Results of a systematic lattice QCD simulation with two degenerate flavors of sea quarks, identified as dynamical \( u \) and \( d \) quarks, are presented. The simulation was performed on a dedicated parallel computer, called CP-PACS, developed at the University of Tsukuba. Clear dynamical quark effects are observed in the light hadron mass spectrum and in the light quark masses: In the light hadron mass spectrum, major parts of the discrepancy between quenched QCD and experiment are shown to be removed by introducing two flavors of dynamical quarks. For the averaged mass of \( u \) and \( d \) quarks, 

\[
    m_{\text{MS}}^{ud}(2\text{GeV}) = 3.44^{+0.14}_{-0.25}\text{MeV}
\]

using the \( \pi \) and \( \rho \) meson masses as physical input, and for the \( s \) quark mass, we obtain 

\[
    m_{\text{MS}}^{s}(2\text{GeV}) = 88^{+4}_{-6}\text{MeV or } 90^{+5}_{-11}\text{MeV}
\]

with the \( K \) or \( \phi \) meson mass as additional input. These values are about 20–30% smaller than the previous estimates in the quenched approximation. We also discuss the \( U(1) \) problem and \( B \) meson decay constants.

1 Introduction

CP-PACS is a dedicated parallel computer designed and developed at the University of Tsukuba for simulations in the physics of fields. With 2048 node processors interconnected with a three-dimensional hypercrossbar network, the CP-PACS achieves a peak performance of 614.4 GFLOPS. Since 1996, intensive calculations of lattice QCD have been performed on the CP-PACS. Among others, the first systematic study including both chiral and continuum extrapolations was attempted for lattice QCD with two flavors of dynamical quarks. In this paper, we report on the results of these studies, focusing on the topics of dynamical quark effects in QCD.

We study lattice QCD formulated on a 4-dimensional hyper-cubic lattice with a finite lattice spacing \( a \). Continuum physics is defined in the limit of large lattice volume and vanishing lattice spacing. Therefore, in order to extract predictions for the real world from the simulations on finite lattices, we have to extrapolate data obtained on a sufficiently large lattice to vanishing lattice spacing (the continuum extrapolation). Furthermore, because the contribution of quarks in the calculation is quite computer-time intensive as we decrease the quark mass, with the current computers and current algorithms, we also have to extrapolate to the physical point of light \( u \) and \( d \) quarks using data at around the \( s \) quark mass region (the chiral extrapolation). It is important to have good control of the systematic errors due to both these extrapolations.

Because of the huge computational power required, majority of calculations have been made in the quenched approximation, in which the effects of dynamical quark loops are ignored. As the first project on the CP-PACS, we made an extensive simulation of quenched QCD. The quality of extrapolations and therefore the precision of the final hadron spectrum were significantly improved over previous studies. From this study, the
existence of systematic errors due to the quenched approximation was clearly demonstrated in the continuum limit.

Therefore, as the next logical step, we then performed a series of “full QCD” simulations, in which the effects of dynamical quarks are taken into account, on the CP-PACS\cite{2}. After chiral and continuum extrapolations, clear dynamical quark effects are observed in the light hadron mass spectrum and in the light quark masses. We also found noticeable effects in B meson decay constants.

In Sec. 2, we summarize the results for the light hadron spectrum from these studies. In Sec. 3, light quark masses are discussed. Sections 4 and 5 are devoted to the U(1) problem and B meson decay constants, respectively. Conclusions are given in Sec. 6.

2 Light hadron spectrum

The precise computation of the hadronic mass spectrum, directly from the first principles of QCD, is one of the main goals of lattice QCD. This provide us with a direct and non-perturbative test of the validity of QCD as the fundamental theory for strong interactions.

