Finite-Size Effect in Lattice QCD Hadron Spectroscopy

M. Fukugita,(1) H. Mino,(2) M. Okawa,(3) and A. Ukawa(4)

(1)*Research Institute for Fundamental Physics, Kyoto University, Kyoto 606, Japan*
(2)*Faculty of Engineering, Yamanashi University, Kofu 400, Japan*
(3)*National Laboratory for High Energy Physics (KEK), Ibaraki 305, Japan*
(4)*Institute of Physics, University of Tsukuba, Ibaraki 305, Japan*
(Received 4 September 1991)

A hadron spectrum calculation with two light dynamical quark flavors was carried out with the Kogut-Susskind quark action at $\beta=5.7$ on lattices of spatial size 8^3, 12^3, and 20^3 for $m_q=0.01$ and 0.02 in lattice units, with emphasis given to a systematic study of the finite-lattice-size effect. It is found that hadron masses on a 16^3 spatial lattice at this β still suffer from a significant finite-lattice effect at least for $m_q=0.01$, showing the importance of a quantitative control over the finite-size effect in comparing simulation results with the experimental hadron masses even for a fairly large lattice. A comparison is also made to the analytic prediction for the finite-size effect from chiral perturbation theory.

PACS numbers: 12.38.Gc

A lattice QCD calculation of the hadron mass spectrum with dynamical quarks [1] requires prodigious computing resources, and the largest computing facilities have been invested towards this goal [2–4]. In spectrum calculations the most fundamental systematic errors arise from finite lattice spacing and from finite extent of the lattice. In the calculations carried out to date the dominant effort is therefore made on the largest possible lattice size at the largest possible value of $\beta=6/g^2$, with which it is hoped that the errors of these origins are reasonably small. As-yet insufficient computing power, however, makes a systematic survey of these effects difficult, and, in particular, little has been studied so far in regard to the finite-size effect.

For the purpose of elucidating those effects we have been carrying out spectroscopic calculations with a variety of values of the coupling constant ranging from $\beta=5.4$ to 5.7 and of lattice sizes from 4^4 to 20^4 with the Kogut-Susskind (KS) staggered fermion action for two effective quark flavors. In this Letter we report on the result for $\beta=5.7$ for the lattice sizes of $8^3\times16$, 12^4, and 20^4, for which we made the most extended runs. For the 16^3 spatial lattice we adopt the high statistics data obtained by the Columbia University group on a $16^3\times32$ lattice [3].

The dynamical effects of two degenerate flavors of quarks are incorporated by the hybrid R algorithm with the even-odd decimation trick [5]. We work with the quark masses of $m_q=0.01$ and 0.02 in lattice units. The molecular-dynamics step size [6] is chosen to be $\delta\tau=0.01$ for $m_q=0.01$ and $\delta\tau=0.02$ for $m_q=0.02$ (we take the normalization of $\delta\tau$ of Ref. [5]). Iterations are made for $\tau\sim600$–1000 for each lattice size with one trajectory corresponding to $\tau=1$. The periodic boundary condition is imposed for quarks and gluons in all four directions. The KS fermion operator D is inverted with the conjugate gradient method, taking $\|\xi-D^\dagger Dx\|^2/3V<10^{-8}$ as the stopping condition [6] with V the space-time lattice volume. The gauge configurations are stored at every $\tau=5$, and hadron propagators are calculated on a lattice doubled or tripled in the time direction. For hadron operators we use the standard local form [7] for π, ρ, and the nucleon (N), adopting the notation [7] π(PS), π(SC), ρ(VT), and ρ(PV) to distinguish the flavor quantum numbers for mesons [we shall denote π(PS) and ρ(VT) simply as π and ρ below]. We also calculate the mass of Δ using the nonlocal operators of Ref. [8]. Two kinds of wall sources [9] are employed: For π and Δ the wall with unit value assigned to all sites on the time slice $t=0$ is taken, and for the other hadrons the unit source is placed on all sites at $t=0$ with even coordinates. These choices are made to enhance the signal-to-noise ratio in hadron propagators. Gauge links are fixed to the Landau gauge on the entire lattice, and those on the wall are further fixed to the Coulomb gauge.

