Lattice QCD with Dynamical up, down and Strange Quarks with the Earth Simulator

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The Standard Model is a unified theory of elementary particles which includes Weinberg-Salam theory for electro-weak interactions and QCD for strong interactions. Lattice QCD and its numerical simulations offer a fundamental tool for verifying and extracting predictions of the model. Our project aims to carry out a large scale lattice QCD simulation in which the three light quarks, up, down and strange, are treated dynamically, thereby fully exonerating quenching effects that have plagued past attempts. This year we have completed the runs on a $20^3 \times 40$ and $16^3 \times 32$ lattices, and have started the run on a $28^3 \times 56$ lattice. The results for the meson spectrum show that the dynamical effects of three quarks are just right to fill in the disagreement of the quenched results from experiment. The light quark masses are significantly lighter than expected phenomenologically, confirming the trend from our earlier results for two dynamical flavors.

Keywords: elementary particle physics, Standard Model, quark, hadron, lattice QCD, Monte Carlo simulation

1. The physics goal of our project

The Standard Model of elementary particles describes all known particle contents and forces in Nature except for gravity. This model includes quantum chromodynamics (QCD) describing strong interactions and Weinberg-Salam theory describing electroweak interactions. Verification of the Standard Model is a crucial step, both to establish the current gauge-theoretic understanding of Nature and to help explore the hierarchy of even finer microscopic scales.

At low energy scales non-perturbative analysis is needed for QCD since the coupling becomes strong toward the infrared due to the remarkable property of asymptotic freedom. The only method versatile enough at present for this purpose is lattice QCD and its numerical simulation.

In lattice QCD simulations in the past, the so-called "quenched approximation", in which vacuum polarization effects of quarks are ignored, have been used. The reason was technical; full QCD simulations treating quarks dynamically requires computational resources two to three orders of magnitude larger than the quenched one. More fundamentally, simulation algorithms for odd number of quarks had not been developed. Fortunately, both these limitations are now overcome.

In our project, we aim to carry out a large-scale three flavor full QCD simulation, in which up, down and strange quarks are treated dynamically, i.e., there is no quenching effect. Among the many important issues which should be addressed in such simulations, we initially concentrate on the followings:

· Verification of the hadron mass spectrum.
· Determination of quark masses and the QCD coupling which are the fundamental parameters of QCD.
· Determination of hadronic weak matrix elements for constraining the Cabibbo-Konayashi-Maskawa quark mixing matrix and for understanding of CP violation.
· Elucidation of the $U(1)$ problem related to the eta' meson mass and gluon field topology, and other long-standing issue of strong interactions.

As a first step we work on an analysis of the light hadron spectrum and quark masses using the unquenched gauge configurations.

2. Gluon configuration generation

In usual lattice full QCD simulations, gluon configuration generation and measurement of physical quantities are performed separately. The Earth Simulator is a powerful tool for the former part which takes large cost computationally. The configurations generated and accumulated are used for off-line measurements of various physical quantities such as hadrons masses, topology and so on.

2.1. Optimization of the PHMC code

In our simulation we assume that up and down quarks are degenerate but that strange quark has a distinct mass. All three quarks are treated dynamically. Therefore, we call this simulation as a 2 + 1 flavor full QCD simulation. For up and down quarks we employ the standard Hybrid Monte Carlo algorithm; for strange quark an odd-flavor algorithm is needed for which we apply the Polynomial Hybrid Monte Carlo (PHMC) algorithm. It is based on a polynomial approximate inversion of the Dirac matrix. A noisy Metropolis test for a correction of the approximation makes this algorithm exact [1].

Our PHMC code was originally developed for Hitachi SR8000 at KEK for which it achieved 40% of peak speed. We have ported this code to the Earth Simulator, and made extensive rewriting and optimizations. In detail, our code uses the strategy in which sites on the z-t plane are numbered by a one-dimensional array and divided by four to realize a large vector length without list vectors [2]. In addition, we use a library supplied by the Earth Simulator support team upon our request which enables an overlap of computations and communications. The use of the library enhances the sustained performance by 12-13%. The total efficiency of the code for Earth Simulator has now reached 46% for our largest lattice size of $28 \times 28 \times 28 \times 56$ used in this year's runs.

