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VERIFYING THE GELL-MANN-OAKES-RENNER RELATION FOR HEAVY SIMULATED QUARKS IN QUENCHED LATTICE QCD

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Abstract. Since its inception in the 1970s, lattice quantum chromodynamics (QCD) has revolutionized the study of quantum particles by allowing extremely difficult quantum field theory (QFT) calculations to be accomplished computationally and by providing an effective way to compare theoretical predictions with experiment. In this paper, we investigate the application of quenched lattice QCD to verify the Gell-Mann-Oakes-Renner (GMOR) relation, which states that the squared pion mass is proportional to the sum of the up and down quark masses. In our simulation, we restricted ourselves to relatively large simulated quark masses. We conclude that several improvements to the simulation are necessary before it can accurately verify the GMOR relation.

1. Introduction

Lattice quantum chromodynamics (QCD) is a powerful tool that discretizes spacetime, the combination of the three dimensions of space and one dimension of time into a single fabric used to describe the location of events, into a 4D lattice of evenly spaced points. Like any other quantum field theory, lattice QCD is described by an action S, a functional (i.e. function of fields) which encodes the interactions, dynamics, and symmetries of a theory. This discretization from a continuous theory into a discrete one, however, requires a lot of care as to preserve all of the symmetries of the continuum theory such as the action's gauge invariance, a purely mathematical redundancy that is essential for constructing a consistent theory. Another restriction on possible lattice QCD actions is that these actions must equate to the continuum QCD action in the limit of small lattice spacing. Such an action must be constructed from link variables $U_\mu(n)$ that impose gauge invariance on the action. Under these restrictions, the Wilson gauge action, the base action used to describe lattice QCD without fermions, can be written as [4]

$$S_G[U] = \frac{\beta}{3} \sum_{n \in \Lambda} \sum_{\mu < \nu} \operatorname{Re} \operatorname{tr} \left[\mathbb{1} - U_{\mu\nu} \right], \tag{1}$$

where the plaquette $U_{\mu\nu}$ is defined as the shortest nontrivial loop of link variables on the lattice, a square in directions μ and ν, where μ and ν are different numbers

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between 0 and 3 corresponding to the x, y, z, t directions respectively, and is given by the expression

$$U_{\mu\nu} = U_\mu(n)U_\nu(n+\hat{\mu})U_\mu(n+\hat{\nu})^\dagger U_\nu(n)^\dagger. \tag{2}$$

Note that the Wilson gauge action is not the only possible lattice QCD gauge action, and there are numerous other improved actions that have been utilized [8].

Special care is required when deriving the Wilson fermion action, the base lattice QCD action for fermions, due to a problematic phenomenon known as the doubling problem [4].

$$S_F[\psi, \bar{\psi}, U] = \sum_{f=1}^{N_f} a^4 \sum_{n,m\in\Lambda} \bar{\psi}^{(f)}(n) D^{(f)}(n|m) \psi^{(f)}(m) \tag{3}$$

where

$$\begin{aligned} D^{(f)}(n|m) = \left(m^{(f)} + \frac{4}{a}\right)\delta_{\alpha\beta}\delta_{ab}\delta_{n,m} - \frac{1}{2a}\sum_{\mu=1}^{4}(\mathbb{1}-\gamma_\mu)_{\alpha\beta}U_\mu(n)\delta_{n+\hat{\mu},m} \\ - \frac{1}{2a}\sum_{\mu=1}^{4}(\mathbb{1}+\gamma_\mu)_{\alpha\beta}U(n-\hat{\mu})^\dagger\delta_{n-\hat{\mu},m} \end{aligned} \tag{4}$$

To clarify the various variables used, $m^{(f)}$ is the fermion mass, the deltas are Kronecker deltas of various indices, and γ_μ are the Dirac gamma matrices. Greek letters are used for spin indices and Latin letters are used for color indices. Note that a represents both an index and the lattice-spacing but it is clear which is which by context.