In Fig. 1 we show the effective mass $m_{\rm eff}(t)$ for π, ρ, and N on a $20^3\times40$ lattice at $m_q=0.01$. These are obtained by fitting the propagator at two (π) or four (ρ,N) successive time slices starting at t with a single (π) or double (ρ,N) exponential taking into account the period-

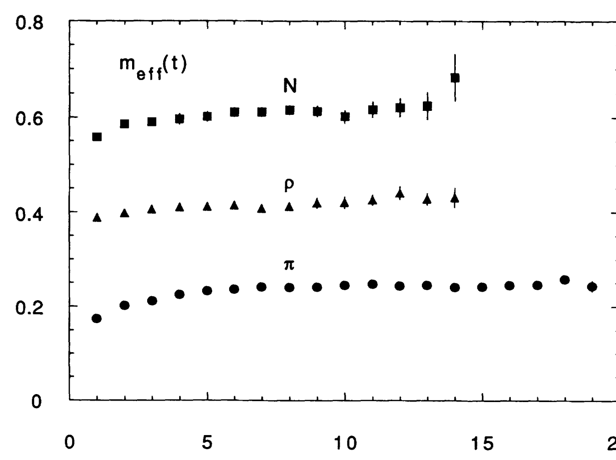

FIG. 1. Effective mass $m_{\rm eff}(t)$ for π, ρ, and nucleon (N) on a $20^3\times40$ lattice at $\beta=5.7$ and $m_q=0.01$.

TABLE I. Hadron masses in lattice units on a $20^3\times(20\times2)$ lattice for $\beta=5.7$. The molecular-dynamics time interval for propagator average is $\tau=250$–950 for $m_q=0.01$ and $\tau=200$–700 for $m_q=0.02$. The bin size for a jackknife error analysis is $\tau=50$. Local operators are used for π, ρ, nucleon (N), and its negative parity partner (N^-). The notation for meson flavor channels follows that of Ref. [7] with $\pi\equiv\pi(\mathrm{PS})$ and $\rho\equiv\rho(\mathrm{VT})$. The first row for Δ is obtained with the nonlocal operator (6.2) of Ref. [8] and the second row through (6.3). The chiral order parameter $\langle\bar{\chi}\chi\rangle$ is normalized so that it approaches $1/m_q$ as $m_q\to\infty$.

	$m_q=0.01$	$m_q=0.02$
m_π	0.244(3)	0.344(3)
$m_{\pi(\mathrm{SC})}$	0.279(5)	0.391(3)
m_ρ	0.417(7)	0.494(5)
$m_{\rho(\mathrm{PV})}$	0.414(11)	0.502(6)
m_N	0.611(10)	0.748(7)
m_{N^-}	0.728(17)	0.970(29)
m_Δ	0.712(38)	0.811(26)
	0.657(15)	0.799(19)
m_π/m_ρ	0.587(7)	0.697(7)
m_N/m_ρ	1.466(18)	1.515(17)
$\langle\bar{\chi}\chi\rangle$	0.02751(13)	0.04865(19)

ic boundary condition and the KS sign factors. Reasonable plateaus are observed for $t\geq8$ (π), $t\geq4$ (ρ), and $t\geq6$ (N), and a wiggle is not apparent in $m_{\mathrm{eff}}(t)$, at least not one as conspicuous as that reported in Ref. [2]. We then extract the hadron masses by a χ^2 fit using the full covariance matrix with a single exponential for $t\geq8$ for the pion in the PS channel, and with two exponentials including the opposite parity state for $t\geq6$ for the other hadrons. The result is given in Table I. The errors are calculated with the jackknife method choosing the bin size of $\tau=50$ where the jackknife errors level off.

In Fig. 2(a) the lattice-size dependence of the meson masses is plotted for $m_q=0.01$ with the data for the spatial size $L=16$ supplemented by the work of Ref. [3]. We see a continuous decrease of both m_π and m_ρ up to $L=20$. In particular, the pion mass drops by 3% (3σ) from $L=16$ to 20, and the ρ mass by 8% (5σ). A more conspicuous decrease is seen in the nucleon mass [Fig. 2(b)]; the decrease from $L=16$ to 20 amounts to 12% (8σ). We also note that the splitting of the negative parity partner (N^-) of the nucleon, expected for spontaneously broken chiral symmetry [10], is observed only for $L\geq16$, and the mass ratio m_{N^-}/m_N increases by 4% from $L=16$ to 20. The plot of mass ratios m_N/m_ρ vs $(m_\pi/m_\rho)^2$ for our data with $L=20$ is shown in Fig. 3, together with the data of Ref. [3] for the size $L=16$ taken at the same $\beta=5.7$. Compared with the latter, our m_N/m_ρ is smaller by 4% at $m_q=0.01$ and the decrease may still be non-negligible at $m_q=0.02$ although a definite conclusion is difficult due to the irregular variation of the data of Ref. [3] for $m_q=0.015$–0.025. The combined plot suggests that a substantial part of the up-

