Charmed baryons at the physical point in 2 + 1 flavor lattice QCD

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(Received 22 January 2013; published 23 May 2013)

We investigate the charmed-baryon mass spectrum using the relativistic heavy-quark action on 2 + 1 flavor PACS-CS configurations previously generated on a $32^3 \times 64$ lattice. The dynamical up-down- and strange-quark masses are tuned to their physical values, reweighted from those employed in the configuration generation. At the physical point, the inverse lattice spacing determined from the Ω baryon mass gives $a^{-1} = 2.194(10)$ GeV, and thus the spatial extent equals $L = 32a = 2.88(1)$ fm. Our results for the charmed-baryon masses are consistent with experimental values, except for the mass of Ξ_{cc}, which has been measured by only one experimental group so far and has not been confirmed yet by others. In addition, we report values of other doubly and triply charmed baryon masses, which have never been measured experimentally.

DOI: 10.1103/PhysRevD.87.094512 PACS numbers: 12.38.Gc

I. INTRODUCTION

Recently, a lot of new experimental results have been reported on charmed baryons [1]. *BABAR* and Belle collaborations have given very accurate results based on their precise analyses. In addition, new experiments such as J-PARC, PANDA, LHCb, and Belle II are expected to give further information on charmed baryons.

The mass spectrum of singly charmed baryons has been determined experimentally with high accuracy. The experimental status of the masses of the ground states is evaluated as being three- or four-star by the Particle Data Group. The excited states have also been investigated fairly well.

In contrast to singly charmed baryons, experimental data for doubly and triply charmed baryons are not well established. A candidate for the doubly charmed baryon, Ξ_{cc}, was reported by the SELEX Collaboration [2] but has not been confirmed yet by *BABAR* [3] and Belle [4]. Further experimental and theoretical confirmations are required to establish Ξ_{cc}. No other doubly charmed baryons or triply charmed baryons have been observed by experiments. In this situation, lattice QCD predictions for the doubly and triply charmed-baryon masses will provide useful information for the experimental discovery of these states.

In lattice QCD, the charmed-baryon spectrum has been mainly investigated using gauge configurations generated with 2 + 1 flavors of dynamical staggered quarks [5–8]. In this case, the choice for light valence quarks requires special care. One may take a fermion formulation other than the staggered for the valence light quarks (the mixed action) to avoid problems due to the complicated flavor structure of staggered quarks. Alternatively, one may construct charmed-baryon operators with the valence naive quark and then rewrite the correlation function of these operators in terms of the staggered propagators [9]. Both approaches violate unitarity of the theory at finite lattice spacing, in addition to the rooting problem of dynamical staggered quarks. Therefore, it is necessary to check their results using other combinations of dynamical and valence quarks, which maintain unitarity at nonzero lattice spacings. Another issue with the existing calculations on dynamical staggered configurations is that the chiral extrapolation suffers from large higher-order corrections. Next-to-leading-order (NLO) SU(2) heavy-baryon chiral perturbation theory is employed to extrapolate data taken at the pion mass of 220–290 MeV to the physical point, but the result shows bad convergence even at $m_\pi = 220$ MeV. A calculation directly at the physical quark masses without chiral extrapolation is the best way to remove this uncertainty.

There are several investigations with other fermion formulations. S. Dürr *et al.* calculated charmed omega baryon masses using smeared improved Wilson and Brillouin fermions for valence strange and charm quarks [10]. Their calculation was performed at single quark mass ($m_\pi = 280$ MeV) and single lattice spacing ($a = 0.07$ fm) on the $N_f = 2$ $O(a)$-improved Wilson quark ensemble. They obtained a result that is consistent with the experimental value for the singly charmed omega baryon (Ω_c) mass.

The ETM Collaboration has studied charmed baryons on ensembles generated with $N_f = 2$ dynamical twisted-mass quarks, employing the same twisted-mass fermion for degenerate up and down valence quarks and Osterwalder-Seiler fermions for strange and charm valence quarks [11]. For a doubly charmed baryon, they found $m_{\Xi_{cc}} = 3.513(23)(14)$ GeV. This is the only lattice QCD result that is consistent with the SELEX experimental value $m_{\Xi_{cc}}^{\mathrm{SELEX}} = 3.519(1)$ GeV, while other results from lattice QCD show deviation from this value. Reasons for this disagreement among lattice QCD results must be understood and should be resolved. One possible source of systematic uncertainties in the ETM Collaboration calculation is a lattice artifact caused by the heavy charm-quark mass at their lattice spacings, $a = 0.09 - 0.06$ fm. Indeed, their results for charmed-baryon masses, especially for $m_{\Omega_{ccc}}$, do not show clear scaling behaviors. To reduce this uncertainty, one must employ a heavy-quark action that allows control over mass-dependent lattice artifacts within the formulation, such as the Fermilab action [12], the relativistic heavy-quark action [13,14], or the highly improved actions. Chiral extrapolation of ETM Collaboration data from $m_\pi = 260$ MeV using the NLO heavy-baryon chiral perturbation theory is another source of systematic uncertainties, as in the case with staggered quarks.