We approach the problem of calculating observables in this theory non-perturbatively, using the following path integral to find expectation values (i.e. average value) of an arbitrary observable O

$$\langle O \rangle = \frac{1}{Z}\int \mathcal{D}[U]e^{-S_G[U]}\mathcal{D}[\psi,\bar{\psi}]e^{-S_F[\psi,\bar{\psi},U]}O[\psi,\bar{\psi},U]. \tag{5}$$

The path integral over Grassmann variables ψ and $\bar{\psi}$, anti-commuting numbers used to encode fermion statistics, can then be evaluated analytically depending on the operator's dependence on ψ and $\bar{\psi}$.

The resulting path integral over link variables must then be evaluated computationally. Seeing as the dimensionality of the integral increases proportionally to lattice volume, using standard numerical integration techniques is not practical for all but the smallest lattices. Therefore, we apply Monte Carlo methods, randomly selecting points according to the probability distribution

$$dP(U) = \frac{e^{-S[U]}\mathcal{D}[U]}{\int \mathcal{D}[U]e^{-S[U]}}, \tag{6}$$

and averaging them over many samples to find the expectation value of the observable via

$$\langle O \rangle = \lim_{n\to\infty}\frac{1}{N}\sum_{n=1}^{N} O[U_n]. \tag{7}$$

In this paper, we focus on evaluating the pion correlation function, an expectation value, which takes the form

$$C(n_t) = \sum_{\vec{n}\in\Lambda_3} -\frac{1}{Z}\int \mathcal{D}[U]e^{-S_G[U]}\,\mathrm{tr}\left[D_u^{-1}\,(n|0)\,D_d^{-1}\,(n|0)^\dagger\right]\det\left[D_d\right]\det\left[D_u\right]. \tag{8}$$

However, the determinants in the equation above are very computationally expensive to calculate. Therefore, we make use of the quenched approximation, setting these both equal to the identity matrix. Here, we consider a lattice with time dimension N_t; n_t is then the location within the time dimension (i.e. $0 \leq n_t \leq N_t$). $C(n_t)$ defined in this manner allows us to extract physical information. Since n_t can be viewed as the time between creation and annihilation of the pion and $C(n_t)$ has to do with the propagation of the pion, it is natural that C depends on n_t.

For large n_t and $N_t - n_t$, $C(n_t)$ is dominated by the simple exponential behavior $e^{-n_t E_0}$ where the ground state energy E_0 corresponds to the mass of the pion [4]. We will utilize this fact to extract the calculated mass, m_{eff}, of the pion based on what we chose as the quark mass in the simulation. m_{eff} is found by obtaining the exponential constant, or alternatively, the slope on a semilog plot, according to

$$m_{\text{eff}} = \ln\left(\frac{C(n_t+1)}{C(n_t)}\right). \tag{9}$$

With m_{eff} determined in this manner, we can test if the relationship between the particle's mass and the sum of masses of the up and down quarks is accurately described by the Gell-Mann-Oakes-Renner (GMOR) relation [7]

$$m_\pi^2 = \frac{\langle q\bar{q}\rangle}{f_\pi^2}\,(m_u + m_d). \tag{10}$$

Equation (10) states that the pion's (i.e. a composite particle) squared mass m_π^2 is proportional to the sum of the mass of the up and down quarks by a constant related to the expectation value of a quark bilinear $\langle q\bar{q}\rangle$ and the squared pion decay constant f_π^2. In other words, GMOR predicts $m_{\text{eff}} = m_\pi \sim (m_u + m_d)^{0.5}$, which we can test computationally.

2. Methods and Materials

2.1. Lattice QCD numerical simulation using Markov chain Monte Carlo method. To create our lattice QCD numerical simulation, we used C++23 in conjunction with the `Eigen` linear algebra library [5]. We utilized the `Eigen` library due to its versatility, speed, reliability, and ample support for sparse matrices [5]. To generate the random numbers necessary for our simulations, we used the random library of C++. Additionally, we ran the program using the flags `-O3 -march=native -funroll-loops -fopenmp -ffast-math -ftree-vectorize` to significantly speed up the linear algebra calculations involved. The source code for the simulation is available at `https://github.com/DavidPevzner17/pion-correlators`. Simulations were run on a Dell Inspiron 14 5410 (Dell Technologies; Round Rock, TX), taking about 5-6 minutes per quark mass combination.