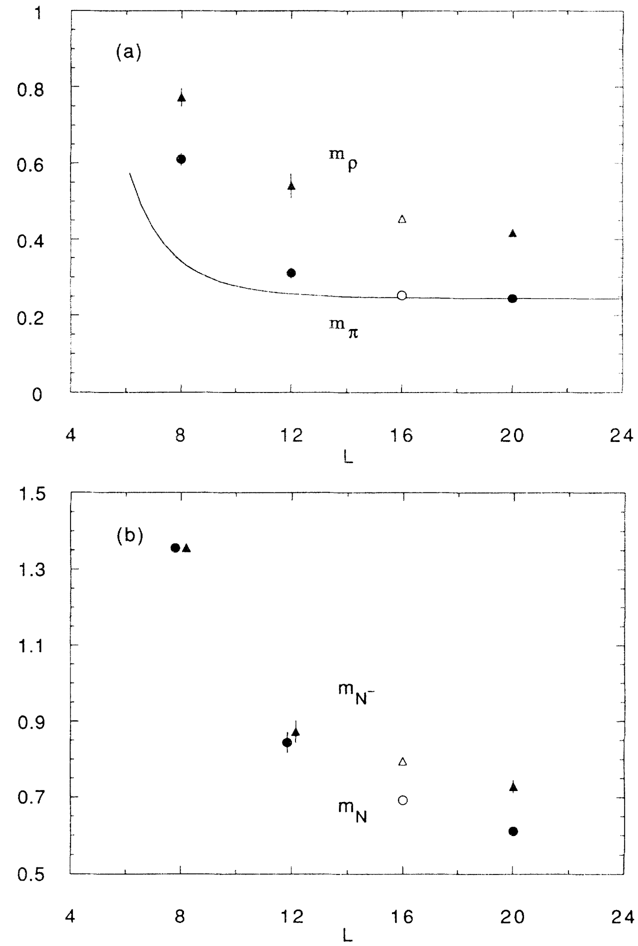

FIG. 2. (a) Meson masses at $\beta=5.7$ and $m_q=0.01$ as a function of the spatial lattice size L. Solid curve is the prediction from chiral perturbation theory for the pion mass (see text). (b) Spatial size dependence of the mass of the nucleon (N) and its parity partner (N^-). The open symbols at $L=16$ are the data of the Columbia University group [3].

ward shift of simulation data relative to the empirical curves is caused by the finite-size effect [12]. From this finding we should conclude that the understanding of the finite-size behavior, in addition to the proper control over the finite-lattice-spacing effect, is indispensable should one extract the continuum values of the hadron masses at the few-percent level.

It may be interesting to compare the finite-size effect seen here with that predicted in chiral perturbation theory [13,14]. In Fig. 2(a) we added the predicted curve [Eq. (26) in the first paper of Ref. [14]] for the pion for the case of $SU(2)\times SU(2)$ chiral symmetry using the value of m_π measured for the spatial size $L=20$ to set the scale and the pion decay constant $f_\pi=0.0403$ in lattice units as determined below. While chiral perturbation theory correctly predicts that m_π decreases with the lattice size, the amount of decrease is less than that seen in the actual simulation data.

