} - \mathbf{d}_{x\alpha b}\Gamma_{\alpha\beta}\mathbf{u}_{x\beta c})$$

where $\Gamma_{\alpha\beta} = -\Gamma_{\beta\alpha}$ such that the diquark op. transforms like a scalar or pseudoscalar.

(i) Scalar: $\Gamma = C\gamma_5$, C is the charge conj. op.
(ii) Pseudoscalar: $\Gamma = C$.

Then local source for diquark-diquark-antiquark can be written as [Sugiyama et al, '03; Sasaki '03]

$$\begin{aligned} \Theta_{x\alpha} &= \epsilon_{cde}\ [\mathbf{u}^T(C\gamma_5)\mathbf{d}]_{xd}\ [\mathbf{u}^T C\mathbf{d}]_{xe}\ (C\bar{\mathbf{s}}^T)_{x\alpha c} \\ \left(\Xi^{--}_{3/2}\right)_{x\alpha} &= \epsilon_{cde}\ [\mathbf{d}^T(C\gamma_5)\mathbf{s}]_{xd}\ [\mathbf{d}^T C\mathbf{s}]_{xe}\ (C\bar{\mathbf{u}}^T)_{x\alpha c} \\ (\Theta_c)_{x\alpha} &= \epsilon_{cde}\ [\mathbf{u}^T(C\gamma_5)\mathbf{d}]_{xd}\ [\mathbf{u}^T C\mathbf{d}]_{xe}\ (C\bar{\mathbf{c}}^T)_{x\alpha c} \end{aligned}$$

while the 3-quark baryon (e.g., Proton) as

$$P_{x\alpha} = [\mathbf{u}^T(C\gamma_5)\mathbf{d}]_{xa}\mathbf{u}_{x\alpha a}$$

Note that for $\Theta, \Xi^{--}_{3/2}$ or Θ_c which is composed of two identical diquarks, one cannot choose both diquark operators to be (pseudo-)scalar, otherwise the interpolating op. is identically zero since diquarks are bosons.

Thus when the orbital angular momentum of this scalar-pseudoscalar-antifermion system is zero (i.e., the lowest lying state), its parity is even rather than odd.

Alternatively, if these two diquarks are located at two different sites, then both diquark op. can be chosen to be scalar, however, they must be antisym in space, $L =$ odd integer. Thus the parity of lowest lying state of this scalar-scalar-antifermion system is even, as suggested in the Jaffe-Wilzcek model.

Three different sources for $\Theta^+(udud\bar{s})$

$$
\begin{aligned}
(O_1)_{x\alpha} &= [\mathbf{u}^T C\gamma_5 \mathbf{d}]_{xc}\ \{(\bar{\mathbf{s}}_{xe}\gamma_5\mathbf{u}_{xe})(\gamma_5\mathbf{d})_{x\alpha c} - (\bar{\mathbf{s}}_{xe}\gamma_5\mathbf{d}_{xe})(\gamma_5\mathbf{u})_{x\alpha c}\} \\
(O_2)_{x\alpha} &= [\mathbf{u}^T C\gamma_5 \mathbf{d}]_{xc}\ \{(\bar{\mathbf{s}}_{xe}\gamma_5\mathbf{u}_{xc})(\gamma_5\mathbf{d})_{x\alpha e} - (\bar{\mathbf{s}}_{xe}\gamma_5\mathbf{d}_{xc})(\gamma_5\mathbf{u})_{x\alpha e}\} \\
(O_3)_{x\alpha} &= \epsilon_{cde}[\mathbf{u}^T C\gamma_5 \mathbf{d}]_{xc}[\mathbf{u}^T C\mathbf{d}]_{xd}(C\bar{\mathbf{s}}^T)_{x\alpha e}
\end{aligned}
$$

where $[\mathbf{u}^T\Gamma\mathbf{d}]_{xa} \equiv \epsilon_{abc}\{\mathbf{u}_{x\alpha b}\Gamma_{\alpha\beta}\mathbf{d}_{x\beta c} - \mathbf{d}_{x\alpha b}\Gamma_{\alpha\beta}\mathbf{u}_{x\beta c}\}$

O_1 is kaon $\otimes$ nucleon operator [Mathur et al.'03]

O_2 is a variant of O_1 [Zhu'03, Csikor et al.'03]

O_3 is the diquark-diquark-antiquark [Sugiyama et al.'03, Sasaki '03]

3×3 Correlation Matrix

$$C_{ij}^{\pm}(t) = \sum_{\vec{x}} \mathrm{tr}\left[\frac{1 \pm \gamma_4}{2}\langle O_i(\vec{x},t)\bar{O}_j(\vec{0},0)\rangle\right]$$

$$\mathcal{C}^{\pm}(t) = \{C_{ij}^{\pm}(t)\} \xrightarrow{diagonalization} \{A_i^{\pm}(t)\} \longrightarrow \{m_i^{\pm}\}$$

Computation of Quark Propagators

The time correlation function

$$C_{ij}(t) = \sum_{\vec{x}} \langle O_i(\vec{x}, t) \bar{O}_j(\vec{0}, 0) \rangle$$

can be expressed in terms of quark prop. (tedious ! a lot of terms !)

In lattice QCD with exact chiral symmetry, quark propagator is of the form $(D_c + m_q)^{-1}$ where D_c is exactly chirally sym. for any finite lattice spacing [TWC,'98], and

$$(D_c + m_q)^{-1} \to [\gamma_\mu(\partial_\mu + iA_\mu) + m_q]^{-1}$$

in the continuum limit.

