Lattice QCD Simulation without Quenched Approximation

Project Representative

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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 gluon configuration generation on $16^3 \times 32$, $20^3 \times 40$ and $28^3 \times 56$ lattices. 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 the Glashow-Salam-Weinberg model for 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, were 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 were not developed. Fortunately, these limitations are now overcome.

In our project, we aim to carry out a large-scale three flavor full QCD simulation, in which all three light quarks in nature, i.e., 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-Kobayashi-Maskawa quark mixing matrix for understanding of CP violation.
- Elucidation of the $U(1)$ problem related to the η' 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 gluon 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 a large computational cost. The configurations generated and accumulated are used for off-line measurements of various physical quantities.

2.1 Optimization of the PHMC code

In our simulation we treat up and down quarks as degenerate and strange quark with a different mass. We call this simulation as 2 + 1 flavor (Nf = 2 + 1) full QCD simulation. For up and down quarks we employ the standard Hybrid Monte Carlo (HMC) algorithm; for strange quark an odd-flavor algorithm is needed for which we apply the Polynomial HMC (PHMC) algorithm. It is based on a polynomial approximation of the inverse square-root of the Dirac matrix. A noisy Metropolis test for 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 an 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 the Earth Simulator has now reached 46% for our largest lattice size of $28^3 \times 56$.

2.2 Simulation parameters for the configuration generation

In our simulation we use a Renormalization Group improved Wilson gauge action (Iwasaki action) and a non-perturbatively $O(a)$ improved Wilson quark action (NPT clover action) [3]. In order to take the continuum limit our simulation is performed at $\beta = 2.05$, 1.90 and 1.83 corresponding to three squared lattice spacings $a^2 \sim 0.005, 0.01, 0.015\ fm^2$, 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 $(2.0\ fm)^3$. In our study 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 or short extrapolation. The distribution of the simulation parameters is shown in Figure 1. The production of gluon configurations, which started in June 2003, was completed in December 2005. The number of HMC trajectories for each simulation parameters are listed in Table 1. The generated gluon configurations are saved at every 10 HMC trajectories.

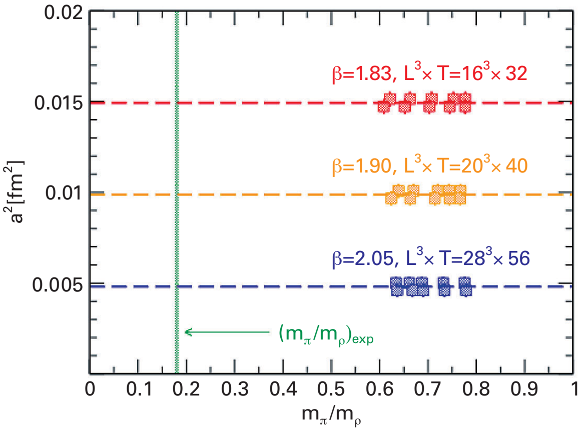

Fig. 1 Distribution of simulation points in $(m_\pi/m_\rho, a^2)$ plane. $(m_\pi/m_\rho)_{\text{exp}}$ represents the experimental value.

Table 1 HMC trajectories for each simulation parameters. κ_{ud} and κ_s represent hopping parameters of quarks.

$\beta = 1.83,\ L^3 \times T = 16^3 \times 32$					
κ_{ud}	κ_s	traj.	κ_{ud}	κ_s	traj.
0.13655		7000	0.13655		7000
0.13710		7000	0.13710		8600
0.13760	0.13710	7000	0.13760	0.13760	8000
0.13800		8000	0.13800		8100
0.13825		8000	0.13825		8100
$\beta = 1.90,\ L^3 \times T = 20^3 \times 40$					
κ_{ud}	κ_s	traj.	κ_{ud}	κ_s	traj.
0.13580		5000	0.13580		5200
0.13610		6000	0.13610		8000
0.13640	0.13580	7500	0.13640	0.13640	9000
0.13680		8000	0.13680		9000
0.13700		8000	0.13700		8000
$\beta = 2.05,\ L^3 \times T = 28^3 \times 56$					
κ_{ud}	κ_s	traj.	κ_{ud}	κ_s	traj.
0.13470		6000	0.13470		6000
0.13510		6000	0.13510		6000
0.13540	0.13510	6000	0.13540	0.13540	6000
0.13550		6500	0.13550		6500
0.13560		6500	0.13560		6500

3. Light hadron spectrum

3.1 Analysis method

Light hadron masses and decay constants are calculated from a correlated fit of meson and baryon correlators. In the calculation single hyperbolic-cosine and hyperbolic-sine fit forms for meson and single exponential fit forms for baryon are used. 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 experimental values of m_π, m_ρ, m_K (K-input) or m_π, m_ρ, m_ϕ (ϕ-input). The lattice spacings are set from m_ρ. The obtained lattice spacings are listed in Table 2.