In Ref. [15], we have shown that the charm-quark mass corrections are under control at $a^{-1} = 2.194(10)$ GeV for the relativistic heavy-quark action of Ref. [13]. It removes the leading cutoff errors of $O((m_Q a)^n)$ and the next-to-leading effects of $O((m_Q a)^n (a\Lambda_{\mathrm{QCD}}))$ for arbitrary order n by tuning a finite number of parameters. Employing this action for the charm quark, we investigated the properties of mesons involving charm quarks with the 2 + 1 dynamical flavor PACS-CS configurations on a $32^3 \times 64$ lattice [16] reweighted to the physical point for up-, down-, and strange-quark masses. We found that our results for charmed meson masses are consistent with experiments at a percent level, and so are those for the decay constants with a few percent accuracy, although our results are obtained at a single lattice spacing. By fixing the charm-quark mass with the spin-averaged $1S$ state of the charmonium, $m(1S) = 3.067(1)(14)$ GeV, which reproduces the experimental value, $M(1S)^{\mathrm{exp}} = 3.068$ GeV [1], we obtained the charmonium hyperfine splitting, $m_{J/\psi} - m_{\eta_c} = 0.1080(14)$GeV. This value underestimates the recent experimental value, $M_{J/\psi}^{\mathrm{exp}} - M_{\eta_c}^{\mathrm{exp}} = 0.1126(8)$ GeV [17], by 4%. Since other lattice QCD calculations show a trend that the hyperfine splitting increases as the lattice spacing decreases, the deviation is expected to become smaller in the continuum limit. Similarly, we calculated the mass differences between charmed mesons and charmonium, for example, $2m_D - m_{J/\psi} = 0.648(20)$ GeV, which agrees with the experimental value, $2M_D^{\mathrm{exp}} - M_{J/\psi}^{\mathrm{exp}} = 0.633$ GeV.

Encouraged by this result, we have extended our investigation to the charmed-baryon sector, for which the results are reported in the present paper. A notable advantage of our investigation over the previous calculations is that the chiral extrapolation is not necessary, since our calculations are performed at the physical point; we are free from the convergence problem of the heavy-baryon chiral perturbation theory. We compare our results for the masses of singly charmed baryons with the corresponding experimental values to check if our method works also for the baryon sector. We then evaluate the doubly and triply charmed baryon spectra, which constitute our predictions. A part of this work has been reported in Ref. [18].

This paper is organized as follows. Section II explains our method and simulation parameters. Section III describes our results for the singly charmed baryon spectrum and comparison with experiments. In Sec. IV, we present our results for doubly and triply charmed baryon masses. Our conclusion is given in Sec. V.

II. SETUP

Our investigation is based on a set of 2 + 1 flavor dynamical lattice QCD configurations generated by the PACS-CS Collaboration [16] on a $32^3 \times 64$ lattice using the nonperturbatively $O(a)$-improved Wilson quark action with $c_{\mathrm{SW}}^{\mathrm{NP}} = 1.715$ [19] and the Iwasaki gauge action [20] at $\beta = 1.90$. The aggregate of 2000 MD time units was generated at the hopping parameter given by $(\kappa_{\mathrm{ud}}^0, \kappa_s^0) = (0.13778500, 0.13660000)$, and 80 configurations separated by 25 MD time units were selected for our calculations. We then reweight those configurations to the physical point given by $(\kappa_{\mathrm{ud}}, \kappa_s) = (0.13779625, 0.13663375)$. It decreases the ud-quark mass by 24%, and the strange-quark mass by 4%. The reweighting shifts the masses of π and K mesons from $m_\pi = 152(6)$ MeV and $m_K = 509(2)$ MeV to $m_\pi = 135(6)$ MeV and $m_K = 498(2)$ MeV, with the cutoff at the physical point estimated to be $a^{-1} = 2.194(10)$ GeV from the Ω baryon mass. An alternative determination of the lattice spacing using the Sommer scale r_0 gives a consistent value, $a_{r_0}^{-1} = 2.182(38)$ GeV [21]. Our parameters and statistics at the physical point are given in Table I.

The relativistic heavy-quark action [13] is designed to reduce cutoff errors of $O((m_Q a)^n)$ with arbitrary order n to $O(f(m_Q a)(a\Lambda_{\mathrm{QCD}})^2)$, once all of the parameters in the

TABLE I. Simulation parameters. MD time is defined as the number of trajectories multiplied by the trajectory length.

β	κ_{ud}	κ_{s}	configuration	MD time
1.90	0.13779625	0.13663375	80	2000

TABLE II. Parameters for the relativistic heavy-quark action.

κ_{charm}	ν	r_s	c_B	c_E
0.10959947	1.1450511	1.1881607	1.9849139	1.7819512

action are determined nonperturbatively, where $f(m_Q a)$ is an analytic function around the massless point $m_Q a = 0$. The action is given by

$$S_Q = \sum_{x,y} \bar{Q}_x D_{x,y} Q_y, \tag{2.1}$$

$$\begin{aligned} D_{x,y} = \delta_{xy} - \kappa_Q \sum_i [(r_s - \nu\gamma_i) U_{x,i} \delta_{x+\hat{i},y} \\ + (r_s + \nu\gamma_i) U^\dagger_{x,i} \delta_{x,y+\hat{i}}] - \kappa_Q [(1-\gamma_4) U_{x,4} \delta_{x+\hat{4},y} \\ + (1+\gamma_4) U^\dagger_{x,4} \delta_{x,y+\hat{4}}] - \kappa_Q \Big[c_B \sum_{i,j} F_{ij}(x) \sigma_{ij} \\ + c_E \sum_i F_{i4}(x) \sigma_{i4} \Big] \delta_{xy}. \end{aligned} \tag{2.2}$$

The parameters r_s, c_B, c_E, and ν have been tuned in Ref. [15]. It should be noticed that, while perturbative estimates are used for r_s, c_B, and c_E [22], the parameter ν is determined nonperturbatively to reproduce the relativistic dispersion relation for the spin-averaged $1S$ state of the charmonium. The charm-quark hopping parameter κ_{charm} is set to reproduce the experimental value of the mass for the spin-averaged $1S$ state. With the value in Table II, we obtain $m(1S) = 3.067(1)(14)$ GeV [15], which agrees with the experimental value, $M(1S)^{\mathrm{exp}} = 3.068$ GeV [1]. The reweighting influences the tuning of charm-quark mass very little, because it is only mildly dependent on sea-quark masses. Our parameters for the relativistic heavy-quark action are summarized in Table II.