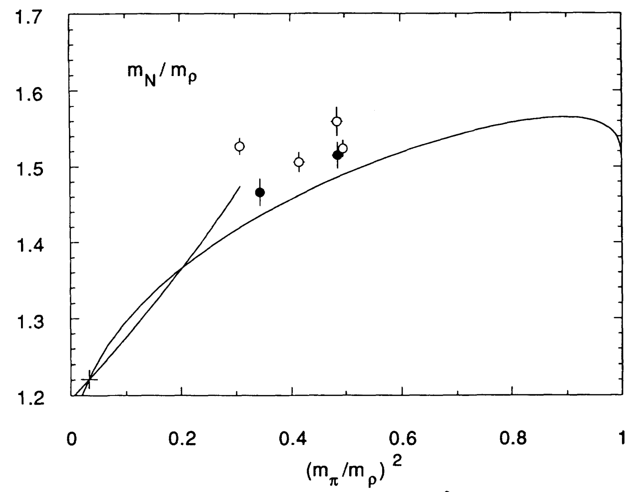

FIG. 3. Mass ratio m_N/m_ρ vs $(m_\pi/m_\rho)^2$ at $\beta=5.7$ for two dynamical flavors of KS fermions. Solid circles are our data for the spatial size $L=20$, while open ones are those of Ref. [3] with $L=16$. Solid curve on the left which is drawn up to 0.3 of the horizontal axis shows the prediction of chiral perturbation theory, and the other curve that runs across the figure is from the empirical quark-model mass formula including hyperfine splitting [11]. The experimental point is marked by a cross.

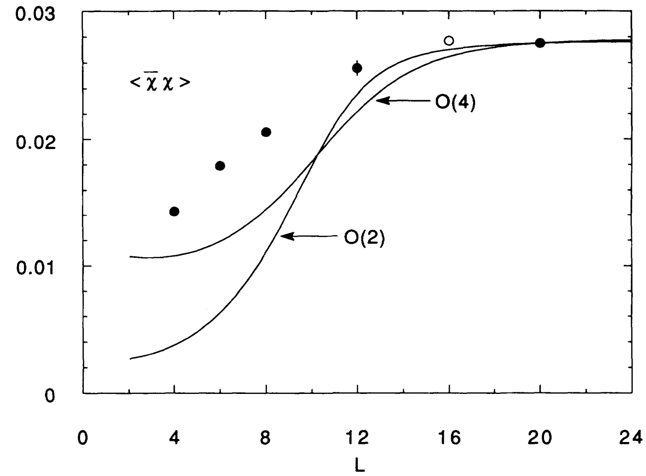

FIG. 4. Chiral order parameter as a function of the lattice size L for $m_q=0.01$ at $\beta=5.7$. Data at $L=4$ and 6 are obtained on 4^4 and 6^4 lattices, and the one at $L=16$ is taken from Ref. [3]. Solid curves are the prediction of chiral perturbation theory for O(2) and O(4) symmetries (see text).

We now discuss some other aspects of hadron spectroscopy with the data on a $20^3\times 40$ lattice. The mass of the pion in the PS channel associated with the U(1) chiral symmetry of the KS fermion satisfies very well the relation expected from PCAC (partial conservation of axial-vector current); if we fit the two points for $m_q=0.01$ and 0.02, we obtain $m_\pi^2=0.0011(28)+5.86(20)m_q$. The constant term is consistent with zero within errors, and is at least smaller by an order of magnitude than that quoted by the Columbia University group [3]. We are then able to extract the pion decay constant f_π with the aid of $f_\pi=[3m_q\langle\bar{\chi}\chi\rangle_{m_q=0}/2m_\pi^2]^{1/2}$, which gives $f_\pi=0.0403(12)$, where we used $\langle\bar{\chi}\chi\rangle=0.00636(32)+2.114(23)m_q$ obtained from our data. If we take the inverse lattice spacing $a^{-1}=2.27(10)$ GeV, determined by the $m_q=0$ extrapolation of the ρ meson mass $[m_\rho=0.340(16)+7.70(90)m_q]$, we find $f_\pi=92(3)$ MeV.

The pion in the SC channel is heavier than π(PS) by 14% at both $m_q=0.01$ and 0.02, which shows the effect of flavor symmetry breaking of the KS fermion at a finite lattice spacing. The mass squared extrapolated to $m_q=0$ $[m_{\pi(\mathrm{SC})}^2=0.0031(65)+7.48(40)m_q]$ is consistent with zero, however, as is the case with the Nambu-Goldstone pion π(PS) discussed above. The flavor degeneracy is considerably better for the ρ meson, for which the masses from the VT and PV channels are degenerate within errors.

For the nucleon our data yield $m_N=0.474(22)+13.7(1.3)m_q$, giving $a^{-1}=1.98(9)$ GeV at $m_q=0$. We have also calculated the mass of Δ with the operators (6.2) and (6.3) of Ref. [8]. The values we obtained are systematically larger than that for the nucleon, supporting that these operators in fact represent the Δ wave function. For $m_q=0.01$, the Δ-N mass difference is 100–200 MeV with a^{-1} determined from m_ρ. Our data, however, are too poor to extrapolate to the physical quark mass.