In order to take continuum limit we assume a scaling linear in a^2, since the quark action is non-perturbatively $O(a)$ improved. For the calculation of quark masses and decay constants, renormalization factors are needed to match the physical quantities on the lattice to that with $\overline{MS}$ scheme in the continuum theory. Since these factors are known only in one-loop perturbation theory for our action combinations, $O(\alpha_s^2 a)$ errors remain in our results, where $\alpha_s = g^2/4\pi$ represents the strong coupling constant. The $O(\alpha_s^2 a)$ errors are assumed to be small and neglected in our study.

In quoting our previous studies [4], in which all quarks are treated in the quenched approximation or only up and down quarks are treated as dynamical ones, we assume a scaling linear in a since the quark action was $O(a)$ improved only in one-loop perturbation theory.

All statistical errors are estimated by the jackknife method. The jackknife bin size is set to 100 HMC trajectories from check of the bin-size dependence of errors.

Table 2 Lattice spacing and physical size.

	K-input		ϕ-input	
β	a [fm]	aL [fm]	a [fm]	aL [fm]
1.83	0.1222(17)	1.955(27)	0.1233(20)	1.973(32)
1.90	0.0993(19)	1.986(38)	0.0995(19)	1.990(38)
2.05	0.0693(26)	1.940(73)	0.0695(26)	1.946(73)

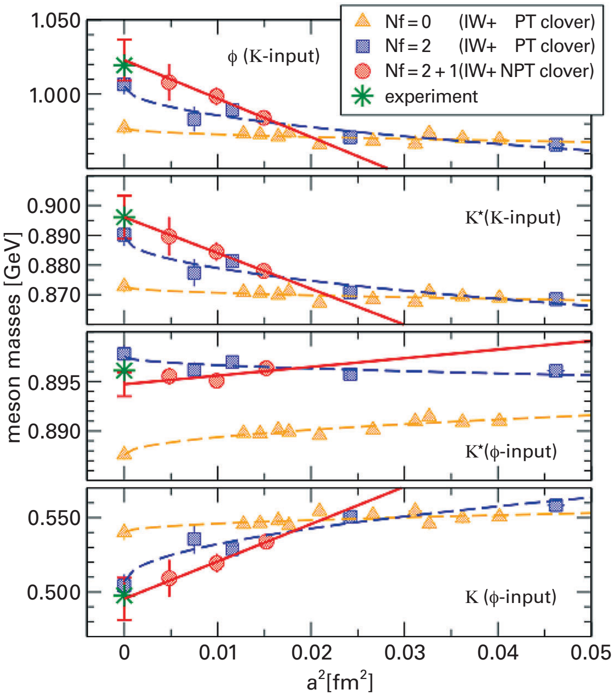

Fig. 2 Continuum extrapolation of light meson masses in 2 + 1 flavor full QCD (Nf = 2 + 1) and its comparison with experimental value. 2 flavor full (Nf = 2) and quenched (Nf = 0) QCD spectrum are also plotted in this figure. Horizontal axis is a^2 and star symbols represent experiment.

3.2 Light meson spectrum

In Fig. 2 we present our results for meson masses. For comparison we also plot the quenched and the 2 flavor full QCD results. The 2 + 1 flavor meson spectrum extrapolated to the continuum is consistent with experiment at a percent level, showing the importance of including the vacuum polarization effects for precision agreement with experiment.

3.3 Light quark masses

The quark masses are fundamental parameters of nature, just like electron mass. These masses cannot be determined by experiment because of the quark confinement property of QCD. At present the only way to determine the quark masses from the first principle is lattice QCD.

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

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

where $A_\mu(t)$ and $P(t)$ are axial-vector and pseudo-scalar current operator respectively. After matching the quark mass on the lattice to that with $\overline{MS}$ scheme in the continuum theory at a scale $\mu = 1/a$, the renormalized quark mass is evolved to $\mu = 2$ GeV using the four-loop renormalization equation.