For Optimal Domain-Wall Fermion [TWC,'02,'03] with $N_s + 2$ sites in the fifth dimension,

$$
\begin{aligned}
D_c &= 2m_0 \frac{1+\gamma_5 S(H_w)}{1-\gamma_5 S(H_w)} \\
S(H_w) &= \frac{1-\prod_{s=1}^{N_s} T_s}{1+\prod_{s=1}^{N_s} T_s} \overset{N_s\to\infty}{\longrightarrow} \frac{H_w}{\sqrt{H_w^2}} \Rightarrow D_c\gamma_5 + \gamma_5 D_c = 0 \\
T_s &= \frac{1-\omega_s H_w}{1+\omega_s H_w}, \quad H_w = \gamma_5 D_w,
\end{aligned}
$$

where D_w is the Wilson Dirac op. plus a neg. parameter $-m_0 \in (-2, 0)$, and $\{\omega_s\}$ are a set of weights specified by an exact formula such that D_c possesses the optimal chiral sym for any given N_s and gauge background [TWC,'02,'03]

$$
\begin{aligned}
\omega_s &= \frac{1}{\lambda_{min}}\sqrt{1-\kappa'^2 \mathrm{sn}^2(v_s;\kappa')}, \quad s = 1, \cdots, N_s \\
\omega_0 &= \omega_{N_s+1} = 0
\end{aligned}
$$

Since

$$(D_c + m_q)^{-1} = \left(1 - \frac{m_q}{2m_0}\right)^{-1} \left[D^{-1}(m_q) - \frac{1}{2m_0}\right]$$

where

$$D(m_q) = m_q + (m_0 - m_q/2)[1 + \gamma_5 S(H_w)],$$

thus the quark propagator can be obtained by solving the system $D(m_q)Y = \mathbb{1}$ with nested conjugate gradient, which turns out to be highly efficient (in terms of precision of chirality vs. CPU time and memory storage) if the inner CG loop is iterated with Neuberger's double pass algorithm. [Neuberger,'98, TWC & Hsieh,'03]

We generate 100 gauge confs with Wilson gauge action at $\beta = 6.1$ on $20^3 \times 40$ lattice.

Fixing $m_0 = 1.3$, we project out 16 low-lying eigenmodes of $|H_w|$ and perform the nested conjugate gradient in the complement of the vector space spanned by these eigenmodes.

For $N_s = 128$, the weights $\{\omega_s\}$ are fixed with $\lambda_{min} = 0.18$ and $\lambda_{max} = 6.3$, where $\lambda(|H_w|) \in [\lambda_{min}, \lambda_{max}]$ for all gauge configurations (after projection of low-lying eigenmodes).

For each configuration, quark propagators are computed for 30 bare quark masses in the range $0.03 \le m_q a \le 0.8$ with stopping criteria 10^{-11} and 2×10^{-12} for the outer and inner conjugate gradient loops respectively. Then the norm of the residual vector of each column of the quark propagator is less than 2×10^{-11}

$$||(D_c + m_q)Y - \mathbb{1}|| < 2 \times 10^{-11},$$

and the chiral symmetry breaking due to finite $N_s (= 128)$ is less than 10^{-14},

$$\sigma = \left| \frac{Y^\dagger S^2 Y}{Y^\dagger Y} - 1 \right| < 10^{-14},$$

for every iteration of the nested CG.

The quark propagators are computed by a Linux PC cluster (with 100 nodes), in which each node computes 1 column for 30 quark masses simultaneously.

Determination of a^{-1} and m_s

We measure the pion time correlation function

$$\begin{aligned} C_\pi(t) &= \sum_{\vec{x}} \mathrm{tr}\{\gamma_5 (D_c + m_q)^{-1}(0,x)\gamma_5 (D_c+m_q)^{-1}(x,0)\} \\ &= \sum_{\vec{x}} \mathrm{tr}\{\left[(D_c+m_q)^{-1}{}^{ab}_{\alpha\beta}(x,0)\right]^* (D_c+m_q)^{-1}{}^{ab}_{\alpha\beta}(x,0)\} \end{aligned}$$

and its average over gauge confs is then fitted by

$$\frac{Z}{2m_\pi a}[e^{-m_\pi a t} + e^{-m_\pi a (T-t)}]$$

to extract pion mass $m_\pi a$ and decay constant

$$f_\pi a = 2 m_q a \frac{\sqrt{Z}}{(m_\pi a)^2} \ .$$

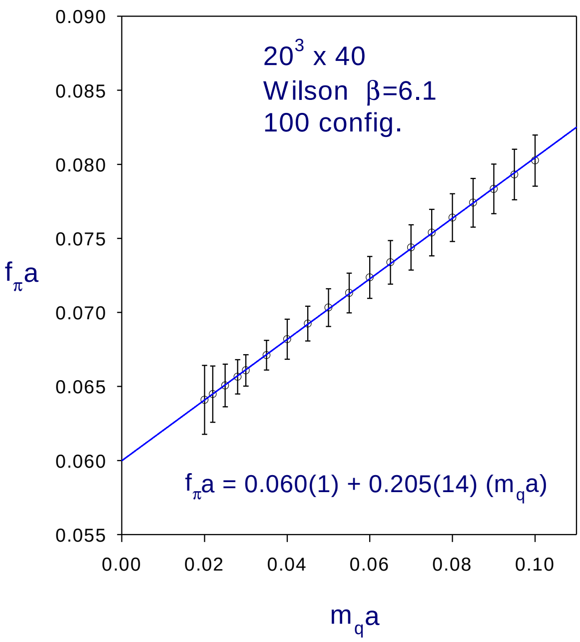
Determine lattice spacing a from pion decay constant.

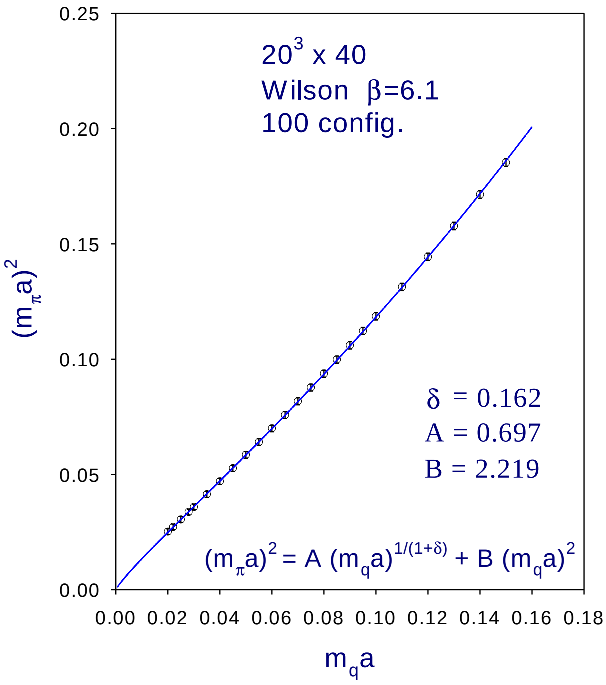
The data of $f_\pi a$ vs. $m_q a$ can be fitted by

$$f_\pi a = 0.060(1) + 0.205(14) \times (m_q a) \qquad (1)$$

Taking $f_\pi a$ at $m_q a = 0$ equal to 0.132 GeV times a, we can determine the lattice spacing a,

$$\begin{aligned} a^{-1} &= \frac{0.132}{f_0} = 2.20(1)\ (\text{GeV}) \\ a &= 0.089(1)\ \text{fm} \end{aligned}$$