2.2. Simulation parameters for the configuration generation

In our simulation we use a Renormalization Group (RG) improved Wilson gauge action and a non-perturbatively $O(a)$ improved Wilson quark action [3]. In order to take the continuum limit our simulation is performed at $\beta = 2.05$, 1.90 and 1.83 corresponding to the three lattice spacings $a \sim \sqrt{1/2} \times 0.1$, 0.1 and $\sqrt{3/2} \times 0.1$ fm, which are at even intervals in a^2. The lattice sizes are $L^3 \times T = 28^3 \times 56$, $20^3 \times 40$ and $16^3 \times 32$ respectively so that the physical volume is fixed at 2.0 fm. Since this volume is not sufficiently large to avoid finite-size effects for baryon masses, we focus on the analysis of the meson sector in this report. We take five values for the degenerate up and down quark mass in the range $m_{PS}/m_V \sim 0.6 - 0.78$ for chiral extrapolation, and two values for strange quark mass around $m_{PS}/m_V \sim 0.7$ for interpolation. Production of gluon configurations at $\beta = 1.90$ was in good progress last year, which we completed early this year. We also carried out some runs for $\beta = 1.83$, but soon decided that this run, being small in lattice size and so demands much less computing resources, can be handled by conventional supercomputers elsewhere. The bulk of our effort this year has been concentrated on the largest $28^3 \times 56$ lattice at $\beta = 2.05$. The simulation parameters and current statistics are listed in Table 1.

Table 1 Simulation parameters. At $\beta = 2.05$, the number of trajectory is 2000 at present. The lattice spacing described in this table represents the current estimate.

β	1.83	1.90	2.05
lattice size	$16^3 \times 32$	$20^3 \times 40$	$28^3 \times 56$
lattice spacing (fm)	0.1223(17)	0.1001(19)	0.0797(92)
# of trajectory	7000-8600 (finished)	5000-9000 (finished)	4000-5000(target) 2000(current)

3. The light hadron spectrum

3.1. Analysis method

Meson masses and decay constants are calculated from a correlated fit of meson correlator using single hyperbolic cosine or hyperbolic sine fit forms. For the chiral extrapolation to obtain the quantities at the physical point, we assume a polynomial fit form in quark masses up to quadratic order. This fit is made to all combinations of valence quarks simultaneously ignoring correlations among these masses. We fix the physical point using the experimental values of m_π, m_ρ, m_K, (K-input) or m_π, m_ρ, m_ϕ (ϕ-input).

We have completed the analyses at $\beta = 1.90$ and 1.83, which are presented below. A preliminary continuum extrapolation using these two points are also made, and compared with provisional values at $\beta = 2.05$.

3.2. Light meson spectrum

In Fig. 1 we present results for meson masses. Since we use a non-perturbatively $O(a)$ improved Wilson quark action, the scaling of meson masses as a function of lattice spacing should be a^2. With this assumption our results are consistent with experiment. This is an encouraging result showing the importance of including the vacuum polarization effects for precision agreement with experiment at a percent level.

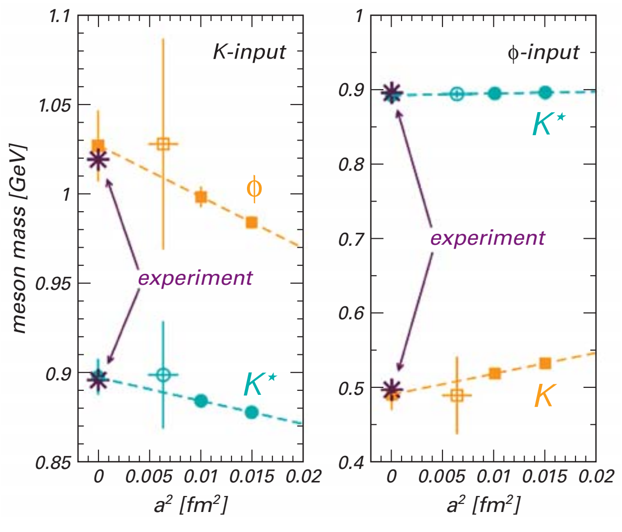

Fig. 1 Continuum extrapolation of light meson masses in 2 + 1 flavor full QCD and its comparison with experimental value. Horizontal axis is a^2 and star symbols represent the experimental value. The results at $a \sim \sqrt{1/2} \times 0.1$ fm in this figure are preliminary and not used for the continuum extrapolation.

3.3. Light quark masses

The quark masses are fundamental parameters in QCD. These masses cannot be determined by experiment because of the quark confinement property of QCD. At present the only way to obtain the quark masses from the first principle is lattice QCD.