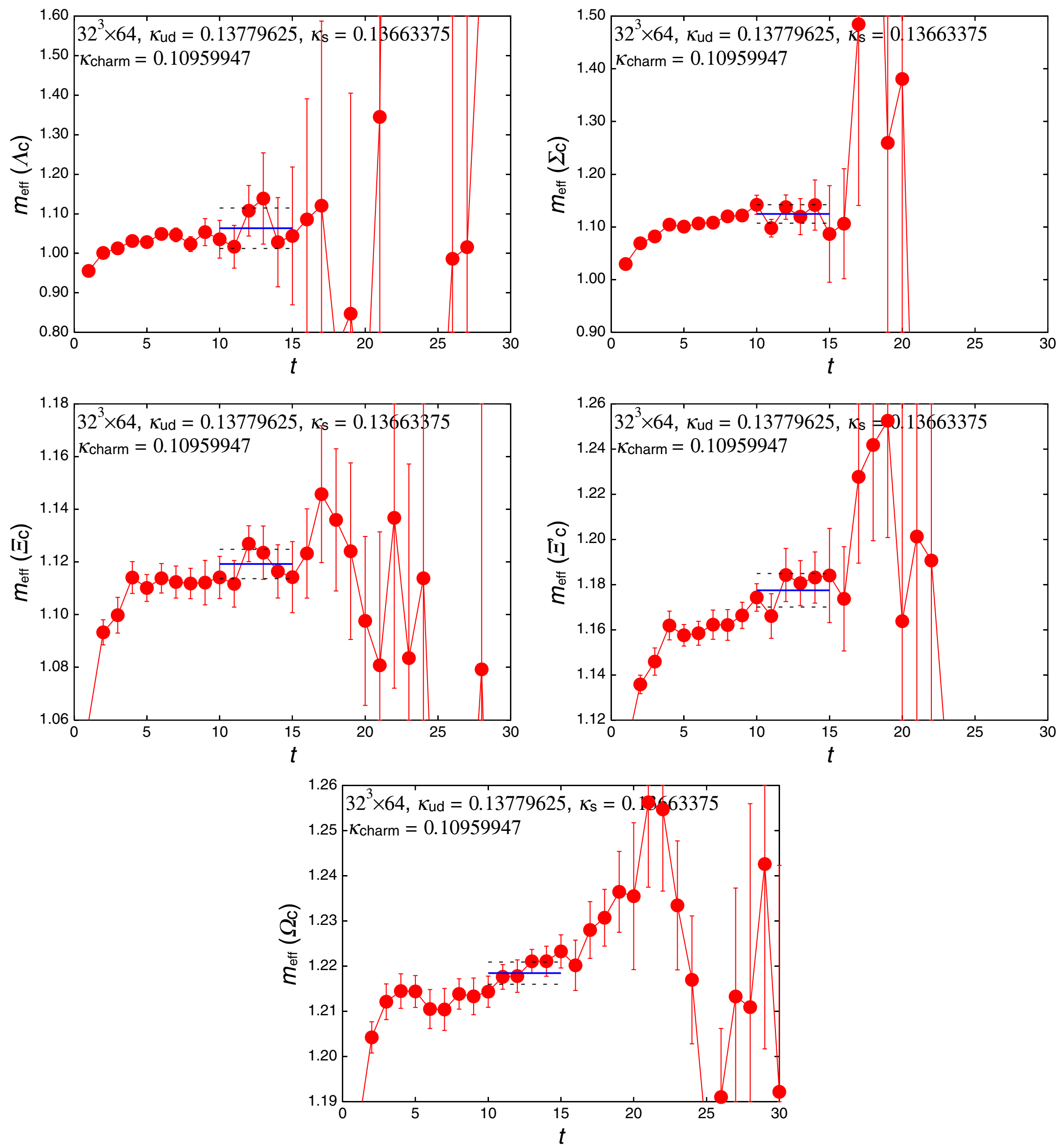

FIG. 1 (color online). Effective masses of $J = 1/2$ singly charmed baryons.

We employ the relativistic operators for charmed baryons as they are natural for the relativistic heavy-quark action used in our calculations. Charmed baryons can be classified under $4 \times 4 \times 4 = 20 + 20_1 + 20_2 + \bar{4}$. In addition to a $J = 3/2$ decuplet-type 20-plet, there are $J = 1/2$ octet-type 20-plet and $\bar{4}$-plet.