The results of quark masses in 2 + 1 flavor full QCD we have obtained are given by

$$m_{up,\,down}^{\overline{MS}}(\mu = 2GeV) = 3.48\,(15)\,MeV,$$
$$m_{strange}^{\overline{MS}}(\mu = 2GeV) = 90.9\,(3.7)\,MeV.$$

The continuum extrapolation leading to these values and a comparison with earlier results in 2 flavor full and quenched QCD cases are shown in Fig. 3. In the continuum limit, our statistical errors are too large to detect possible changes from 2 flavor to 2+1 flavor simulations.

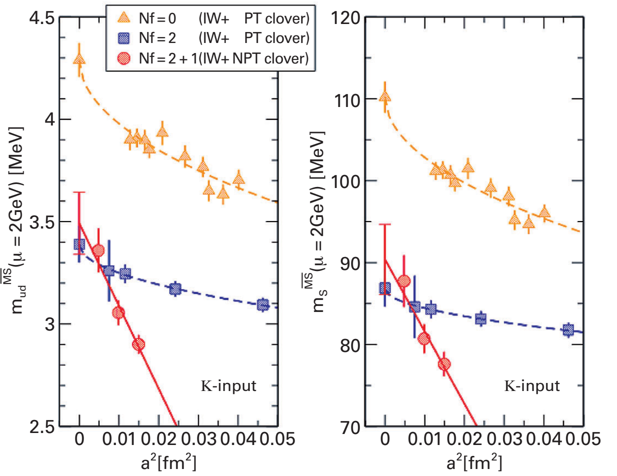

Fig. 3 Continuum extrapolation of ud quark masses (left) and strange quark masses (right) in 2 + 1 flavor full QCD (Nf = 2 + 1) compared with 2 flavor full (Nf = 2) and quenched (Nf = 0) QCD.

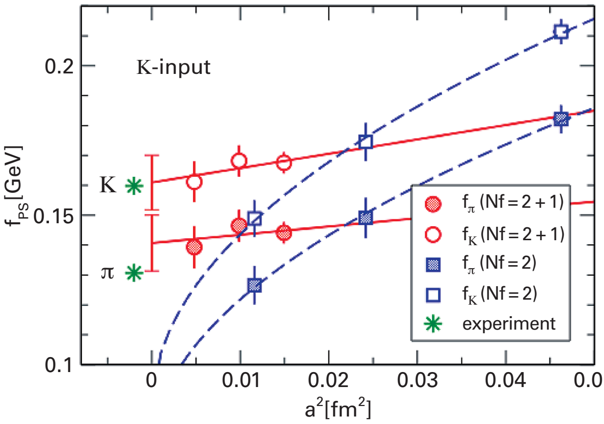

Fig. 4 Continuum extrapolation of pseudo-scalar decay constants f_π and f_K in 2 + 1 flavor full QCD (Nf = 2 + 1) comparing with 2 flavor full (Nf = 2) and quenched (Nf = 0) QCD. Star symbols represent experiment.

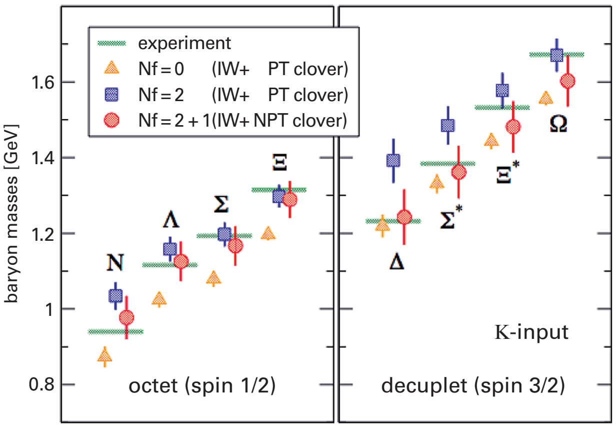

Fig. 5 Light baryon spectrum in 2 + 1 flavor full QCD (Nf = 2 + 1) comparing with 2 flavor full (Nf = 2) and quenched (Nf = 0) QCD. Fat horizontal lines represent experiment.

3.4 Light meson decay constants

The decay constant of pseudo-scalar meson f_{PS} is defined through

$$\langle 0 | A_4 | PS\ meson \rangle = f_{PS}\, m_{PS}.$$

Fig. 4 shows our current results for f_π and f_K. We also plot the results in 2 flavor full QCD in this figure. Historically, previous simulations using the Wilson type quark actions have not reproduced well the experimental value of the pseudo-scalar decay constants, as exemplified by the blue data points in the figure for 2 flavor full QCD. We can state that we find a much more reasonable results in the 2 + 1 flavor case.