We calculate the physical quark mass m_q using the axial-vector Ward-Takahashi identity (AWI) definition:

$$m_q^{AWI} = \lim_{t\to\infty} \frac{\langle \partial_4 A_4(t) P(0) \rangle}{\langle P(t) P(0) \rangle}.$$

An alternative definition employs the vector Ward-Takahashi identity (VWI). In our analysis we apply the AWI definition since the scaling violation of the quark mass is empirically smaller than that in the VWI definition. The renormalization factors which match the quark mass on the lattice to that with $\overline{MS}$ scheme in the continuum theory are calculated perturbatively. Hence $O(\alpha_s^2 a)$ errors remain in our result where $\alpha_s = g^2/4\pi$ represents the strong coupling constant. The renormalized quark masses are evolved to μ = 2 GeV using the 4-loop β-function. We assume that the remaining $O(\alpha_s^2 a)$ effects are small, and take the a^2 continuum limit in our current analysis.

The preliminary estimate for the continuum value for quark masses in 2 + 1 flavor full QCD are given by

$$m_{up,down} = 3.41(24) MeV,$$
$$m_{strange} = 88.6(7.1) MeV$$

The continuum extrapolation leading to these values and a comparison with earlier results in two-flavor full and quenched QCD cases are shown in Fig. 2. The 2 + 1 flavor full QCD results are somewhat smaller than those of two-flavor full QCD at finite lattice spacings, but the difference are not visible after the continuum extrapolation. Precision results at our finest lattice at β = 2.05 are needed to settle the continuum value.

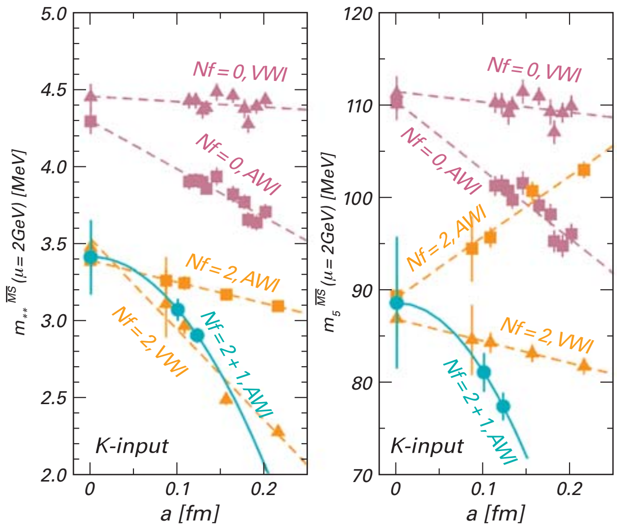

Fig. 2 Continuum extrapolation of up and down quark masses (left) and strange quark mass (right) in 2 + 1 flavor full QCD (Nf = 2 + 1) compared with 2 flavor full (Nf = 2) and quenched (Nf = 0) QCD [4]. Horizontal axis denotes lattice spacing a. The quark masses defined by VWI are also shown for Nf = 2 and 0 cases for comparison.

3.4. Meson decay constants

The decay constants of pseudo-scalar meson and vector meson are defined through

$$\langle 0 | A_4 | PS\ meson \rangle = f_{PS}\, m_{PS},$$
$$\langle 0 | V_i | Vector\ meson \rangle = \varepsilon_i\, f_V\, m_V$$

where ε_i is a polarization vector. Historically, previous simulations using the Wilson type quark action have not reproduced well the experimental values of the decay constants. In this analysis we use a local current for A_4 and a conserved current for V_i. The advantage of using the conserved vector current is that a renormalization factor is not needed. Our calculation of the decay constants has $O(a)$ errors; we assume that they are small and employ a^2 scaling in taking continuum limit as in the quark masses.

Fig. 3 shows our current values, exhibiting a reasonable

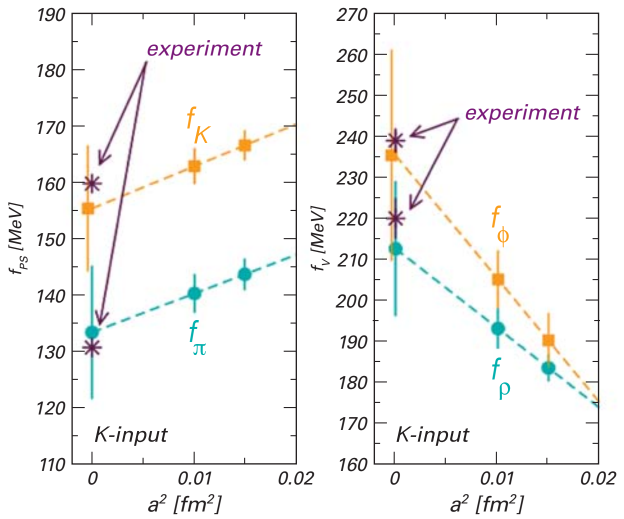

Fig. 3 Continuum extrapolation of pseudo-scalar decay constant (left) and vector decay constant (right). Horizontal axis is a^2. Star symbols represent the experimental value.

agreement with experiment within the limitation of the two-point continuum extrapolation and large statistical errors. The final results at $\beta = 2.05$ are needed for further analyses.