The $J = 1/2$ octet-type baryon operators are given by

$$O^{fgh}_{\alpha}(x) = \epsilon^{abc}((q^a_f(x))^T C\gamma_5 q^b_g(x))q^c_{h\alpha}(x), \tag{2.3}$$

$$C = \gamma_4\gamma_2, \tag{2.4}$$

where f, g, and h are quark flavors and a, b, and c are quark colors. The index $\alpha = 1, 2$ labels the z component of the spin. The Σ-type and Λ-type are distinguished as

$$\Sigma\text{-type:} \quad -\frac{O^{[fh]g} + O^{[gh]f}}{\sqrt{2}}, \tag{2.5}$$

$$\Lambda\text{-type:} \quad \frac{O^{[fh]g} - O^{[gh]f} - 2O^{[fg]h}}{\sqrt{6}}, \tag{2.6}$$

where $O^{[fg]h} = O^{fgh} - O^{gfh}$.

The decuplet-type $J = 3/2$ baryon operators are expressed as

$$D^{fgh}_{3/2}(x) = \epsilon^{abc}((q^a_f(x))^T C\Gamma_+ q^b_g(x))q^c_{h1}(x), \tag{2.7}$$

$$D^{fgh}_{1/2}(x) = \epsilon^{abc}[((q^a_f(x))^T C\Gamma_0 q^b_g(x))q^c_{h1}(x) - ((q^a_f(x))^T C\Gamma_+ q^b_g(x))q^c_{h2}(x)]/3, \tag{2.8}$$

$$D^{fgh}_{-1/2}(x) = \epsilon^{abc}[((q^a_f(x))^T C\Gamma_0 q^b_g(x))q^c_{h2}(x) - ((q^a_f(x))^T C\Gamma_- q^b_g(x))q^c_{h1}(x)]/3, \tag{2.9}$$

$$D^{fgh}_{-3/2}(x) = \epsilon^{abc}((q^a_f(x))^T C\Gamma_- q^b_g(x))q^c_{h2}(x), \tag{2.10}$$

$$\Gamma_{\pm} = (\gamma_1 \mp i\gamma_2)/2, \qquad \Gamma_0 = \gamma_3. \tag{2.11}$$

Two-point functions for these charmed-baryon operators are calculated with exponentially smeared sources and a local sink. The smearing function is given by $\Psi(r) = A\exp(-Br)$ at $r \neq 0$ and $\Psi(0) = 1$. We set $A = 1.2$, $B = 0.07$ for the ud quark, $A = 1.2$, $B = 0.18$ for the strange quark, and $A = 1.2$, $B = 0.55$ for the charm quark. The number of source points is eight per configuration, and polarization states are averaged over to reduce statistical fluctuations. Statistical errors are analyzed by the jackknife method with a bin size of 100 MD time units (four configurations), as in the light quark sector [16]. We extract charmed-baryon masses by fitting two-point functions with a single exponential form. Figures 1–3 show our effective masses. We take the fitting interval for charmed baryons as far as possible away from the origin,

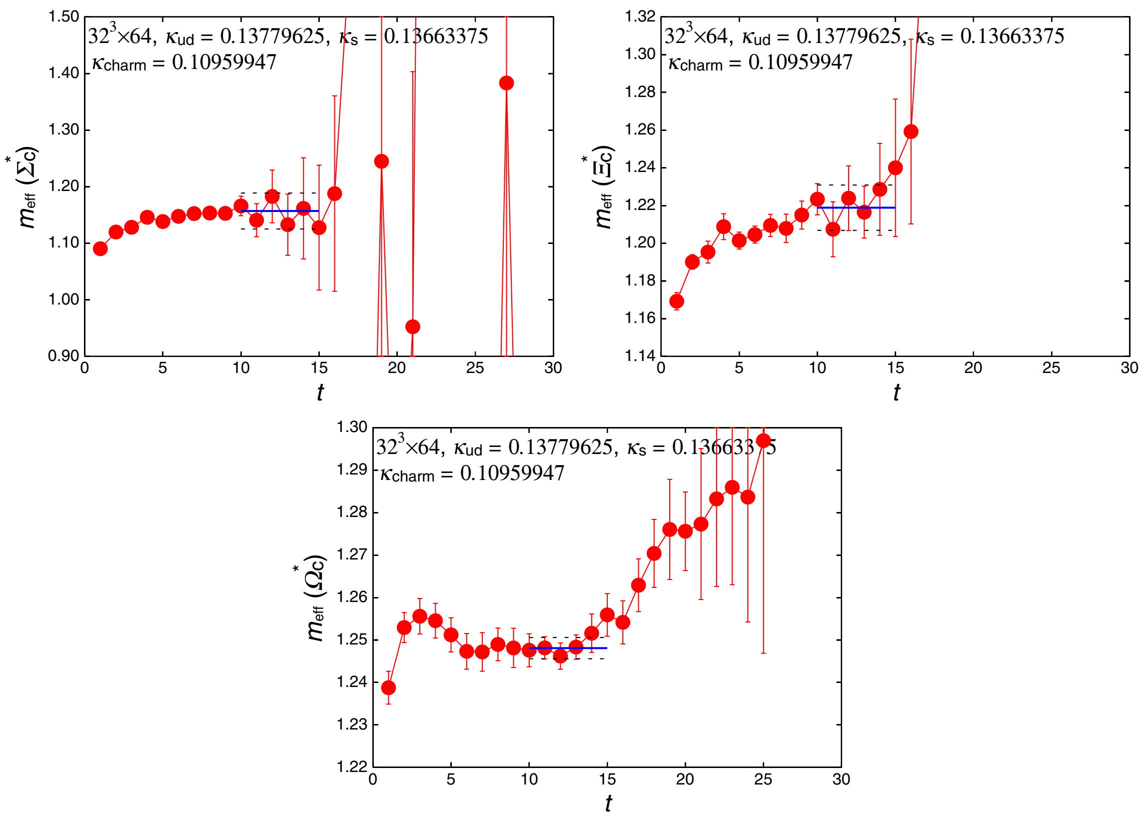

FIG. 2 (color online). Effective masses of $J = 3/2$ singly charmed baryons.