In Fig. 1, the latest results for the light hadron spectrum in the quenched approximation of QCD are summarized\cite{3}. Simulations are made on four lattices $32^3 \times 56$ to $64^3 \times 112$ with lattice spacings in the range $a \approx 0.1-0.05$ fm. The spacial lattice size was fixed to be about 3 fm, with which the finite size effects are estimated to be maximally 0.5% in the spectrum. The $u$ and $d$ quarks were treated as degenerate. On each lattice, five quark masses, corresponding to the pseudoscalar-to-vector mass ratio $m_{PS}/m_{V} \approx 0.75-0.4$, were studied. The $u$, $d$ quark mass $m_{ud}$ and the lattice spacing $a$ were fixed using the experimental values for $m_{\pi}$ and $m_{\rho}$ as inputs, while the $s$ quark mass was fixed either by $m_{K}$ (K-input) or $m_{\phi}$ ($\phi$-input). Errors in Fig. 1 include statistical as well as systematic errors from chiral and continuum extrapolations, but do not include the errors from the quenched approximation.

From Fig. 1, we see that, although the global pattern of the experimental spectrum is correctly reproduced, there remain systematic discrepancies of up to about 10% (7 standard deviations). The resulting spectrum is different depending on the choice of input for $s$ quark mass; the $K$-input or the $\phi$-input. These discrepancies and ambiguities are due to the quenched approximation.

Because this limitation of the quenched approximation was made clear, the next log-
ical step is to perform a “full QCD” calculation removing the quenched approximation. As the first step towards the realistic QCD, we performed a series of QCD simulations with two degenerate flavors of sea quarks, identified as dynamical $u$ and $d$ quarks, while the $s$ quark is treated in the quenched approximation ($N_f = 2$ QCD).4

A key ingredient in avoiding a rapid increase of the computer time is the improvement of the lattice theory, with which lattice artifacts are reduced on computationally less intensive coarse lattices. We adopted the combination of an RG-improved gauge action and a “clover”-type improved Wilson quark action, and carried out the first systematic investigation of full QCD to perform both continuum and chiral extrapolations. Our preparatory full QCD study6 shows that this action leads already to small lattice artifacts at $a \sim 0.2$ fm. Therefore, we have chosen the simulation parameters as summarized in Table 1. The spacial lattice size was fixed to be about 2.5 fm for all lattices.

Recently, we have doubled the statistics on the finest lattice at $a \approx 0.1$ fm. All results, except for the $B$ meson decay constants, presented in this paper are based on this full statistics.

Figure 2 shows the lattice spacing dependence of $K^*$ and $\phi$ meson masses from $N_f = 2$ QCD, compared with the results of quenched calculations. For the quenched masses, two different data sets are shown: Those denoted as “$N_f = 0$ Standard” are the results of the quenched simulation, mentioned before, using the standard lattice action. Because the action used in the full QCD calculation is different from the original quenched calculation, we carried out an additional quenched simulation using the same improved action as for the full QCD runs. The results are denoted as “$N_f = 0$ Improved” in the figure.

Our data for hadron spectrum confirms the expectation that both quenched calculations must lead to universal values in the continuum limit. The quenched results, however, show discrepancies from the experimental values, as discussed before. On the other hand, when we introduce two flavors of dynamical quarks, the discrepancies are much reduced. This means also that the ambiguities from the choice of input for $s$ quark mass are much reduced in $N_f = 2$ QCD. The remaining small difference might be caused by the quenching of the $s$ quark.

3 Light quark masses

Although quark masses are the most fundamental parameters of QCD, due to the confinement, it is impossible to measure them directly by an experiment. They have to be indirectly inferred from hadronic observables using a non-perturbative theoretical relation between these hadronic quantities and QCD parameters. A lattice QCD determination of the hadron spectrum provides us with such a theoretical relation directly from the first principles of QCD.

