CURRENT STATUS TOWARD THE PROTON MASS CALCULATION IN LATTICE QCD

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The proton mass calculation is still a tough challenge for lattice QCD. We discuss the current status and difficulties based on the recent PACS-CS results for the hadron spectrum in 2+1 flavor QCD.

1 Introduction

The proton mass calculation has a profound meaning in lattice QCD: To distinguish the proton mass from the neutron one we need to incorporate the isospin breaking effects with the different up and down quark masses and the electromagnetic interactions. This is still out of reach for current lattice QCD calculations. The accomplishment of the first principle calculation of the proton mass inevitably means that other physical quantities should be calculated with similar precision on the same configurations.

In this report we show the recent progress in lattice QCD based on the 2+1 flavor lattice QCD results obtained by the PACS-CS Collaboration who are currently aiming at the physical point simulation. We discuss the difficulties in lattice QCD from a view point of the systematic errors. The toughest problem is the rapid increase of computational cost with the up-down (ud) quark mass reduced toward the physical value. We explain why the direct simulation on the physical point is required in order to avoid the problems in the chiral extrapolation method.

2 Difficulties in Lattice QCD Calculation

Most fundamental quantities in lattice QCD are Green functions in the path-integral formalism:

\[
\langle O[U, q, \bar{q}] \rangle = \frac{1}{Z} \int DU Dq D\bar{q} O[U, q, \bar{q}] e^{-S_{\text{QCD}}[U, q, \bar{q}]},
\]

where \( S_{\text{QCD}} \) represents the QCD action defined on the discretized four-dimensional space time. \( U \) is the so-called link variable which contains the gauge fields. \( q \) and \( \bar{q} \) denote the quark and the anti-quark fields. Only the Monte Carlo method makes feasible the nonperturbative evaluation of the above expression. With appropriate choices of the operator \( O \) we can extract various physical quantities, e.g., the hadron spectrum.

There exists two types of errors in lattice QCD: One is the statistical one due to the Monte Carlo technique. The other is the systematic ones. The former is arbitrarily reduced according to \( 1/\sqrt{N} \) with \( N \) the number of the independent configurations (Monte Carlo samples). The
We have four major systematic errors: (i) finite volume effects, (ii) finite lattice spacing effects, (iii) quench approximation and (iv) chiral extrapolation. It is rather straightforward to diminish the first and the second errors with the use of larger and finer lattices. For almost twenty years after the first lattice QCD calculation of the hadron masses in 1981, most of the large-scale simulations were carried out in the quenched approximation where the sea quark effects are neglected. The primary reason is that the 2+1 flavor lattice QCD simulation requires $O(10^2)$ times as much computational cost as the quenched approximation. In late 90s the CP-PACS collaboration performed a detailed investigation of the quenching effects. The systematic study of the hadron spectrum in the quenched approximation with other systematic errors under control reveals that the results deviate from the experimental values at a 10% level. The comparison are depicted in Fig. 1, where the physical inputs are a set of $m_\pi, m_\rho, m_K$ (closed triangles) or $m_\pi, m_\rho, m_\phi$ (open triangles) to determine the averaged up-down quark mass, the strange one and the lattice spacing $a$. The confirmation of the discrepancy between the quenched results and the experimental values drove us to embark on the 2+1 flavor QCD simulations.

Now the remaining task is to remove the systematic error associated with the chiral extrapolation. Figure 2 illustrates the difficulty: The solid line represents the empirical cost estimate for the 2+1 flavor lattice QCD simulation with the Hybrid Monte Carlo (HMC) algorithm given by Ukawa in 2001. The cost seems to almost diverge as the $m_\pi/m_\rho$ ratio approaches the physical point. It was obvious that we definitely need not only the increase of the computational power but also the algorithmic improvements. Years later the difficulty is overcome by the Domain-Decomposed Hybrid Monte Carlo (DDHMC) algorithm. Blue circles denote the measured computational cost in our simulation armored with several other algorithmic improvements, which clearly shows that the direct simulation at the physical point is allowed with the current computational resources.

