Abstract

We investigate the mass spectrum of Nucleon and Delta (and its counterparts with strange and charm), and their excited states, in quenched lattice QCD with exact chiral symmetry. For each light baryon, we use 23 masses to determine the coefficients of the mass formula in quenched chiral perturbation theory. By chiral extrapolation to $m_{\pi} = 135$ MeV, we obtain $M_N = 958(26)$ MeV, $M_{N^*} = 1553(42)$ MeV, $M_\Delta = 1216(32)$ MeV and $M_{\Delta^*} = 1611(17)$ MeV, which are identified with $N(939)P_{11}$, $N(1535)S_{11}$, $\Delta(1232)P_{33}$ and $\Delta(1620)S_{31}$ respectively. Further, we directly measure the masses of $\Omega^-$, $M_{\Omega} = 1648(60)$ MeV, and its excited state, $M_{\Omega^*} = 1935(48)$ MeV; as well as the triply charmed baryon $\Omega^{++}_{cc}$, $M_{\Omega^{++}_{cc}} = 4931(22)$ MeV, and its excited state, $M_{\Omega^{++}_{cc}^*} = 5185(35)$ MeV.
One of the objectives of lattice QCD is to compute the hadron masses nonperturbatively from the first principles. For hadrons composed of charm and strange quarks (i.e., without $u, d$ light quarks), their masses can be directly measured on presently accessible lattices. However, for hadrons containing $u, d$ light quarks, the performance of the present generation of computers is still quite remote from what is required for computing their masses at the physical scale (e.g., $m_\pi \simeq 135$ MeV), on a lattice with enough sites in each direction such that the discretization errors as well as the finite volume effects are both negligible comparing to the statistical ones. Nevertheless, even with lattices of moderate sizes, lattice QCD can determine the values of the parameters in the hadron mass formulas of the (quenched) chiral perturbation theory. Then one can use these formulas to evaluate the hadron masses at the physical scale, as well as to determine the quark masses.

In this paper, we study spin 1/2 and spin 3/2 baryons containing three quarks of the same mass\(^1\), and obtain their masses for 30 quark masses in the range $0.03 \leq m_q a \leq 0.8$ (i.e., from $m_s/2$ to $m_c$).

For spin 3/2 baryons composed of three strange quarks ($\Omega^-$), and three charm quarks ($\Omega_{ccc}^{++}$), as well as their excited states, we can measure their masses directly on the lattice. Here the strange quark bare mass ($m_s a = 0.06$) and charm quark bare mass ($m_c a = 0.8$) are fixed by requiring the masses of the corresponding vector mesons to agree with the masses of $\phi(1020)$ and $J/\psi(3097)$.

For baryons composed of light quarks, we use 23 masses to determine the coefficients in the baryon mass formula in quenched chiral perturbation theory\(^1\)

\[ M = c_0 + c_1 m_\pi + c_L m_\pi^2 \ln(m_\pi) + c_2 m_\pi^2 + c_3 m_\pi^3 + O(m_\pi^4 \ln m_\pi) \] (1)

Then, extrapolating to the physical pion mass $m_\pi = 135$ MeV, we obtain the masses of $N(1/2^+), N^*(1/2^-), \Delta(3/2^+)$, and $\Delta^*(1/2^-)$ respectively. For our data, we find that we have to set $c_1 = 0$, otherwise the errors of some coefficients would become unacceptable ($> 100\%$). For $\Delta^*$, we also have to set $c_3 = 0$. Evidently, if one can measure more baryon masses in the chiral regime ($m_\pi \ll 2\sqrt{2}\pi f_\pi$), then the coefficients can be determined more precisely. However, one should limit $m_\pi L > 3 \sim 4$, otherwise the baryon masses would suffer from finite size effects, which in turn would lower the reliability of the resulting coefficients. For our lattice of size $20^3 \times 40$ at $\beta = 6.1$, we find that $m_q a \geq 0.03$ gives $m_\pi L > 4$ in the spatial direction, which should be sufficient to suppress the finite size effects.