Considering our relatively coarse lattice of $8 \times 8 \times 8 \times 16$ ($8^3 \times 16$, for 3 spatial dimensions plus time), we chose a relatively large lattice spacing of 0.30. We can then find $\beta = 5.48$ which is related to the strength of the coupling constant using the Necco-Sommer scaling relation [9, 6], which relates the lattice spacing and β.

$$\ln(2a) = -1.6804 - 1.7331(\beta - 6) + 0.7849(\beta - 6)^2 - 0.4428(\beta - 6)^3. \tag{11}$$

The simulation has two main phases: first, equilibrating the Markov chain for generating link variables according to the probability distribution in (6) using the Metropolis Monte Carlo algorithm [2] and, second, using this Markov chain to compute the observable. The pseudocode for this is shown in Algorithm 1. Note that the majority of the code are support functions, used for updating the link variable and computing the observable (i.e. correlation function $C(n_t)$ in our case).

Algorithm 1: Structure of a program for lattice QCD

```
// Phase 1, equilibrate Markov chain
Initialization
for n = 1 to n_equil do
    Update the global link variable U using Algorithm 2
end
// Phase 2, repeatedly sample the observable
for n = 1 to n_measure do
    Compute the observable C(n_t)
    for n = 1 to n_lag do
        Update the global link variable U using Algorithm 2
    end
end
```

In the first phase, we generate the global link variable as a 5D array of 3×3 matrices from a cold start then perform $n_{\text{equil}} = 5000$ sweeps. For each link in the array, the sweep proposes a new link variable and then accepts this new link with probability $e^{-\Delta S_G}$ where $\Delta S_G = S_G[U_\mu(n)'] - S_G[U_\mu(n)]$. The proposed link is generated by scaling the old link by a randomly selected SU(3) matrix from an array of $n_{\text{set}} = 10000$ SU(3) matrices that are created by embedding SU(2) matrices into 3×3 matrices. The generation of these SU(2) matrices is done according to a parameter ϵ which can be adjusted as needed to maximize efficiency. For our purposes, we have set $\epsilon = 0.12$ so that our acceptance rate of proposed links is around 70%. Note that this set consists half of unique SU(3) matrices and half of these matrices' adjoints so as to ensure a symmetric selection probability. After many sweeps, this Markov chain will reach an equilibrium distribution described by (6), allowing us to sample from it. Algorithm 2 gives pseudocode that describes how the global link variable is updated.

As the second phase of the calculation, we then perform $n_{\text{measure}} = 10$ measurements of the correlation function. In this case, a measurement is done by evaluating the trace in (8). Rather than calculating and storing the full propagators $D_u^{-1}(n|m)_{ba}^{\beta\alpha}$ and $D_d^{-1}(n|m)_{ba}^{\beta\alpha}$, we calculate each column of the propagators by considering fixed indices α_0, a_0, and m_0 so that

$$D^{-1}(n|m)_{ba_0}^{\beta\alpha_0} = \sum_{m,\alpha,a} D^{-1}(n|m)_{ba}^{\beta\alpha} S^{(m_0,\alpha_0,a_0)}(m)_a^\alpha, \tag{12}$$

where we have introduced point sources

$$S^{(m_0,\alpha_0,a_0)}(m)_a^\alpha = \delta(m - m_0)\delta_{aa_0}\delta_{\alpha\alpha_0}. \tag{13}$$

Algorithm 2: Metropolis Monte Carlo algorithm sweep function for updating global link variable U

```
Initialization
for all points i on the lattice do
    Generate random SU(3) matrix
    Multiply ith link U(i) by this matrix to get updated link
    Generate random integer R from 0 to 1
    if e^{-ΔS_G} ≥ R // lower energy solution
     then
        Change link to updated link
    end
end
```

This way, propagator columns G can be calculated by solving the equation

$$DG = S \tag{14}$$

using the biconjugate gradient stabilized method, often abbreviated as BiCGSTAB [10]. Nonetheless, performing these propagator calculations is by far the most time-consuming part of the program.