3.5 Light baryon spectrum

Fig. 5 shows the baryon spectrum calculated in 2 + 1 flavor full QCD and compared with quenched and 2 flavor full QCD. Historically, a clear and systematic deviation of the quenched spectrum compared to experiment revealed in this figure provided a decisive impetus toward full QCD simulations in recent years. It is gratifying to observe an overall agreement of the full QCD results with experiment, albeit statistical errors are large. We should also bear in mind that the physical volume of (2.0 *fm*)^3 used in the current 2 + 1 flavor runs is too small to contain finite lattice size effects.

4. Summary

4.1 Light hadron results

This project started in the second half of JFY2002. Over the span of three years since then, we have generated gluon configurations including the vacuum polarization effects of all three light quarks at three lattice spacings as originally planned. The light hadron spectrum measurement and analyses have been completed, and we have found the meson spectrum in agreement with experiment at a percent level in the continuum limit, and the light quark masses considerably smaller than the widely used phenomenological estimations. These findings have been reported at a number of international workshops and conferences this year [5, 6].

We need to note that our quarks, while dynamical, are still relatively heavy compared to experiment as shown in Fig. 1. Estimates of systematic errors that arise from the need for a long chiral extrapolation to reach the physical point is an important issue with our result. In particular chiral fits using the fit form derived from Wilson Chiral Perturbation Theory (WChPT) [7, 8], which includes explicit breaking effect of chiral symmetry in the Wilson type quark actions, are needed. This analysis is in progress, and we hope to report on results in the near future.

4.2 Further physical quantities

There are a large number of physical quantities of interest which we wish to calculate on the generated gluon configurations. We have so far calculated meson decay constants. Toward their precision determination, a non-perturbative calculation of renormalization factors and $O(a)$ improvement coefficients of currents are needed. We plan to calculate the former quantity using the Schrodinger functional method. The latter calculation has been recently completed and its application to analysis for quark masses and decay constants is in progress.

Additionally, we have started calculations of (1)η and η' meson masses, and (2) heavy meson quantities using a relativistic heavy quark action [9].

4.3 World-wide sharing of the gluon configurations

International Lattice Data Grid (ILDG) [10] is a project to build a data grid of lattice QCD gluon configurations so that they can be shared by the lattice QCD community. We plan to put the 2 + 1 flavor gluon configuration to our Lattice QCD Archive [11] which is the Japanese site of the ILDG.

5. Future plan

The algorithmic advances and the computing power of the Earth Simulator have allowed us to carry out a fully dynamical simulation of lattice QCD and reach the point m_π/m_ρ ~0.6, corresponding to m_{ud}/m_s ~0.5 in the present project. This point is still away from the point corresponding to nature m_π/m_ρ ~0.18, and we wish to further approach the physical point both to reduce systematic errors due to a long chiral extrapolation and to explore physics of strong interactions at more physical setting. Since the computational cost grows rapidly toward light quarks, algorithmic advances are needed. The Domain Decomposition HMC (DDHMC) recently proposed by M. Luscher [12] is a promising candidate in this direction. We plan to implement this algorithm in our program and carry out simulations with it on the PACS-CS computer being developed at Center for Computational Sciences of University of Tsukuba as the successor to the CP-PACS computer [13, 14]. Our estimates show that we can hopefully reach m_{ud}/m_s ~0.2 for quark masses and the volume ~$(0.3\,fm)^3$. Such calculations extends the 2 + 1 full QCD calculations opened by the current project using the Earth Simulator, and bring in further deepening of understanding of the physics of strong interaction and the Standard Model.

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クエンチ近似を取り除いた格子量子色力学の数値シミュレーション

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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。グルーオン配位は(格子サイズ, 格子間隔[fm])$=(28^3\times 56, \sqrt{0.5}\times 0.1), (20^3\times 40, 0.1), (16^3\times 32, \sqrt{1.5}\times 0.1)$ の3点で、各々10種類のクォーク質量パラメータで生成を行った。このグルーオン配位上でクエンチ近似のない様々な物理量の計算がなされる。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、次の様な結果を得た。

- 軽い中間子スペクトル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過去に行われたアップ・ダウンクォークのみ真空偏極効果を取り入れた数値シミュレーションの結果と同程度である。
- 軽い中間子の崩壊定数は統計誤差の範囲内で実験値と矛盾しない。
- 軽い重粒子スペクトルは設定した空間体積が十分でないこともあり、確定的な結果を示すことはできないが、スペクトルのパターンは実験を再現している。

これらの結果を基礎データとし、現在は、U(1)問題に関連するη'中間子質量の計算、相対論的重クォーク作用を用いた重い中間子に関する種々の物理量の計算を行っている。

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