Table 1. Simulation parameters for $N_f = 2$ QCD on the CP-PACS. $L_s$ is the spacial size of the lattice. On each lattice, four sea quark masses in the range $m_{PS}/m_V \approx 0.8$–0.6 were simulated. For each sea quark mass, we studied hadrons using five valence quarks in the range $m_{PS}/m_V \approx 0.8$–0.5.

| lattice | $a$ (fm) | $L_s$ (fm) | $N_{\text{trajectory}}$ |
|---------|---------|-----------|-------------------|
| $12^3 \times 24$ | 0.215(2) | 2.58(3) | 5000–7000 |
| $16^3 \times 32$ | 0.153(2) | 2.48(3) | 5000–7000 |
| $24^3 \times 48$ | 0.108(2) | 2.58(3) | 4000 |

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Fig. 3 summarizes the lattice spacing dependence of the average $u$ and $d$ quark mass $m_{ud}$ and the $s$ quark mass $m_s$, in $N_f = 2$ full QCD and in quenched QCD. On the lattice, there exist several alternative definitions for the quark mass. In the figures, they are denoted as VWI (vector Ward identity quark masses), AWI (axial-vector Ward identity quark masses), etc. See Table 1 for details. While different definitions of quark masses lead to results that differ at finite lat-
Table 2. Light quark masses in the $\overline{\text{MS}}$ scheme at 2 GeV.

| $N_f$          | $m_{ud}$ (MeV) | $m_s$ (MeV)  | $m_s$ (MeV) (K-input) | $m_s$ (MeV) ($\phi$-input) |
|----------------|----------------|--------------|------------------------|-----------------------------|
| 0 standard     | 4.57±0.18      | 116±3        |                        | 144±6                       |
| 0 improved     | 4.36±0.17      | 110±4        |                        | 132±4                       |
| 2              | 3.44±0.14      | 88±4         |                        | 90±5                        |

Errors include our estimates for systematic errors from chiral and continuum extrapolations and renormalization factors. First, we note that the two quenched calculations lead to universal values, as in the case of the light hadron spectrum. However, the quenched value for $m_s$ differs by about 20% between $K$-input and $\phi$-input. We find that this discrepancy between the inputs disappears within an error of 10% by the inclusion of two flavors of sea quarks.

The most interesting point is that the values predicted through $N_f = 2$ QCD are 20–30% smaller than those in the quenched QCD. In particular, our $s$ quark mass in $N_f = 2$ QCD is about 90 MeV, which is significantly smaller than the value $\approx$ 150 MeV often used in hadron phenomenology, and almost saturating an estimate of the lower bound from QCD sum rules using the positivity of spectral functions. On the other hand, our result for the $u, d$ to $s$ quark mass ratio, $m_s^{\overline{\text{MS}}}/m_{ud}^{\overline{\text{MS}}}$ = 26±2, is consistent with 24.4 ± 1.5 from one loop chiral perturbation theory.
4 U(1) problem

The clarification of the mechanism for a large \( \eta' \) meson mass is an important issue in QCD. Propagators of a flavor non-singlet meson consist of a loop of a valence quark propagator, while propagators of the flavor singlet \( \eta' \) meson have an additional contribution with two disconnected valence quark loops. The fact that the \( \eta' \) is much heavier than the corresponding non-singlet meson \( \pi \) means that the two-loop contribution should exactly cancel the \( \pi \) pole of the one-loop contribution, leaving the heavy \( \eta' \) pole. This phenomenon is considered to be related with the anomalous violation of the flavor singlet axial U(1) symmetry and with the topological structure of gauge field configurations.

The calculation of the two-loop contribution requires a large amount of computations on the lattice. For this reason only limited results are available. In an approximation ignoring the mixing with the \( s\bar{s} \) state, we studied one and two-loop contributions, and performed, for the first time, both chiral and continuum extrapolations. We obtain \( m_{u\bar{u}+d\bar{d}} = 972 \pm 97 \) MeV for the flavor-singlet \( u\bar{u} + d\bar{d} \) meson. See Fig. 1. In the real world, the \( u\bar{u} + d\bar{d} \) state mixes with the \( s\bar{s} \) state to lead to \( \eta'(547) \) and \( \eta'(958) \) mesons. We are extending the study to inspect the mixing with the \( s\bar{s} \) state and the relation to the topological structures.

5 B mesons on the lattice

The decay constant for the \( B_q \) meson is defined by \( \langle 0|\bar{b}\gamma_\mu\gamma_5q|B_q(p)\rangle = i f_{B_q} p_\mu \), where \( q \) denotes either \( d \) or \( s \) quark. The non-perturbative determination of \( f_{B_q} \) and also the bag parameters \( B_{B_q} \) is quite important for a precise determination of CKM matrix elements. Therefore, intensive lattice calculations have been made.