The interpolating operators for Nucleon and $\Delta$ can be written as

\[ N_{xa} = \epsilon_{abc} u_{xab}^T (C \gamma_5)_{\alpha\beta} d_{x\beta c} u_{xaa} \] (2)

\(^1\)In this paper, we work in the isospin limit, $m_u = m_d$. 

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and
\[ \Delta_{xo; \mu} = \epsilon_{abc} d_{xab}^T (C \gamma_5 \gamma_\mu)_{ab\delta} d_{x\beta c} d_{x\alpha a}, \quad \mu = 1, 2, 3 \] (3)

where \( u \) and \( d \) denote the quark fields, the superscript \( T \) denotes the transpose of the Dirac spinor, \( C \) is the charge conjugation operator, \( \epsilon_{abc} \) is the completely antisymmetric tensor, and \( x, \{a, b, c\} \) and \( \{\alpha, \beta\} \) denote the lattice site, color, and Dirac indices respectively. For \( \Delta(\Delta^*) \), we average over \( \mu = 1, 2, 3 \) to increase the statistics. Note that the “diquark” operator in (3) transforms like a vector, thus the even parity state of (3) can overlap with \( \Delta(3/2^+) \), in which the quarks are in S-wave; while its odd parity state can overlap with \( \Delta^*(1/2^-) \), in which the quarks are in P-wave.

Now it is straightforward to work out the baryon propagator in terms of quark propagators. In lattice QCD with exact chiral symmetry, quark propagator with bare mass \( m_q \) is of the form \( (D_c + m_q)^{-1} \) \[ 3 \], where \( D_c \) is exactly chirally symmetric at finite lattice spacing. In the continuum limit, \( (D_c + m_q)^{-1} \) reproduces \( \left[ \gamma_\mu (\partial_\mu + iA_\mu) + m_q \right]^{-1} \). For optimal domain-wall fermion \[ 2 \] with \( N_s + 2 \) sites in the fifth dimension,

\[
D_c = 2m_0 \frac{1 + \gamma_5 S(H_w)}{1 - \gamma_5 S(H_w)},
\]

\[
S(H_w) = \frac{1 - \prod_{s=1}^{N_s} T_s}{1 + \prod_{s=1}^{N_s} T_s},
\]

\[
T_s = \frac{1 - \omega_s H_w}{1 + \omega_s H_w}, \quad H_w = \gamma_5 D_w,
\]

where \( D_w \) is the standard Wilson Dirac operator plus a negative parameter \(-m_0 \) \( (0 < m_0 < 2) \), and \( \{\omega_s\} \) are a set of weights specified by an exact formula such that \( D_c \) possesses the optimal chiral symmetry \[ 2 \]. Since

\[
(D_c + m_q)^{-1} = (1 - rm_q)^{-1} [D^{-1}(m_q) - r], \quad r = \frac{1}{2m_0}
\]

thus the quark propagator can be obtained by solving the system \( D(m_q)Y = 1 \) with nested conjugate gradient \[ 4 \], which turns out to be highly efficient (in terms of the precision of chirality versus CPU time and memory storage) if the inner conjugate gradient loop is iterated with Neuberger’s double pass algorithm \[ 5 \]. For more details of our scheme of computing quark propagators, see Ref. \[ 6 \].

We generate 100 gauge configurations with Wilson gauge action at \( \beta = 6.1 \) on the \( 20^3 \times 40 \) 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 $\lambda_{\text{min}} = 0.18$ and $\lambda_{\text{max}} = 6.3$, where $\lambda_{\text{min}} \leq \lambda(|H_w|) \leq \lambda_{\text{max}}$ for all gauge configurations. For each configuration, quark propagators are computed for 30 bare quark masses in the range $0.03 \leq m_q a \leq 0.8$, with stopping criteria $10^{-11}$ and $2 \times 10^{-12}$ 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 $2 \times 10^{-11}$

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

and the chiral symmetry breaking due to finite $N_s$ 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 conjugate gradient.