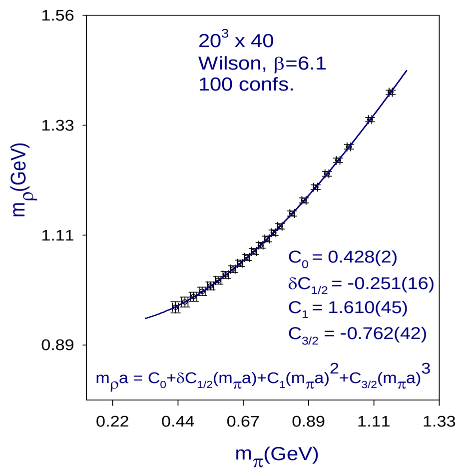




The bare mass of strange quark is determined by extracting the mass of vector meson from

$$C_V(t) = \frac{1}{3}\sum_{\mu=1}^{3}\sum_{\vec{x}} \text{tr}\{\gamma_\mu (D_c + m_q)^{-1}_{x,0}\gamma_\mu (D_c + m_q)^{-1}_{0,x}\}$$

At $m_q a = 0.06$, $M_V a = 0.4638(32)$, which gives $M_V = 1025(7)$ MeV, in good agreement with the mass of $\phi(1020)$. Thus we take $m_s a = 0.06$. Then we have 6 quark masses smaller than m_s, i.e., $m_q a = 0.03, 0.035, 0.04, 0.045, 0.05, 0.055$.
Here we work in the isospin limit $m_u = m_d$.



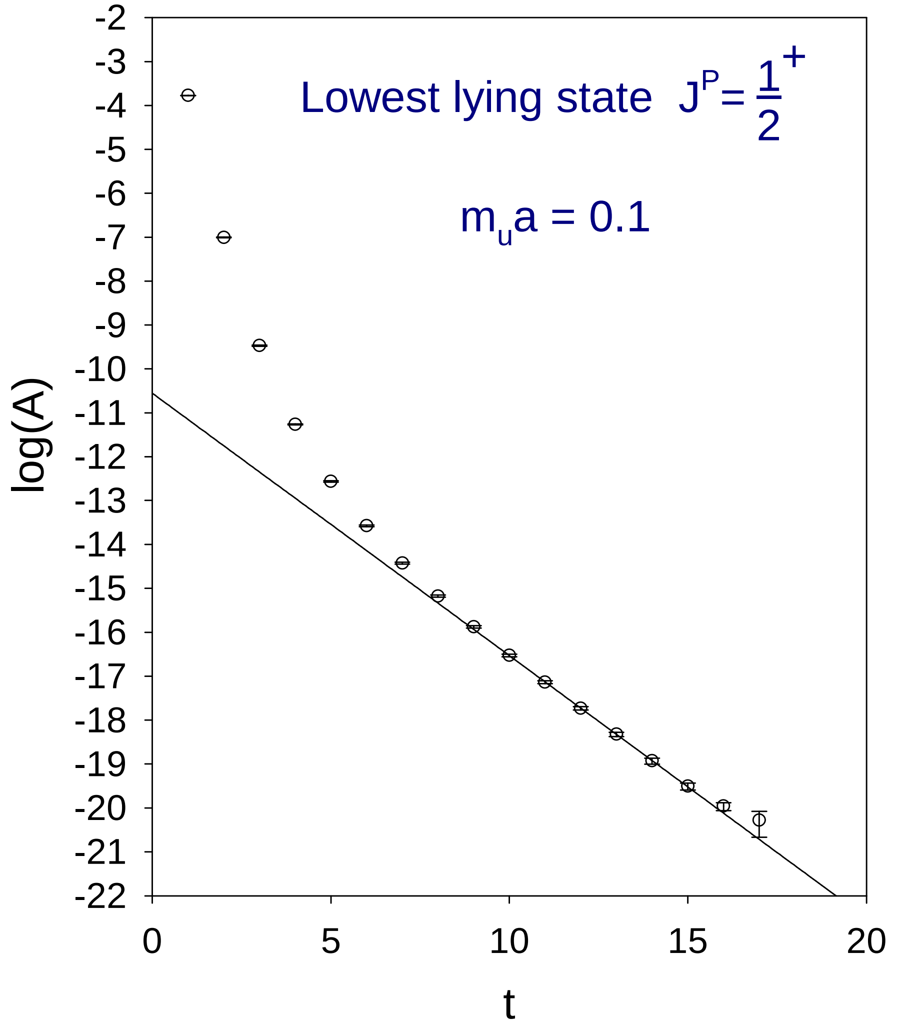
Mass Spectrum of 3×3 Correlation Matrix

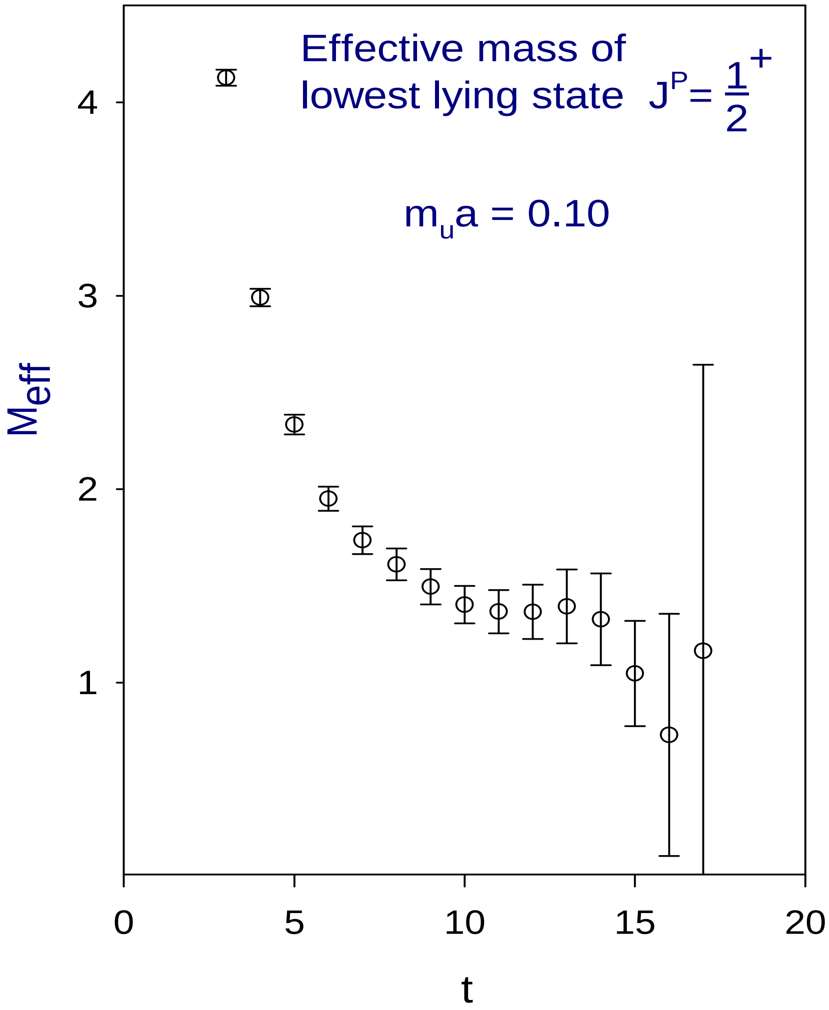
$$C^{\pm}_{ij}(t) = \sum_{\vec{x}} \mathrm{tr}\left[\frac{1 \pm \gamma_4}{2} \langle O_i(\vec{x}, t) \bar{O}_j(\vec{0}, 0) \rangle \right]$$