The chiral condensate $\langle\bar{\chi}\chi\rangle$ for $m_q=0.01$ is shown in Fig. 4 as a function of the lattice size L. The decrease towards smaller sizes reflects the fact that spontaneous breakdown of chiral symmetry does not occur for small volumes. The figure shows a smooth increase with the lattice size and an appreciable size effect at least up to $L=16$. In this figure we also plotted the curve predicted from chiral perturbation theory [Eq. (35) in the second paper of Ref. [14]] with the parameters given above. Here we present curves both for the O(4)=SU(2)$\times$SU(2) and the O(2) cases, since the identification of the effective symmetry group is ambiguous. Neither of them, however, lends a good fit to the simulation result. It is possible that the pion mass in our simulation is still too large relative to the other hadron masses to apply the analysis of chiral perturbation theory. The same comment also applies to the pion mass discussed above.

In conclusion, we have demonstrated that a proper understanding of finite-size effects is important not only for phase-transition analyses at finite temperatures [15] but also for spectroscopy carried out close to the continuum limit. A lattice size of $La\sim 1.4$ fm corresponding to $L=16$ with $a^{-1}=2.27$ GeV at $\beta=5.7$ is clearly insufficient, and even $La\sim 1.8$ fm for $L=20$ may not be sufficient especially for the nucleon mass, for which at least a 2% accuracy is required for further progress. We also failed to confirm the validity of the predictions from analytic formula for the finite-size effect. Full details of the present calculation will be published elsewhere.

The numerical computation was made on HITAC

S820/80 at KEK. This work is supported in part by the Grant-in-Aid of the Ministry of Education (No. 03640270).

[1] For some earlier attempts, see M. Fukugita, Y. Oyanagi, and A. Ukawa, Phys. Rev. Lett. **57**, 953 (1986); Phys. Rev. D **36**, 824 (1987); M. Campostrini *et al.*, Phys. Lett. B **193**, 78 (1987); H. Hamber, Phys. Lett. B **193**, 292 (1987); S. Gottlieb *et al.*, Phys. Rev. D **38**, 2245 (1988).

[2] K. M. Bitar *et al.*, Phys. Rev. D **42**, 3794 (1990).

[3] F. R. Brown *et al.*, Phys. Rev. Lett. **67**, 1062 (1991); H. Chen, in *Lattice 90* [Nucl. Phys. B (Proc. Suppl.) **20**, 370 (1991)].

[4] R. Gupta *et al.*, Phys. Rev. D **44**, 3272 (1991).

[5] S. Gottlieb *et al.*, Phys. Rev. D **35**, 2537 (1987).

[6] The systematic errors due to our choice of the step size and conjugate gradient accuracy are not detected beyond statistical fluctuations. Our test runs on a 16^4 lattice produced results consistent with those of Ref. [3] which used a smaller step size and a more stringent stopping condition.

[7] K. C. Bowler *et al.*, Nucl. Phys. **B284**, 299 (1987).

[8] M. F. L. Golterman and J. Smit, Nucl. Phys. **B255**, 328 (1985).

[9] G. W. Kilcup, in *Lattice 89* [Nucl. Phys. B (Proc. Suppl.) **17**, 201 (1990)]; R. Gupta *et al.*, Los Alamos Report No. LA-UR-90-3050, 1990 (to be published).

[10] C. DeTar and J. B. Kogut, Phys. Rev. D **36**, 2828 (1987).

[11] S. Ono, Phys. Rev. D **17**, 888 (1978).

[12] Our m_N/m_ρ are lower than those of Ref. [2] obtained at $\beta=5.6$ on 12^4 and 16^4 lattices. Since the physical lattice sizes for the two simulations are similar, we think that the difference is more likely to be caused by the finite-lattice-spacing effect rather than the finite-lattice-size effect.

[13] M. Lüscher, Commun. Math. Phys. **104**, 177 (1986).

[14] J. Gasser and H. Leutwyler, Phys. Lett. B **184**, 83 (1987); **188**, 477 (1987); P. Hasenfratz and H. Leutwyler, Nucl. Phys. **B343**, 241 (1990).

[15] M. Fukugita, H. Mino, M. Okawa, and A. Ukawa, Phys. Rev. Lett. **65**, 816 (1990).