Each measurement is then followed by $n_{\text{lag}} = 5$ sweeps to generate a new state for the link variables, reducing autocorrelation errors [1]. All of these measurements are then averaged to get an approximation of the correlation function for a particular n_t.

A problem that arises with the above method is that of exceptional configurations; we may end up with small eigenvalues for the operator $D[U]$, causing the inversion of $D[U]$ to break down. To remedy this, we need to decrease the magnitude of fluctuations of the eigenvalues by smearing over the gauge field. That is, we need to replace link variables by local averages over neighboring links, ultimately keeping the long distance behavior the same. In particular, we have used Albanese Parisi Evertz (APE) smearing where the link becomes [3]

$$U_\mu(n)' = P_{\text{SU(3)}} \left\{ (1-\alpha)U_\mu + \frac{\alpha}{6} \sum_{\nu \neq \mu} C_{\mu\nu}(n) \right\}, \tag{15}$$

where

$$C_{\mu\nu}(n) = U_\nu(n)U_\mu(n+\hat{\nu})U_\nu(n+\hat{\mu})^\dagger + U_\nu(n-\hat{v})^\dagger U_\mu(n-\hat{\nu})U_\nu(n+\hat{\mu}-\hat{\nu}) \tag{16}$$

and the matrix is being projected to SU(3) via a procedure involving the Gram-Schmidt process. We set the parameter α as $\alpha = 0.5$.

2.2. **Finding pion mass and verifying the GMOR relation.** In this paper, we have collected data from this simulation for three trials of 16 different combinations of up and down quark mass on a $8^3 \times 16$ lattice with the parameter values discussed above. From the correlation functions ($C(n_t)$), we can find the effective pion mass (m_{eff}) as the absolute value of the slope of the correlation function for large n_t and $N_t - n_t$, obtained via (9), effectively, the midpoint slope on a semilog plot. Therefore, for a particular choice of m_u and m_d we calculate m_{eff} by averaging over

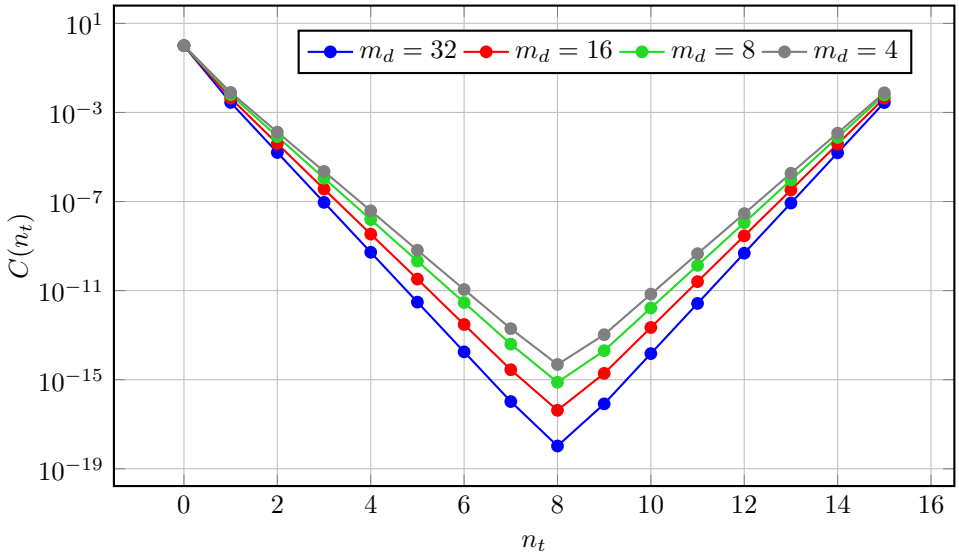

FIGURE 1. Correlation functions $C(n_t)$ vs. n_t for $m_u = 32$ and $m_d = 32, 16, 8, 4$, with lines connecting the points to guide the eye. Masses are given in lattice units. $n_{measure} = 10$. V shape indicates simple exponential behavior at large n_t and $N_t - n_t$ [4].