$$\mathcal{C}^{\pm}(t) = \{C^{\pm}_{ij}(t)\} \xrightarrow{diagonalization} \{A^{\pm}_i(t)\} \longrightarrow \{m^{\pm}_i\}$$

(1) Lowest-lying state with $J^P = 1/2^+$

The effective mass attains a plateau for $t \in [9, 14]$. Its mass can be extracted by single exp fit. It behaves like usual resonances encountered in quenched lattice QCD.

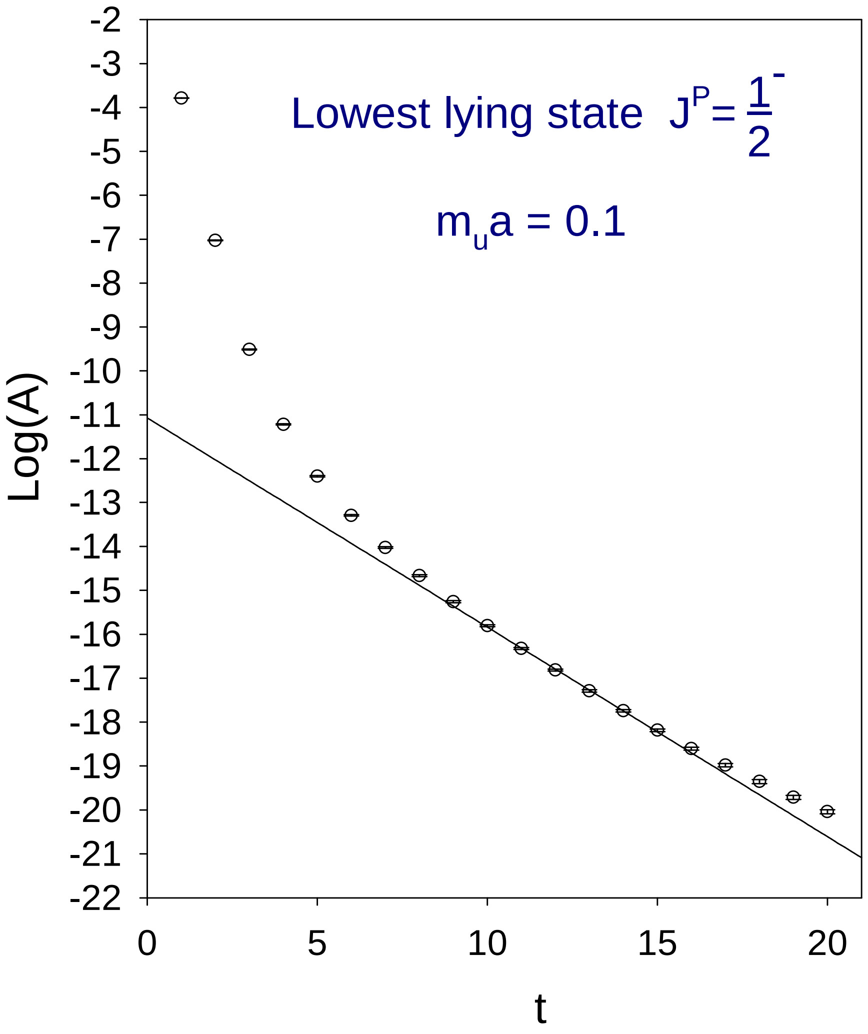

Lowest lying state $J^P = \frac{1}{2}^+$
$m_u a = 0.1$
log(A)
t
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
-15
-16
-17
-18
-19
-20
-21
-22
0
5
10
15
20


Effective mass of
lowest lying state $J^P = \frac{1}{2}^+$
$m_u a = 0.10$
M_{eff}
t
4
3
2
1
0
5
10
15
20

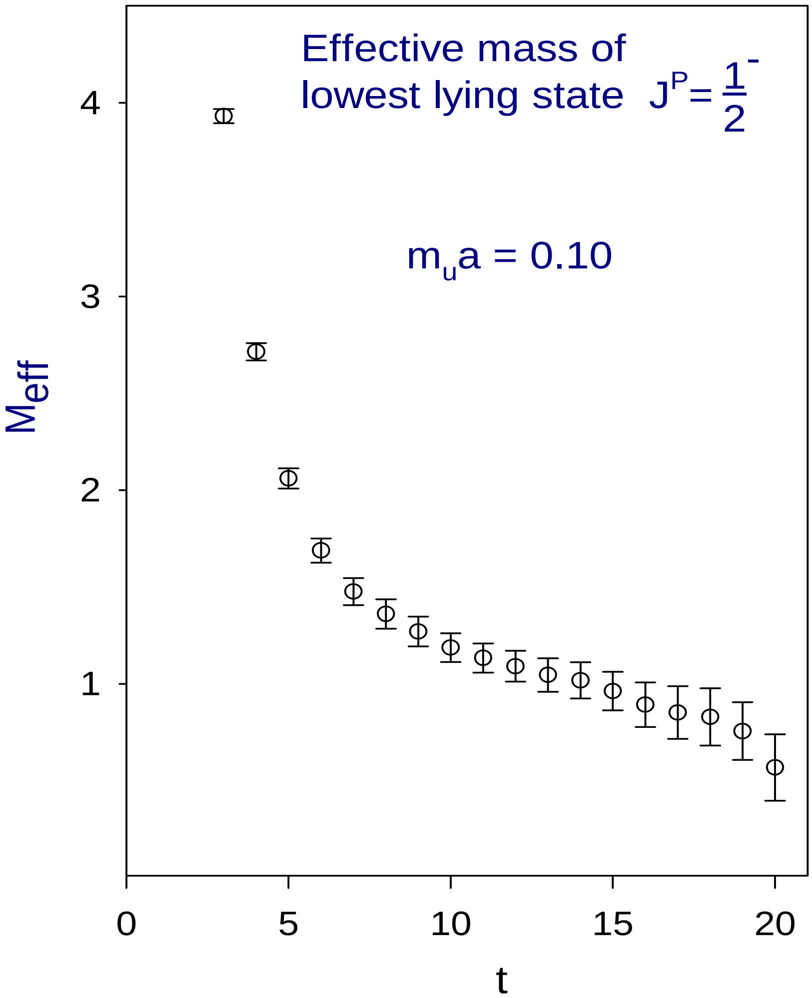
(2) Lowest lying state with $J^P = 1/2^-$