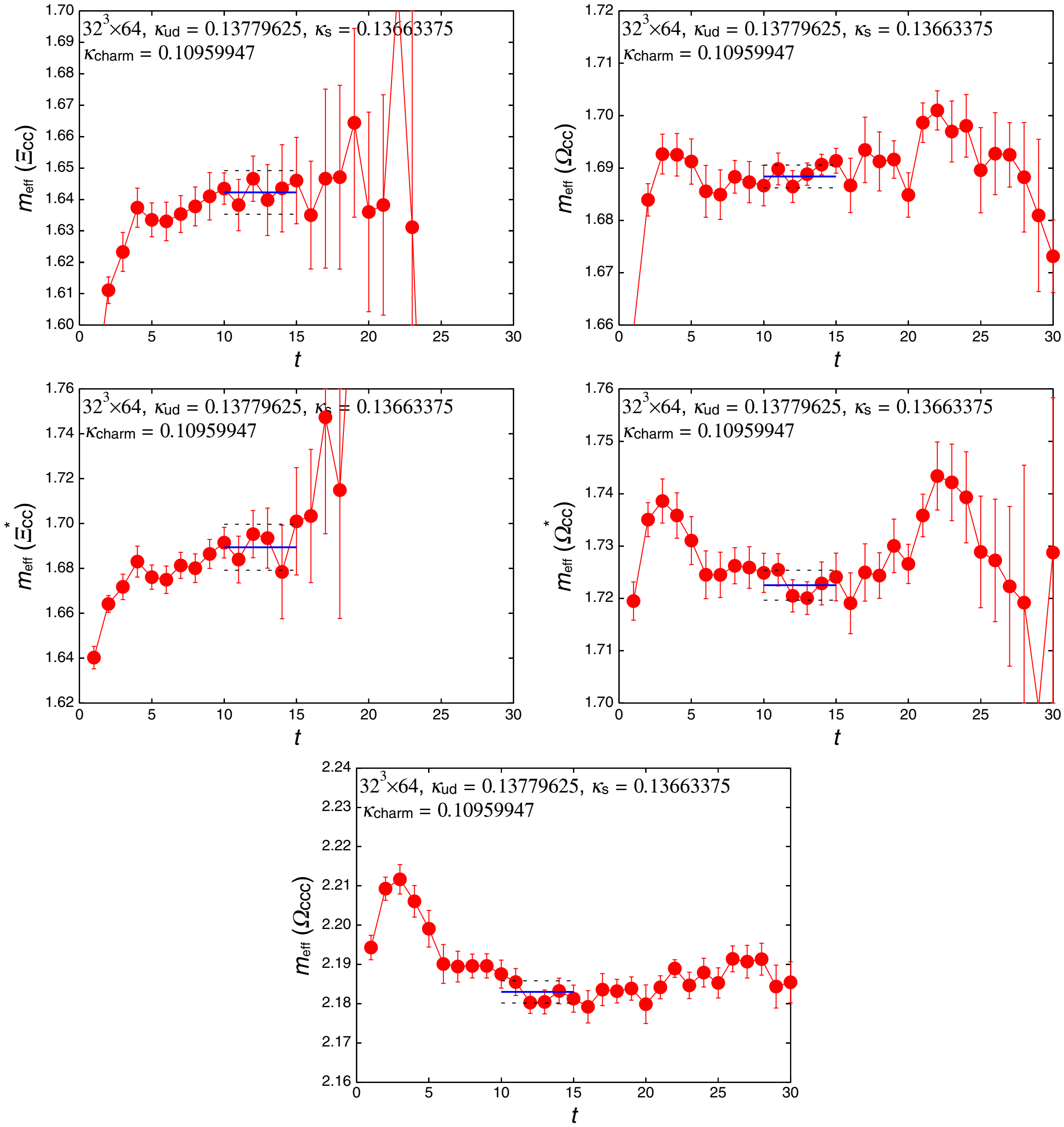

FIG. 3 (color online). Effective masses of doubly and triply charmed baryons.

$[t_{min}, t_{max}] = [10, 15]$, to avoid possible contaminations from excited states. The charmed-baryon masses are converted into the physical unit by multiplying M_Ω^{exp}/m_Ω. Our results are compiled in Tables III and IV.

III. SINGLY CHARMED BARYON SPECTRUM

Our result for the singly charmed baryon spectrum at the physical point is summarized in Fig. 4. All of our values for the charmed-baryon masses are predictions from lattice QCD, since the physical charm-quark mass has already been fixed by the mass for the spin-averaged $1S$ charmonium state, and no other experimental inputs are required for calculating the charmed-baryon masses. We note that several systematic errors have not been fully evaluated yet for these results. First, finite size effects are not taken into account. The NLO heavy-baryon chiral perturbation theory predicts that finite-size effects for charmed baryons are less than 1%. Higher-order terms may give significant contributions, however. In addition, we may need a formulation that goes beyond p-regime heavy-baryon chiral perturbation theory, because of the smallness of our $m_\pi L \sim 2$. A direct confirmation in lattice QCD by comparing spectra among different lattice volumes is desirable. Second, strong decays such as $\Sigma_c \rightarrow \Lambda_c \pi$ are not taken into account in our analysis, since $\Sigma_c \rightarrow \Lambda_c \pi$ is kinematically prohibited on our lattice volume. Last but not least, our results are obtained at a single lattice spacing without

TABLE III. Our results for singly charmed baryon masses. The first error is statistical, and the second is from the scale determination. Experimental values from PDG [1] are also listed.