the slope over between all points except between 0 and 1, 7 and 8, 8 and 9; the censored points are endpoints or cusps in $m_u + m_d$.

To verify the validity of the GMOR relation, we plotted our calculated pion mass vs. the sum of our simulated quark masses on log-log axes. If the GMOR holds true, we would expect to see a linear line with a slope of 0.5, i.e. $m_{\text{eff}} \sim (m_u + m_d)^{0.5}$, based on (10).

3. Results

To give an idea of the shape of our correlation functions and effective mass plots, we have included them Figures 1 and 2 for various simulated masses of the up and down quarks. Figure 1 shows $C(n_t)$ as a function of n_t. The V shaped curve is to be expected and reflects how the correlation function $C(n_t)$ is dominated by simple exponential behavior $e^{-n_t E_0}$ for large n_t and $N_t - n_t$ [4]. Figure 2 shows the midpoint slope of segments in Figure 1 as a measure of m_{eff}, obtained from (9).

Table 1 summarizes effective pion masses for various combinations of up and down quark masses, using the data of Figures 1 and 2.

4. Discussion

4.1. **Finding pion mass.** Analyzing the data in Table 1, it is clear that the pion mass (m_{eff}) is a function of the sum of the up and down quark masses ($m_u + m_d$) because there is no significant statistical difference between pion masses whenever the quark mass sum is the same, i.e. cross-diagonal terms are equal in Table 1. For

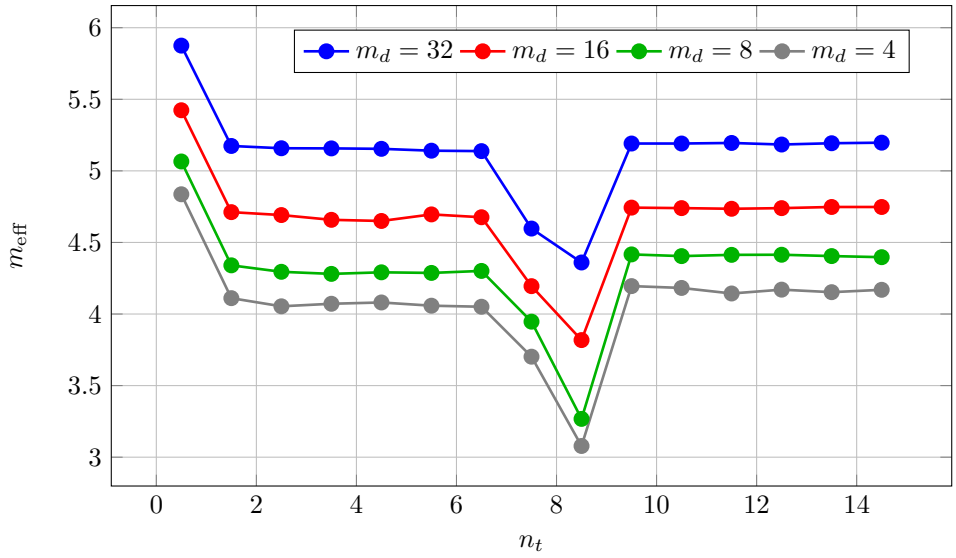

FIGURE 2. m_{eff} vs n_t for $m_u = 32$ and $m_d = 32, 16, 8, 4$. Masses are given in lattice units. $n_{measure} = 10$. Points here are the midpoint slope of segments in Figure 1. Slopes at the endpoints and cusp are ignored in subsequent analyses.