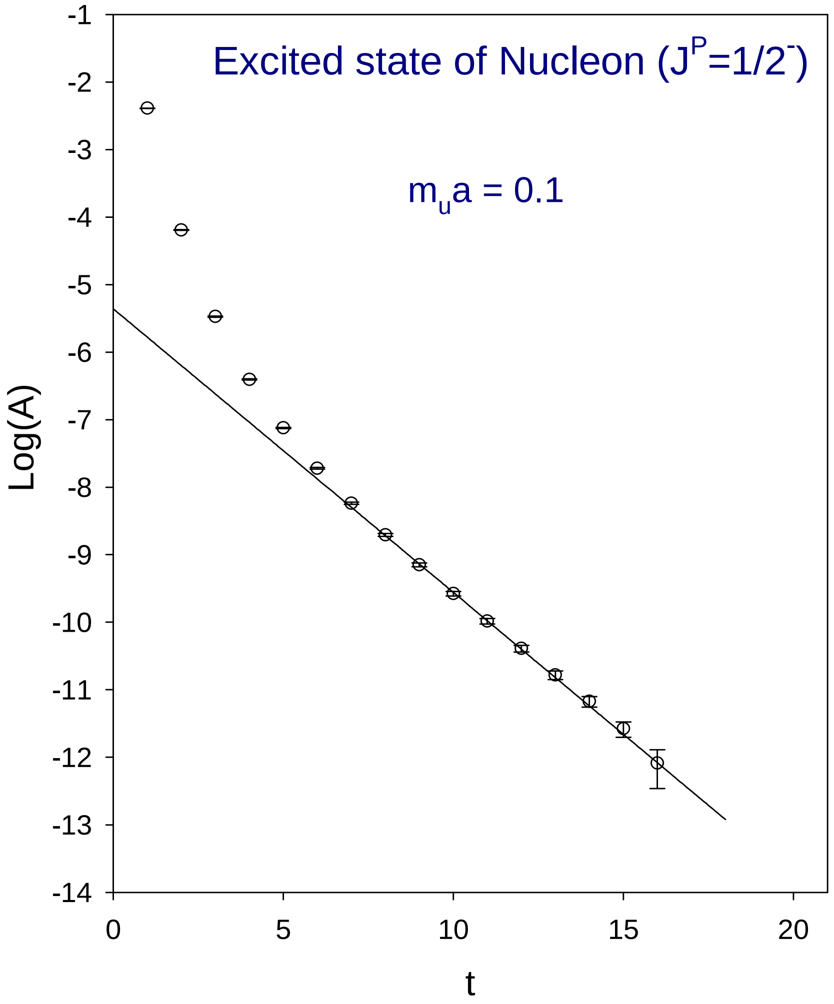
The M_{eff} decreases monotonically, no plateaus. This implies that it is very unstable, and decays rapidly into two or many particles. So its decay width must be very large ! [Note that the S-wave of $(udud\bar{s})$ can easily fall apart into K^+ and n !]

To estimate the lower bound of its width by comparing its $A(t)$ and $M_{eff}(t)$ with those of the excited state ($J^P = 1/2^-$) of nucleon, $N^*(1535)$ which has $\Gamma \sim 100 - 200$ MeV.

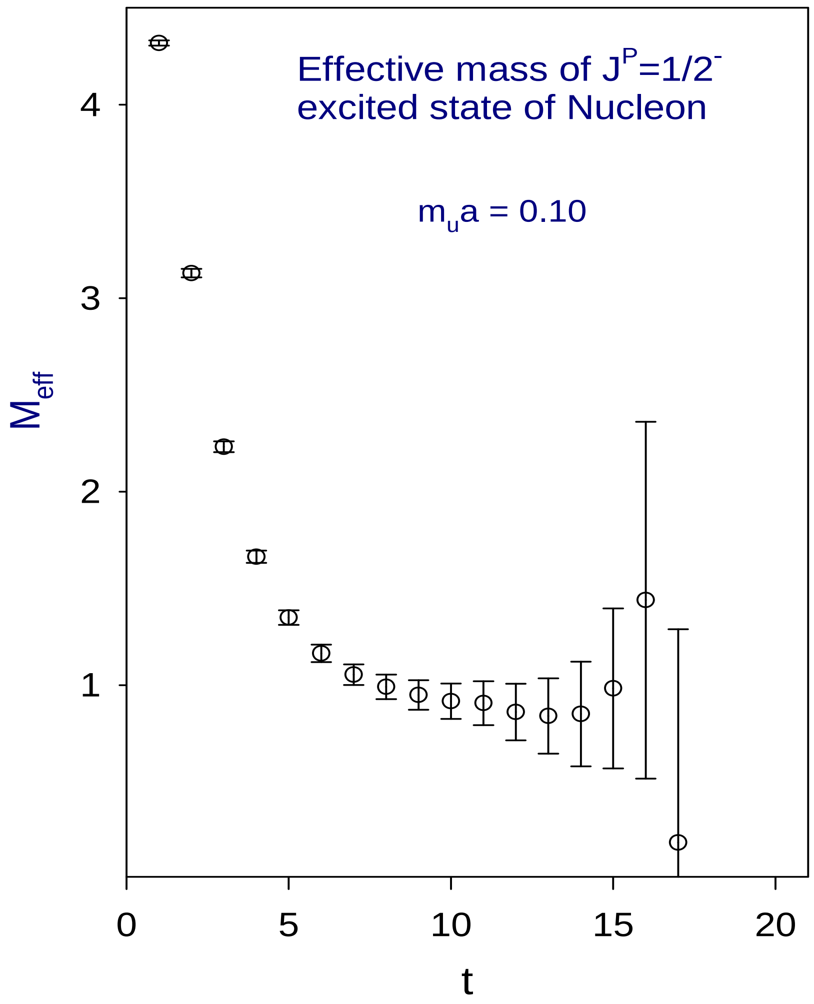


Lowest lying state $J^P = \frac{1}{2}^-$
$m_u a = 0.1$
Log(A)
t
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
-15
-16
-17
-18
-19
-20
-21
-22
0
5
10
15
20