After the quark propagators have been computed, we first measure the pion propagator and its time correlation function, and extract the pion mass ($m_\pi a$) and the pion decay constant ($f_\pi a$). With the experimental input $f_\pi = 132$ MeV, we determine the inverse lattice spacing $a^{-1} = 2.21(3)$ GeV. (Our procedure has been described in Ref. [6].)

Next we compute the nucleon propagator $\langle N_x \bar{N}_y \rangle$ and its time correlation function $C(t)$. Then the average of $C(t)$ over gauge configurations is fitted by the usual formula

$$\frac{1 + \gamma_4}{2} (Z_+ e^{-m_+ a(T-t)} - Z_- e^{-m_- a(T-t)}) + \frac{1 - \gamma_4}{2} (Z_+ e^{-m_+ a(T-t)} - Z_- e^{-m_- a(T-t)})$$

where $m_\pm$ are the masses of even and odd parity states. Thus, one can use parity projector $(1 \pm \gamma_4)/2$ to project out two amplitudes,

$$A_+(t) \equiv Z_+ e^{-m_+ a(T-t)} - Z_- e^{-m_- a(T-t)},$$

$$A_-(t) \equiv Z_+ e^{-m_+ a(T-t)} - Z_- e^{-m_- a(T-t)}.$$

Now the problem is how to extract $m_\pm$ from $A_\pm$ respectively. Obviously, for sufficiently large $T$, there exists a range of $t$ such that, in $A_\pm$, the contributions due to the opposite parity state are negligible. Then $m_\pm$ can be extracted by a single exponential fit to $A_\pm$, for the range of $t$ in which the effective mass $m_{\text{eff}}(t) = \ln(A_\pm(t)/A_\pm(t + 1))$ attains a plateau. On the other hand, if $T$ is not so large, then it may turn out that the heavier mass, say $m_- \text{ (assuming } m_- > m_+)$, could not be easily extracted from $A_-$ due to the non-negligible contributions of the (lowest lying) even parity state. Further, if $T$ is too small, then one even has difficulties to extract the mass of the lowest lying state. For our lattice with $T = 40$, it is sufficiently large to extract both $m_+$ and $m_-$ from $A_+$ and $A_-$ respectively.
In Fig. 1, the nucleon masses of even and odd parity states are plotted versus \((m_{\pi}a)^2\), for \(m_{\pi}\) smaller than the chiral cutoff \(\Lambda_{\chi} = 2\sqrt{2}\pi f_{\pi}\). For the \(J^{\Pi} = 1/2^+\) ground state nucleon, the 23 nucleon masses can be fitted by

\[
M_N a = 0.417(13) - 1.350(168) \times (m_{\pi}a)^2 \ln(m_{\pi}a) + 0.727(134) \times (m_{\pi}a)^2 \\
+ 0.458(144) \times (m_{\pi}a)^3
\]

(4)

with \(\chi^2/\text{d.o.f.} < 0.003\). At the physical pion mass \(m_{\pi} = 135\) MeV (the y-axis), (4) gives \(M_N = 958(26)\) MeV, which is naturally identified with \(N(939)P_{11}\).

For the \(J^{\Pi} = 1/2^-\) excited nucleon, the 23 masses can be fitted by

\[
M_{N^*} a = 0.689(21) - 0.949(291) \times (m_{\pi}a)^2 \ln(m_{\pi}a) + 0.904(236) \times (m_{\pi}a)^2 \\
+ 0.211(250) \times (m_{\pi}a)^3
\]

(5)

with \(\chi^2/\text{d.o.f.} < 0.007\). At \(m_{\pi} = 135\) MeV, (5) gives \(M_{N^*} = 1553(42)\) MeV, which is identified with \(N(1535)S_{11}\).
At this point, it is instructive to examine whether our data of nucleon mass can accommodate the linear term \(c_1 m_\pi\). To this end, we take the square of the nucleon mass, then the higher order terms are further suppressed, and the linear term (if any) would become more prominent, especially at small \(m_\pi a\). In Fig. 2 we plot \((M_N a)^2\) and \((M_N^* a)^2\) versus \((m_\pi a)^2\), which turn out to be well fitted by

\[
(M_N a)^2 = 0.196(9) + 2.388(55) \times (m_\pi a)^2 \quad (6)
\]
\[
(M_N^* a)^2 = 0.5174(192) + 2.829(124) \times (m_\pi a)^2 \quad (7)
\]