Before physical point simulations, we should examine the logarithmic quark mass dependence in the pseudoscalar meson sector predicted by the Chiral Perturbation Theory (ChPT). This is a good testing ground to check whether or not the light quark simulations are properly performed. In Fig. 3 we plot the ratio $m_\pi^2/m_{ud}$ as a function of $m_{ud}$ in lattice unit together with the previous CP-PACS/JLQCD results for comparison. The curvature observed near the chiral limit is explained by the SU(2) ChPT prediction:

$$
\frac{m_\pi^2}{2m_{ud}} = B \left\{ 1 + \frac{1}{16\pi^2} \frac{2m_{ud}B}{f^2} \ln \left( \frac{2m_{ud}B}{\mu^2} \right) + 4 \frac{2m_{ud}B}{f^2} l_3 \right\},
$$

where $B, f, l_3$ are the low energy constants and $\mu$ is the renormalization scale. Figure 4 compares
our results for $\bar{l}_3$, which is defined by $\bar{l}_3 = -64\pi^2 l_3$ at $\mu = m_\pi$, with currently available data given by other groups.\cite{6,7} Black symbol denotes the phenomenological estimate.\cite{8} Red closed (open) symbols are for the results obtained by the SU(3) (SU(2)) ChPT fit on 2+1 flavor dynamical configurations. All the results for $\bar{l}_3$ reside between 3.0 and 3.5, except for the MILC result which is sizably smaller and marginally consistent with others within a large error.

![Figure 3: $m_\pi^2/m_{ud}$ as a function of $m_{ud}$. Solid line is just for guiding your eyes.](image)

![Figure 4: Comparison of $\bar{l}_3$ obtained by the 2+1 flavor dynamical simulations. See text for details.](image)

3 Why is the Physical Point Simulation Necessary?

Chiral extrapolation with the use of ChPT as a guiding principle is currently the most popular strategy to estimate the results at the physical point. The simulation points are usually ranging from 200 – 300 MeV to 600 – 700 MeV for $m_\pi$. There are several problems in this procedure. Firstly, it is numerically difficult to trace the logarithmic quark mass dependence of the physical quantities predicted by ChPT. High precision measurements are required for the reliable extrapolation. Secondly, it is not always possible to resort to the ChPT analyses. A typical example is SU(3) Heavy Baryon ChPT which completely fails to describe the lattice results for the octet baryon masses.\cite{9} Figure 5 shows the next-to-leading order (NLO) fit result for the nucleon mass. This difficulty may be practically avoided by the use of the polynomial fit function instead of ChPT. We apply a simple linear function of $m^H = m^H_0 + \alpha m_{ud} + \beta m_s$ to the lattice data obtained at 156 MeV $\leq m_\pi \leq$ 410 MeV. In Fig. 6 we compare our results for the hadron spectrum with the experimental values. Most of them are consistent within the error bars, though some cases show 2 – 3% deviations at most. Note that we are left with the $O((\Lambda_{QCD} \cdot a)^2)$ finite lattice spacing effects thanks to the nonperturbative $O(a)$-improvement employed in our formulation.\cite{10} This encouraging result, however, does not mean the polynomial extrapolation is a sufficient solution. Since we know that $m_{ud} = 0$ is a singular point in ChPT, the convergence radius of the analytic expansion around the physical ud quark mass is just $0 < m_{ud} < 2m_{ud}^{\text{physical}}$, which roughly corresponds to 0 MeV $< m_\pi <$ 190 MeV. Thirdly, it is impossible to make a proper treatment of resonances, e.g. $\rho$ meson, with the extrapolation method. The reason is quite simple: Lattice QCD calculation shows that the pion mass quickly becomes heavier as the ud quark mass increases so that the kinematical condition $2m_\pi < m_\rho$ is not satisfied anymore at the unphysically large ud quark mass. It is theoretically difficult to predict the real world, where the $\rho \to \pi\pi$ decay is allowed, by the chiral extrapolation from the virtual world with the decay

\[\text{Similar hadron spectrum is obtained by the BMW Collaboration.}\]

It is likely that their continuum extrapolation using the simulations at three lattice spacings succeeds in removing the $O(\Lambda_{QCD} \cdot a)$ errors which are the leading finite lattice spacing effects in their formulation.
forbidden. Fourthly, our final destination is to simulate the different up and down quark masses, which is an essential ingredient for the proton mass calculation. The isospin breaking effects are so tiny that the reliable evaluation would be difficult with the chiral extrapolation method.

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure5}
\caption{Nucleon result of SU(3) Heavy Baryon ChPT fit up to NLO for the octet baryon masses.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure6}
\caption{Light hadron spectrum in 2+1 flavor QCD with $m_\pi$, $m_K$, $m_\Omega$ as physical inputs.}
\end{figure}

4 Conclusion and Future Plan

In the history of lattice QCD simulation the computational cost has been a big issue preventing us from the direct simulation at the physical point. The chiral extrapolation method, which is just a compromise due to the lack of computational power, has intrinsic problems to be avoided. Thanks to the rapid increase of computational power and the algorithmic improvements in last decade the PACS-CS Collaboration are now able to simulate the physical point directly on a (6 fm)$^3$. We are going to incorporate the up-down quark mass difference and the electromagnetic interactions in the next step.

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