Effective mass of
lowest lying state $J^P = \frac{1}{2}^-$
$m_u a = 0.10$
M_{eff}
4
3
2
1
0
5
10
15
20
t

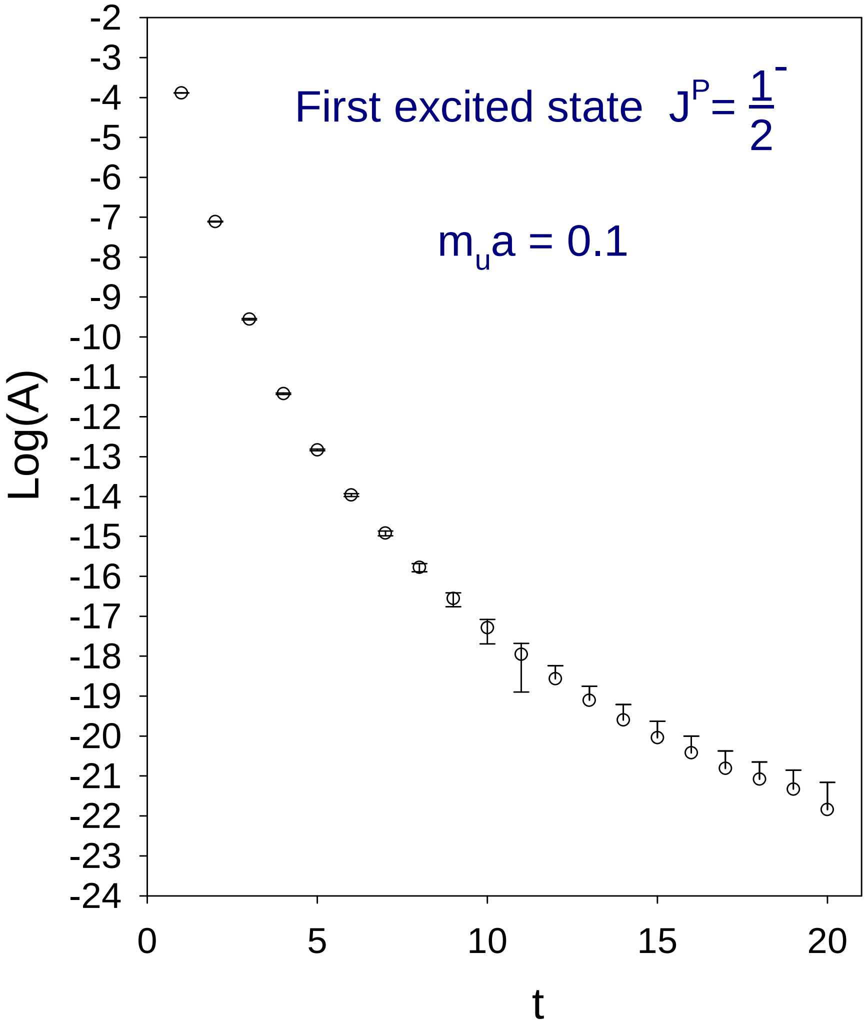


Excited state of Nucleon ($J^P=1/2^-$)
$m_u a = 0.1$
Log(A)
t
-1
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
0
5
10
15
20

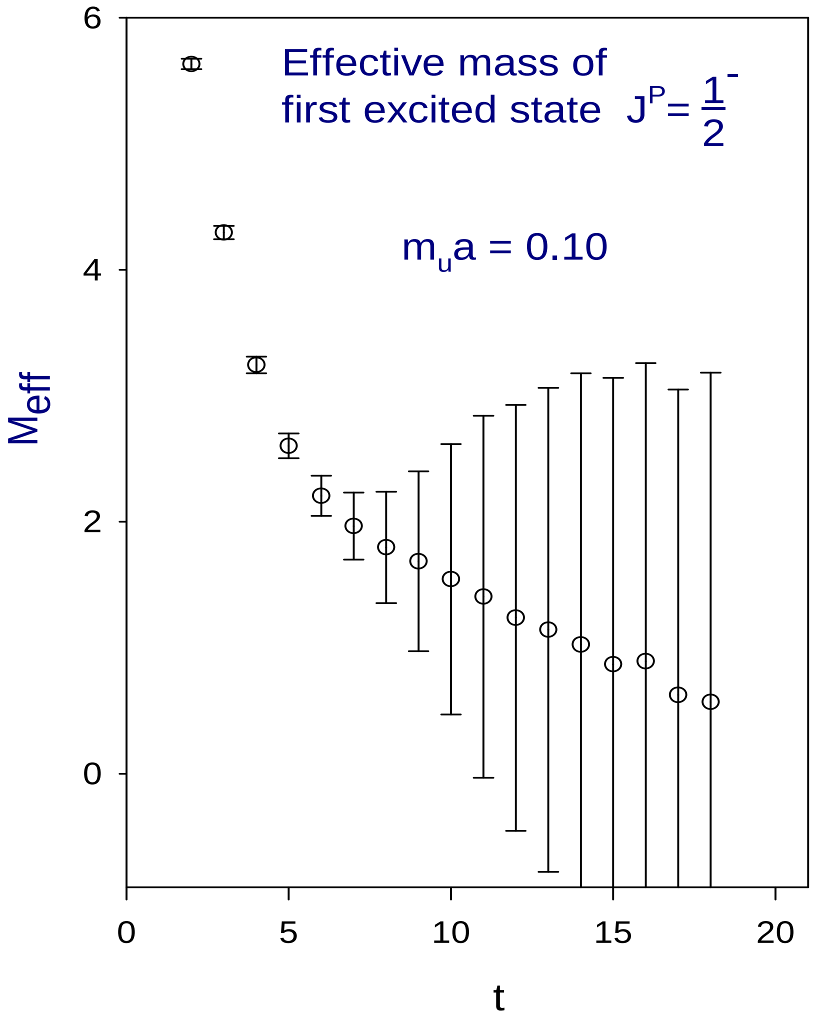

Effective mass of J^P=1/2^-
excited state of Nucleon
m_u a = 0.10
M_eff
t
0
5
10
15
20
1
2
3
4

(3) First Excited State with $J^P = 1/2^-$

The $A^-(t)$ and the effective mass of the first excited state with $J^P = 1/2^-$ are similar to those of the lowest lying state. This rules out the possibility that the negative parity channel of $(udud\bar{s})$ could be a candidate for Θ^+ (with width $<$ 15 MeV).