	J^P	(I, S, C)	Lattice	Experiment
m_{Λ_c} [GeV]	$\frac{1}{2}^+$	(0,0,1)	2.333(112)(10)	2.286(0)
m_{Σ_c} [GeV]	$\frac{1}{2}^+$	(1,0,1)	2.467(39)(11)	2.454(0)
m_{Ξ_c} [GeV]	$\frac{1}{2}^+$	$(1/2, -1, 1)$	2.455(12)(11)	2.471(1)
$m_{\Xi'_c}$ [GeV]	$\frac{1}{2}^+$	$(1/2, -1, 1)$	2.583(16)(11)	2.578(3)
m_{Ω_c} [GeV]	$\frac{1}{2}^+$	$(0, -2, 1)$	2.673(5)(12)	2.695(2)
$m_{\Sigma_c^*}$ [GeV]	$\frac{3}{2}^+$	(1,0,1)	2.538(70)(11)	2.519(1)
$m_{\Xi_c^*}$ [GeV]	$\frac{3}{2}^+$	$(1/2, -1, 1)$	2.674(26)(12)	2.646(1)
$m_{\Omega_c^*}$ [GeV]	$\frac{3}{2}^+$	$(0, -2, 1)$	2.738(5)(12)	2.766(2)

TABLE IV. Our results for doubly and triply charmed baryon masses. The first error is statistical, and the second is from the scale determination. An experimental value from SELEX [2] is also listed.

	J^P	(I, S, C)	Lattice	Experiment
$m_{\Xi_{cc}}$[GeV]	$\frac{1}{2}^+$	$(1/2, 0, 2)$	3.603(15)(16)	(3.519(1))
$m_{\Omega_{cc}}$[GeV]	$\frac{1}{2}^+$	$(0, -1, 2)$	3.704(5)(16)	$\cdots$
$m_{\Xi_{cc}^*}$[GeV]	$\frac{3}{2}^+$	$(1/2, 0, 2)$	3.706(22)(16)	$\cdots$
$m_{\Omega_{cc}^*}$[GeV]	$\frac{3}{2}^+$	$(0, -1, 2)$	3.779(6)(17)	$\cdots$
$m_{\Omega_{ccc}}$[GeV]	$\frac{3}{2}^+$	(0,0,3)	4.789(6)(21)	$\cdots$

continuum extrapolation. Although a naive order counting gives a percent level of cutoff effects from $O(\alpha_s^2 f(m_Q a) \times (a\Lambda_{\mathrm{QCD}}), f(m_Q a)(a\Lambda_{\mathrm{QCD}})^2)$ terms in the relativistic heavy-quark action, the continuum extrapolation is necessary to remove this uncertainty. Additional calculations should be performed in the future to remove all systematic errors mentioned above.

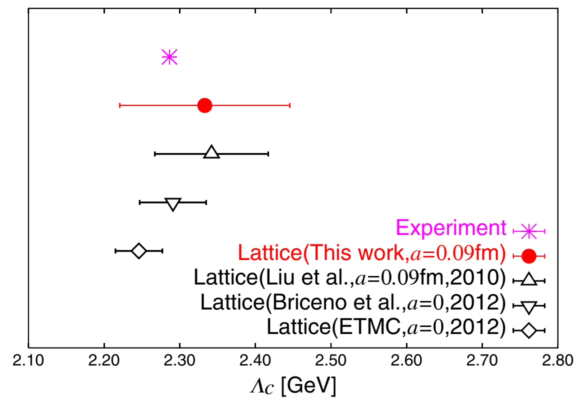

FIG. 5 (color online). Comparison of Λ_c mass. The results of Briceno *et al.* [7] and the ETM Collaboration [11] include systematic errors such as those associated with the continuum extrapolation, while those of this work and Liu *et al.* [6] give statistical errors only.

As can be seen from Fig. 4, our prediction for the singly charmed baryon spectrum in lattice QCD at a single lattice spacing is in reasonable agreement with the experimental one. In Fig. 5, we also compare our value for Λ_c with other results obtained in recent lattice QCD simulations using the dynamical staggered quarks [5–7], and the twisted mass quarks [11]. All results are consistent with each other, although the statistical error is larger for our result due to the conservative choice of our fitting interval.

Figure 6 displays mass differences. Our results are consistent with experimental values within 2 σ uncertainty. These agreements indicate that the decomposition of $J = 1/2$ Σ-type and Λ-type baryons, as well as that of $J = 3/2$ and $J = 1/2$ charmed baryons, have been made successfully in our calculation.