Obviously, the term \(c_1 \sqrt{(m_\pi a)^2}\) does not exist in our data of nucleon masses, otherwise, we would see deviations from the fitted lines at small \((m_\pi a)\).

Note that (3) and (4) give \(M_N = 1001(22)\) MeV and \(M_N^* = 1607(30)\) MeV at \(m_\pi = 135\) MeV, in good agreement with the masses of \(N(939)P_{11}\) and \(N(1535)S_{11}\). This seems to justify the ansatz, namely, if the number of
baryon mass data points is too small (e.g., less than 10) and/or the baryon masses are measured only at large quark masses, then they may not feasible for fitting the mass formula (1), however, they still could be used for the linear fit: \((Ma)^2 = A + B(m_\pi a)^2\), which may turn out to provide a good extrapolation to the physical \(m_\pi\).

For recent quenched lattice QCD studies of \(N\) and \(N^*\), see Refs. [7]-[12].

![Figure 3: The \(\Delta\) masses versus the pion mass square, for \(\Delta(J^{\Pi} = 3/2^+)\) and \(\Delta^*(J^{\Pi} = 1/2^-)\) respectively. The solid lines are fits to (1), with \(c_1 = 0\) for \(\Delta\), and with \(c_1 = c_3 = 0\) for \(\Delta^*\).](image)

Next we compute the time correlation function of \(\Delta\), and extract the masses of even and odd parity states.

In Fig. 3 we plot the masses of \(\Delta\) versus \(m_\pi^2\) for even and odd parity states respectively. The lowest lying state has even parity, which implies that it has \(J^{\Pi} = 3/2^+\) since its three quarks are in S-wave, and symmetric in spin. Using (1) with \(c_1 = 0\) to fit the 23 masses of \(\Delta\), we obtain
Figure 4: The Delta mass square versus the pion mass square, for $\Delta(J^\pi = 3/2^+)$ and $\Delta^*(J^\pi = 1/2^-)$ respectively. The solid lines are linear fits.

\[ M_{\Delta} a = 0.530(16) - 1.685(218) \times (m_\pi a)^2 \ln(m_\pi a) + 0.552(176) \times (m_\pi a)^2 \]
\[ + 0.682(187) \times (m_\pi a)^3 \quad (J^\pi = 3/2^+) \] (8)

At $m_\pi = 135$ MeV, (8) gives $M_\Delta = 1216(32)$ MeV, which is identified with $\Delta(1232)_{P33}$.

For the negative parity state $\Delta^*$, its quarks are in P-wave, thus its $J^\pi = 1/2^-$. Using (1) with $c_1 = c_3 = 0$ to fit the 23 masses of $\Delta^*$, we obtain

\[ M_{\Delta^*} a = 0.717(8) - 0.724(34) \times (m_\pi a)^2 \ln(m_\pi a) + 1.156(12) \times (m_\pi a)^2 \] (9)

At $m_\pi = 135$ MeV, (9) gives $M_{\Delta^*} = 1611(17)$ MeV, which is identified with $\Delta(1620)_{S31}$. This is the first lattice QCD determination of the mass of $\Delta(1620)_{S31}$. 
Again, we check the ansatz of baryon mass square versus pion mass square. In Fig. 4, we plot $(M_{\Delta}a)^2$ and $(M_{\Delta^*}a)^2$ versus $(m_\pi a)^2$. They can be fitted by the straight lines:

\[
\begin{align*}
(M_{\Delta}a)^2 &= 0.330(13) + 3.078(87) \times (m_\pi a)^2 \quad [J^H = 3/2^+] \\
(M_{\Delta^*}a)^2 &= 0.536(17) + 3.000(109) \times (m_\pi a)^2 \quad [J^H = 1/2^-]
\end{align*}
\]

At $m_\pi = 135$ MeV, they give $M_{\Delta} = 1292(25)$ MeV and $M_{\Delta^*} = 1635(26)$ MeV, in good agreement $\Delta(1232)P_{33}$ and $\Delta(1620)S_{31}$ respectively.