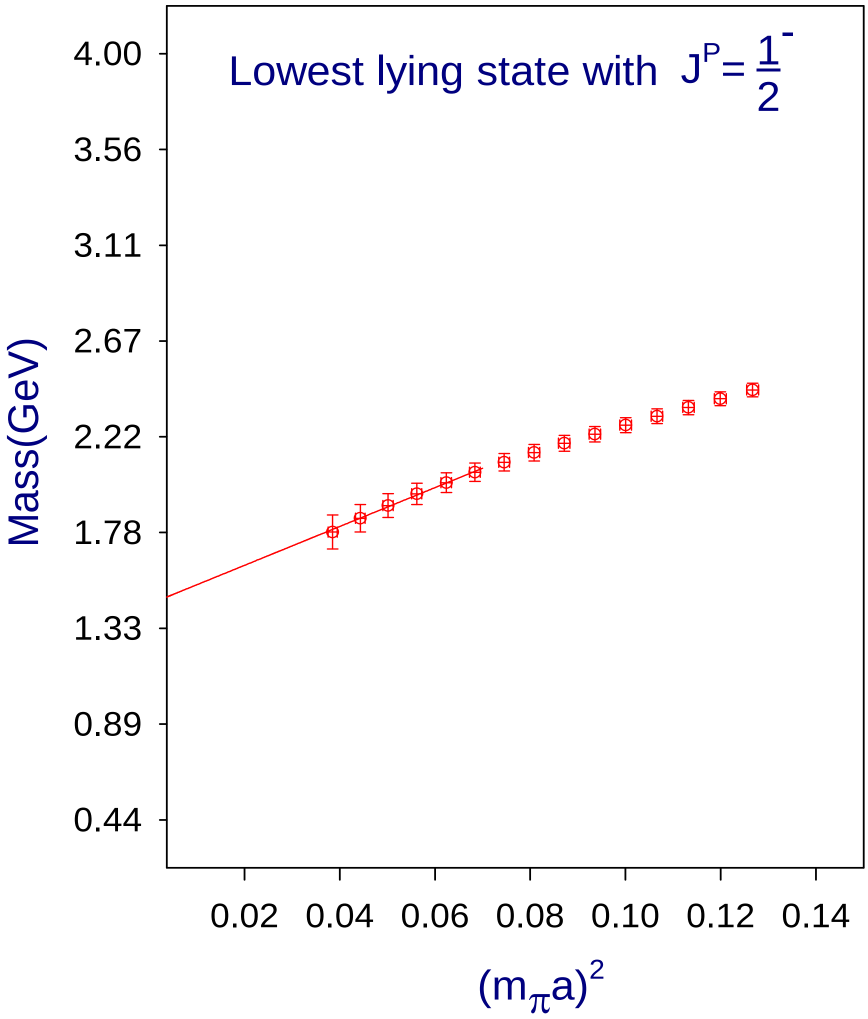
First excited state $J^P = \frac{1}{2}^-$
$m_u a = 0.1$
Log(A)
t
-2
-3
-4
-5
-6
-7
-8
-9
-10
-11
-12
-13
-14
-15
-16
-17
-18
-19
-20
-21
-22
-23
-24
0
5
10
15
20


Effective mass of
first excited state $J^P = \frac{1}{2}^-$
$m_u a = 0.10$
M_{eff}
t
0
2
4
6
0
5
10
15
20

Mass of lowest lying state with $J^P = 1/2^-$

Assuming the mass of a resonance can be estimated by single exp fit to the central region of t where M_{eff} attains a quasi-plateau, one can extract the masses of $J^P = 1/2^-$ states from $\{A^-(t), 10 \le t \le 15\}$.

Using the 4 smallest masses for linear extrap. to $m_\pi = 135$ MeV, we obtain $M_{1/2^-} = 1433(57)$ MeV, which is close to $m_K + m_N = 1430$ MeV. This seems to suggest that it may be a weakly bound two particle system, or even the KN scattering state.