IV. DOUBLY AND TRIPLY CHARMED BARYON SPECTRUM

For doubly and triply charmed baryons, an experimental value has been reported only for Ξ_{cc}, and the experimental

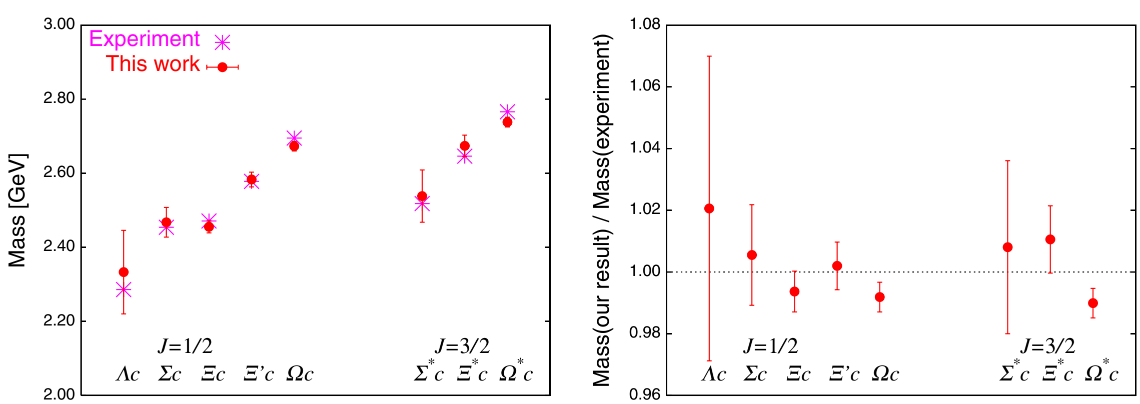

FIG. 4 (color online). Our results for the singly charmed baryon spectrum (left panel) and those normalized by the experimental values (right panel).

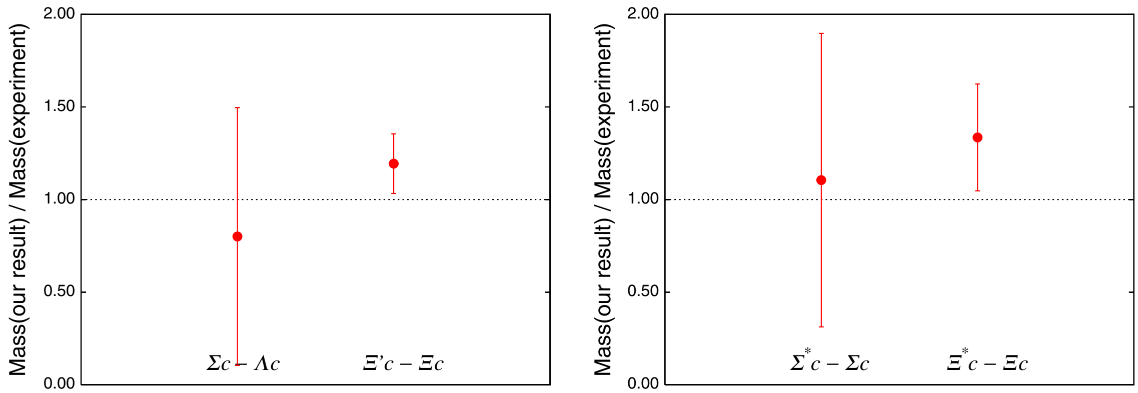

FIG. 6 (color online). Comparison of mass differences of $\Sigma_c - \Lambda_c$ types (left panel) and $\Sigma_c^* - \Sigma_c$ types (right panel).

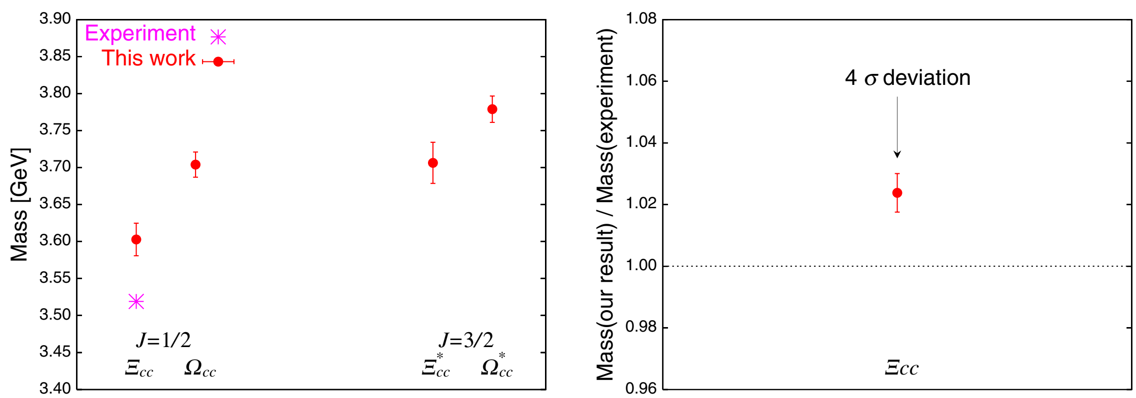

FIG. 7 (color online). Our results for the doubly charmed baryon spectrum (left panel) and those normalized by the experimental value (right panel).

status is controversial. In the other channels, the lattice QCD result gives predictions before experimental mass measurements.

Figure 7 shows our results for the doubly charmed baryons. Our estimate for $m_{\Xi_{cc}}$ clearly deviates from the experimental value by the SELEX Collaboration [2]. The difference is 4σ, as shown in the right figure. Our result for $m_{\Xi_{cc}}$ is consistent with results from other lattice QCD calculations except the ETM Collaboration, as shown in Fig. 8. This discrepancy needs to be understood and should be resolved.

Similarly, Fig. 9 displays lattice QCD results for the triply charmed baryon from several groups. Our prediction agrees with that by others except the ETM Collaboration. A marginal discrepancy is observed between our value and that of Ref. [8] for $m_{\Omega_{ccc}} - 3/2m_{J/\psi}$ mass difference (the right figure).