On the lattice, however, the simulation of the heavy \( b \) quark is not a trivial extension of light quark simulations, because \( m_b \sim 4 \) GeV is larger than the lattice cutoff \( \sim 1–4 \) GeV to date. Two methods have been developed to simulate heavy quarks on the lattice. One is based on a non-relativistic effective theory of QCD (NRQCD) defined through an expansion in the inverse heavy quark mass. Another employs a relativistic action and reinterprets it in terms of a non-relativistic Hamiltonian (Fermilab method). Because the both methods include an effective treatment of heavy quarks, the consistency of the results among them should be checked.

Majority of the lattice studies are done in the quenched approximation. On the other hand, a chiral perturbation theory suggests sizable corrections from dynamical quarks in the values of \( f_{B_q} \). The first full QCD calculations of \( f_{B_q} \) were made by the MILC Collaboration using the Fermilab method, and by Collins et al. using the NRQCD method. In these studies, configurations were generated using the staggered sea quarks, which is different from the valence light quark (the Wilson quark or the clover quark).

Using the CP-PACS computer, we studied heavy meson decay constants applying a consistent formulation for sea and valence light quarks, the clover quark, and applied both the NRQCD method and the Fermilab method. Our best estimates of heavy meson decay constants for \( N_f = 2 \) and

| \( f_{B_d} \) | \( f_{B_s} \) | \( f_{D_s} \) | \( f_{D_s} \) |
|---|---|---|---|
| Fermilab | NRQCD | Fermilab | NRQCD |
| \( f_{B_d} \) | 188±3±9 | 208±10±11 | 205±8±15 | |
$N_f = 0$ (with improved action) are summarized in Table 3. Because the Fermilab method is applicable also for the $c$ quark, we also computed $f_{D_d}$ and $f_{D_s}$ with this method. The fact that our $f_{D_s}$ for $N_f = 2$ is consistent with the recent experimental results, $285\pm20\pm40$ MeV (ALEPH) and $280\pm19\pm44$ MeV (CLEO3), is quite encouraging.

From the table, we see that Fermilab and NRQCD methods are consistent with each other. We also note that $N_f = 2$ results for B mesons are about 10–15% larger than the quenched values, while $f_{D_d}$ and $f_{D_s}$ are less sensitive to $N_f$. Increase of the B meson decay constants affects the determination of several CKM matrix elements through the $B_q - \overline{B}_q$ mass difference $\Delta M_q$. Our results for $f_{B_d}$ and $f_{B_s}$ are consistent with the hypothesis that the Wolfenstein parameter $\rho$ is positive.

6 Conclusions

We performed the first systematic study of lattice QCD with two flavors of dynamical quarks. We found that dynamical quark effects are quite important in the hadron physics. The effect is as large as 20–30% in the values of light quark mass and about 10–15% in B meson decay constants. Both of the shifts has significant implications to phenomenological studies of the standard model. It is urgent to evaluate dynamical quark effects in other hadronic quantities, such as the bag parameters $B_{B_q}$. It is also important to study the effects of dynamical $s$ quark. Further intensive studies on the lattice are under way to clarify the precise structure of the standard model.

Acknowledgments

The studies presented here were performed by the CP-PACS Collaboration. I thank other members of the Collaboration; A. Ali Khan, S. Aoki, Y. Aoki, G. Boyd, R. Burkhalter, S. Ejiri, M. Fukugita, S. Hashimoto, N. Ishizuka, Y. Iwasaki, T. Izubuchi, T. Kaneko, Y. Kuramashi, T. Manke, K. Nagai, J. Noaki, M. Okamoto, M. Okawa, H.P. Shanahan, Y. Taniguchi, A. Ukawa, and T. Yoshié, for discussions. This paper is in part supported by the Grants-in-Aid of Ministry of Education, Science and Culture (No. 10640248) and JSPS Research for Future Program.

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