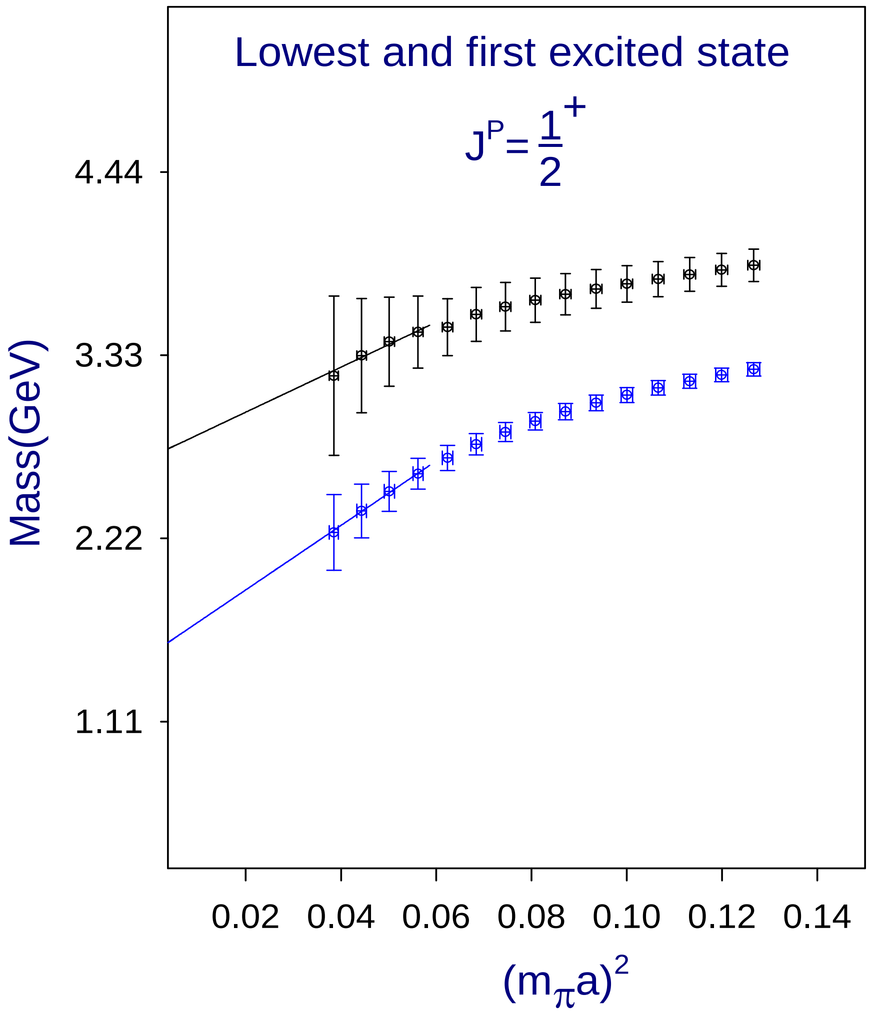

Lowest lying state with $J^P = \frac{1}{2}^-$
4.00
3.56
3.11
2.67
2.22
1.78
1.33
0.89
0.44
Mass(GeV)
0.02
0.04
0.06
0.08
0.10
0.12
0.14
$(m_\pi a)^2$

Masses of lowest lying and 1st excited state with $J^P = 1/2^+$

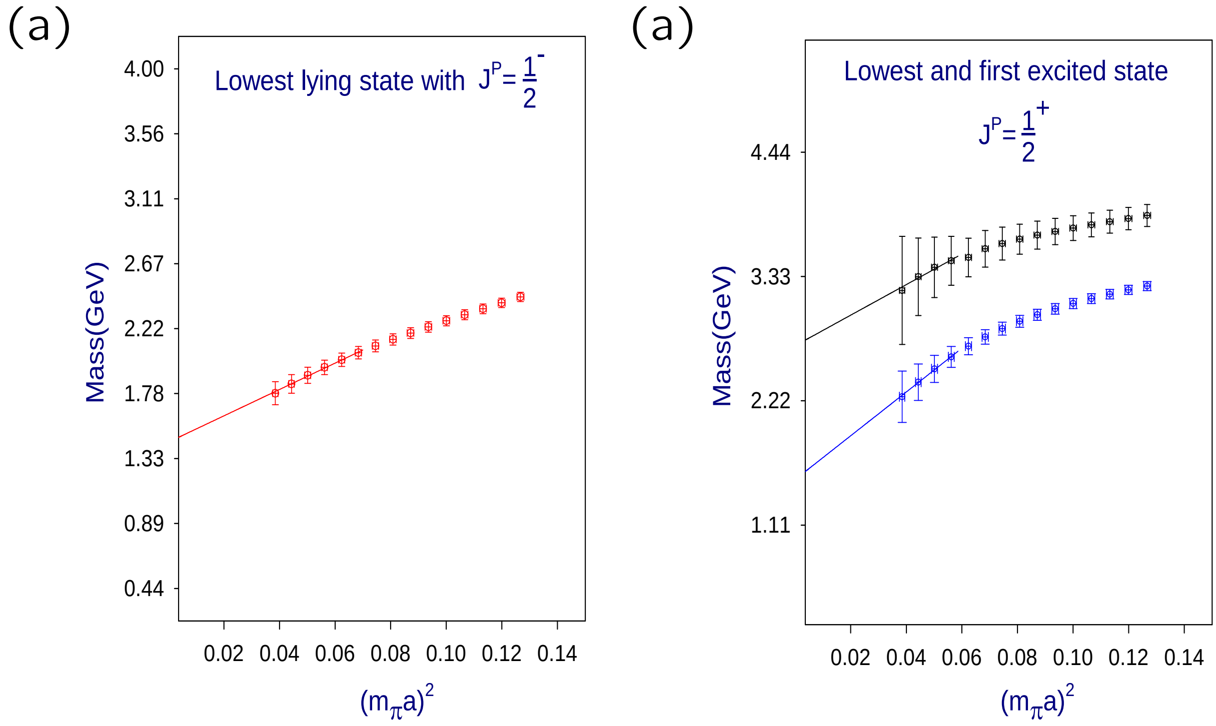
All masses are obtained by single exp fit:
$t \in [8, 13]$ for the lowest lying ones
$t \in [7, 10]$ for the first excited ones

Using the four smallest masses (i.e., with $m_u a = 0.03, 0.035, 0.04, 0.045$) for linear extrapolation to $m_\pi = 135$ MeV, we obtain the mass of the lowest lying $J^P = 1/2^+$ state:

$$M_{1/2^+} = 1583 \pm 121 \text{ MeV}$$



Lowest and first excited state
$J^P = \frac{1}{2}^+$
4.44
3.33
2.22
1.11
Mass(GeV)
0.02
0.04
0.06
0.08
0.10
0.12
0.14
$(m_\pi a)^2$



(a) The masses of the lowest $J^P = 1/2^-$ state. The solid line is the linear fit using four smallest masses. (b) The masses of the lowest and the first excited state with $J^P = 1/2^+$. The solid lines are linear fits using four smallest masses.

Concluding Remarks

Computed 3×3 correl matrix of 3 different interpolating op for Θ^+, and obtain eigenvalues $\{A_i^\pm(t)\}$ for $\pm$ parity.

For $J^P = 1/2^-$ states, $A^-(t)$ deviates from pure exp decay even at large t, and $M_{eff}(t)$ decays monotonically. Thus it cannot be a resonance with narrow decay width, and is ruled out as a candidate of $\Theta^+(1540)$.

For $J^P = 1/2^+$ states, $A^+(t)$ behaves like usual resonances seen in quenched lattice QCD. The mass of the lowest lying $J^P = 1/2^+$ state is determined to be 1583 ± 121 MeV, in agreement with $\Theta^+(1540)$. Whether one can identify this state with $\Theta^+(1540)$ depends on whether its Γ could turn out to be as small as 20 MeV.

The remaining challenge is to determine its decay width, in which the incorporation of dynamical quarks seems to be crucial.