4. Plan for Fiscal 2005

4.1. Runs and analyses

This year, we have completed the gluon configuration generations at β = 1.83 and 1.90. The results so far obtained from these configurations are quite encouraging, as we reported here, and also at a number of international workshops and conferences this year [5-9]. We think that this calls for accelerated configuration generations and analyses of the β = 2.05 run. So far, we have accumulated 2000 trajectories at 10 quark parameter sets at β = 2.05. In fiscal 2005 we hope to increase the number up to 4000-5000 trajectories. Using the full set of configurations we hope to report the final result of the light hadron spectrum by the end of fiscal 2005.

Achieving this goal requires a control of chiral and continuum extrapolations. For the chiral extrapolation, we intend to pursue Wilson chiral perturbation theory which will provide the chiral fit function including infrared chiral logarithms and finite lattice spacing corrections to them [10]. For the continuum extrapolation, we are calculating renormalization factors and $O(a)$ improved coefficients non-perturbatively.

This year we have separately carried out extensive tests of a relativistic heavy quark action using quenched and two-flavor full QCD [11]. Application of this framework to 2 + 1 flavor full QCD to calculate heavy meson quantities will also be pursued

4.2. Sharing of the gauge configurations

International Lattice Data Grid (ILDG) [12] is a project to build a data grid of lattice QCD gauge configuration archive so that they can be shared by the lattice QCD community. We plan to put the 2 + 1 configurations to our Lattice QCD Archve [13] which is the Japanese site of the ILDG.

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地球シミュレータによる格子上の素粒子標準模型の研究

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素粒子標準模型は強い相互作用を記述する量子色力学(QCD)と、弱電磁相互作用を記述するWeinberg-Salam理論を統合した低エネルギーでの素粒子を記述する模型である。この模型を確立し、さらに、標準模型を超えたよりミクロ階層の物理を探るには、第一原理からの計算によって物理の再現性を確かめることが必要であり、また、この模型を規定する種々のパラメータの決定も重要である。素粒子標準模型を構成しているQCDでは、漸近自由性という特有な性質のために低エネルギー領域では摂動論が破綻する。よって非摂動的手法が必要であるが、これを可能にしたのが格子QCD であり、その数値シミュレーションである。格子QCD によってあらゆる物理量の計算が原理的には可能であるが、実際は様々な問題を抱えている。特に計算機性能の制限、あるいは計算アルゴリズムの不整備から、従来、クォークの真空偏極効果を無視したクエンチ近似という手法が使用されてきた。この近似法から導かれる結果はある程度は自然を再現してはいるものの、実験値との差異も確認されている。この様な状況の中で、本プロジェクトではクエンチ近似を全て取り除いた格子QCDの数値シミュレーションに取り組んでいる。計算アルゴリズムに関しては我々のグループが実用化したPHMC法を用いることにより、軽いクォークであるアップ・ダウン・ストレンジ全ての真空偏極効果を取り入れることに成功した。クエンチ近似を取り除いた数値シミュレーションで取り組むべき課題は沢山あるが、我々は特に軽いハドロンスペクトル、CPの破れ等の重いクォークの物理、U(1)問題等の解決に力を注いでいる。その第一段階として軽いハドロンスペクトルについての解析を行い、現時点で次の様な結果を得ている。
・軽い中間子スペクトルの計算結果は実験値を良く再現している。これはクエンチ近似を取り除いた効果であると考えられる。
・アップ・ダウン・ストレンジクォークの質量は現象論で用いられてきた値に比べて20 −30%軽い。
・軽い中間子の崩壊定数は大きな統計誤差の範囲内で実験値と矛盾しない。
これらの結果を確定するため、現在さらに細かい格子間隔でのゲージ配位の生成を行っており、2005年度中には最終結果がを得ることを目標としている。また、重いクォークについては、相対論的な定式化のテストがほぼ終了し、2005年度にはその応用をも行う予定である。

キーワード：素粒子物理学，素粒子標準模型，クォーク，ハドロン，格子量子色力学，モンテカルロシミュレーション