For a more detailed comparison, the precise evaluation of all systematic errors are required. In particular, the

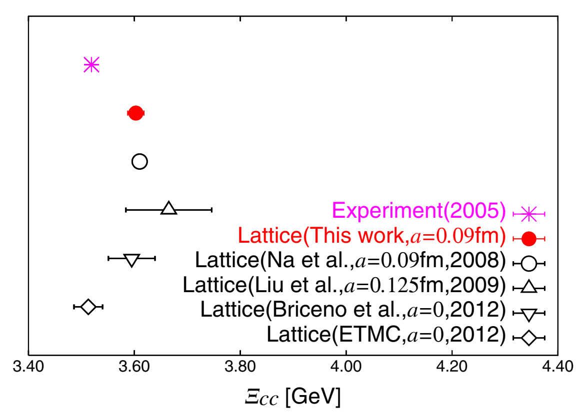

FIG. 8 (color online). Comparison of Ξ_{cc}. The results of Briceno *et al.* [7] and the ETM Collaboration [11] include systematic errors such as those associated with the continuum extrapolation, while those of this work, Na *et al.* [5], and Liu *et al.* [6] give statistical errors only.

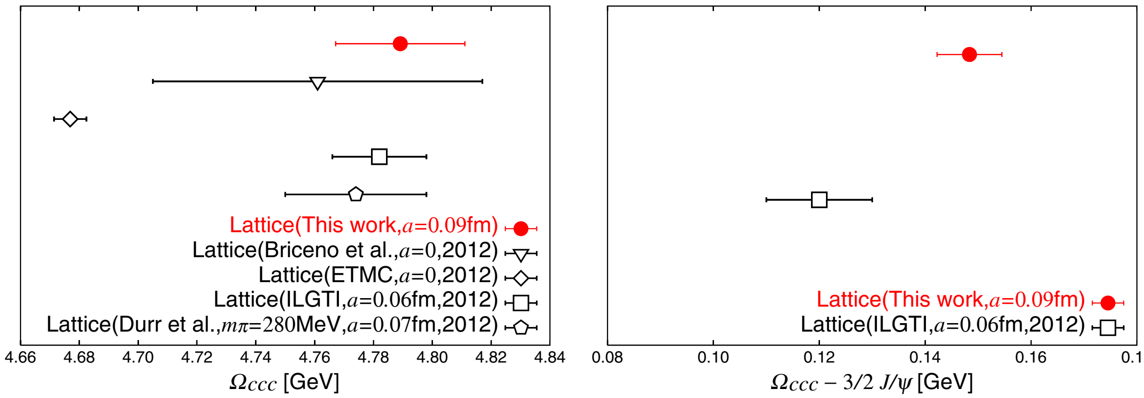

FIG. 9 (color online). Comparison of Ω_{ccc} (left panel) and $\Omega_{ccc} - 3/2J/\psi$ (right panel). The results of Briceno *et al.* [7] and the ETM Collaboration [11] include systematic errors such as those associated with the continuum extrapolation, while those of this work, ILGTI [8], and Dürr *et al.* [10] give statistical errors only.

largest source of systematic errors for our calculation is the lattice artifact, which should be removed by the continuum extrapolation.

V. CONCLUSIONS

We have studied the charmed-baryon spectrum in $N_f = 2 + 1$ dynamical lattice QCD at a lattice spacing of $a^{-1} = 2.194(10)$ GeV. The reweighting technique allows us to perform mass measurements directly at the physical point. This avoids systematic errors associated with chiral extrapolations in charmed-baryon masses, which prevented previous lattice QCD calculations from predicting precise values for charmed-baryon masses.

Our results for the mass spectrum of singly charmed baryons are consistent with experiment within 2 σ uncertainty. This confirms that we are able to control charm-quark mass corrections successfully, not only in the meson sector [15] but also in the baryon sector, by use of the relativistic heavy-quark action of Ref. [13].

We then extract predictions for doubly charmed baryons. Our result for $m_{\Xi_{cc}}$ is consistent with values of other lattice QCD calculations employing the dynamical staggered quarks but disagree with the estimation by the ETM Collaboration. Moreover, our Ξ_{cc} mass is different from the SELEX experimental value, approximately by 85 MeV, which corresponds to a 4σ deviation. A similar deviation between the ETM Collaboration and our result is also observed in the triply charmed baryon mass, $m_{\Omega_{ccc}}$. Precise estimations of all systematic errors, especially the lattice artifacts, are required to resolve these discrepancies.

ACKNOWLEDGMENTS

Y. N. thanks Yasumichi Aoki, Carleton DeTar, and Nilmani Mathur for valuable discussions and Stephan Dürr for his comment on this manuscript. Numerical calculations for the present work have been carried out on the PACS-CS computer under the "Interdisciplinary Computational Science Program" of the Center for Computational Sciences, University of Tsukuba. This work is supported in part by Grants-in-Aid of the Ministry of Education, Culture, Sports, Science and Technology (MEXT)-Japan (Grants No. 18104005, No. 20340047, No. 20540248, No. 21340049, No. 22244018, and No. 24540250), the Grants-in-Aid for Scientific Research on Innovative Areas (Area No. 2004: Grants No. 20105001, No. 20105002, No. 20105003, and No. 20105005), and SPIRE (Strategic Program for Innovative REsearch).

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