Finally, we turn to the heavy baryons which can be measured directly on our lattice. Now replacing the down quark in $\Delta^-$ with the strange quark, we have the $\Omega^-$. Similarly, replacing the up quark in $\Delta^{++}$ with the charm quark, we obtain the triply charmed baryon $\Omega^{++}_{ccc}(J^H = 3/2^+)$, which so far has not been discovered in high energy experiments.

To determine the bare masses of strange quark and charm quark, we extract the mass of vector meson from the time correlation function

\[
C_\rho(t) = \frac{1}{3} \sum_{\mu=1}^3 \sum_{\vec{x}} \text{tr}\{\gamma_\mu(D_c + m_q)^{-1}(0, \vec{x})\gamma_\mu(D_c + m_q)^{-1}(x, 0)\}
\]

At $m_q a = 0.06$, the vector meson has mass $M a = 0.4638(32)$, which gives $M = 1025(7)$ MeV, in good agreement with the mass of $\phi(1020)$. Thus, at $m_q a = 0.06$, $\Delta^-$ becomes $\Omega^-$, and its mass can be extracted from the time correlation function. Our result is $M a = 0.746(27)$, which yields

\[
M_{\Omega^-} = 1648(60)\text{MeV}
\]

in good agreement with the mass of $\Omega^-(1672)$.

Similarly, at $m_q a = 0.80$, the vector meson has mass $M a = 1.3830(15)$, which gives $M = 3056(3)$ MeV, in good agreement with the mass of $J/\Psi(3097)$. Thus, at $m_q a = 0.80$, $\Delta^{++}$ actually is $\Omega^{++}_{ccc}$, the triply charmed baryon with $J^H = 3/2^+$, which has not been observed in experiments. However, we can determine its mass from the time correlation function, and our result is $M a = 2.23(1)$, which gives

\[
M_{\Omega^{++}_{ccc}} = 4931(22)\text{MeV} \quad [\text{quark content}=(ccc), \ J^H = 3/2^+]
\]

Also, for the corresponding $J^H = 1/2^-$ excited baryons, our results are

\[
\begin{align*}
M_{\Omega^*} &= 1935(48)\text{MeV} \quad [\text{quark content}=(sss), \ J^H = 1/2^-] \\
M_{\Omega^{++}_{ccc}} &= 5185(35)\text{MeV} \quad [\text{quark content}=(ccc), \ J^H = 1/2^-]
\end{align*}
\]

Note that [13]-[15] are the first lattice QCD predictions for the masses of these baryons. Even though we have not estimated the errors due to quenched approximation, discretization, and finite lattice size, we suspect that the resulting
error in each mass of (13)-(15) is less than 80 MeV. A possible candidate for the $\Omega^*$ in (14) could be the $\Omega^-(2250)$ [13].

Finally we transcribe the bare masses of strange quark ($m_s a = 0.06$) and charm quark ($m_c a = 0.80$) to $\overline{\text{MS}}$ at $\mu = 2$ GeV. Using the lattice renormalization constant $Z_m = Z_s^{-1}$ (where $Z_s$ is the renormalization constant for $\bar{\psi}\psi$) to one loop order [14], we obtain

\begin{align*}
m_{s,\overline{\text{MS}}}(2 \text{ GeV}) &= 114(9) \text{ MeV} \\
m_{c,\overline{\text{MS}}}(2 \text{ GeV}) &= 1520(38) \text{ MeV}
\end{align*}

where the errors are estimates based on the errors of the vector meson masses with respect to $\phi(1020)$ and $J/\Psi(3097)$.

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