TABLE 1. 95% confidence intervals for mean effective mass m_{eff} of the pion for various combinations of m_u and m_d values. Masses are given in lattice units. $n_{measure} = 10$.

m_u \ m_d	4	8	16	32
4	2.97(5)	3.25(3)	3.63(4)	4.12(4)
8	3.25(6)	3.51(1)	3.87(1)	4.36(2)
16	3.64(3)	3.89(2)	4.24(2)	4.71(4)
32	4.12(1)	4.35(1)	4.71(1)	5.17(1)

differing quark mass sums, where $m_u \neq m_d$, or moving along diagonals, there is a noticeable difference. To quantify this difference, we constructed a table of m_{eff} vs $m_u + m_d$ by combining confidence intervals of equal mass sum in Table 1 (i.e. taking union of intervals), as shown in Table 2.

Using the data of Table 2, we can create a graph (Figure 3) on log-log axes of the pion mass (m_{eff}) vs the sum of the simulated quark masses ($m_u + m_d$), to verify the scaling of m_{eff} versus $m_u + m_d$ predicted by the GMOR relation of (6).

4.2. **Verifying the GMOR relation.** If the GMOR relation holds we would expect to see a linear line with a slope of 0.5 in Figure 3. However, we found that the data were well described by a regression line of slope 0.26 with $r^2 = 0.98$. That is, the pion mass was proportional to $(m_u + m_d)^{0.26}$ rather than $(m_u + m_d)^{0.5}$, which

TABLE 2. 95% confidence intervals for mean effective mass m_{eff} of the pion for various $m_u + m_d$ values. Masses are given in lattice units.

$m_u + m_d$	8	12	16	20	24
m_{eff}	2.97(5)	3.25(6)	3.51(1)	3.63(4)	3.89(2)

$m_u + m_d$	32	36	40	48	64
m_{eff}	4.24(2)	4.12(4)	4.36(2)	4.71(4)	5.171(5)

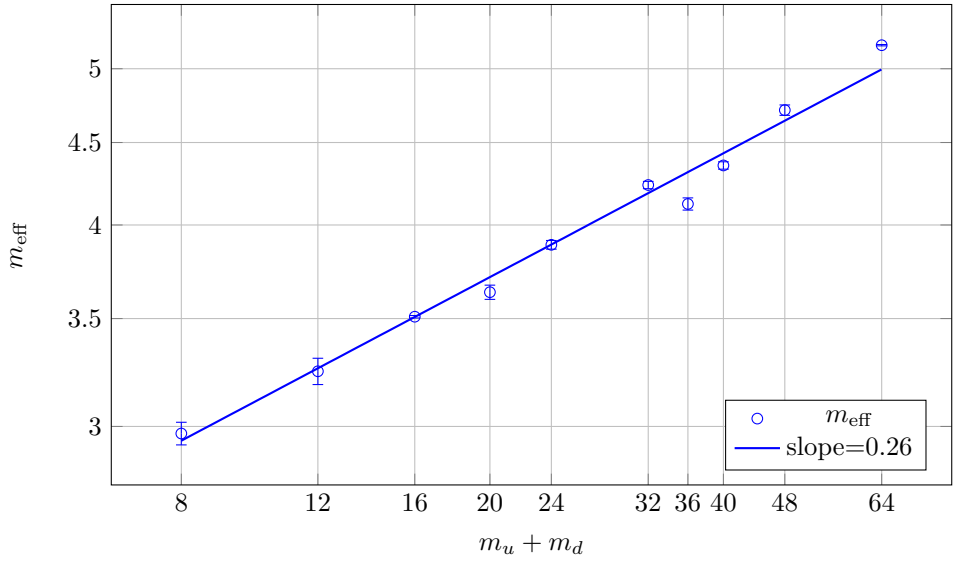

FIGURE 3. Log–log plot of m_{eff} vs. $m_u + m_d$ with 95% confidence intervals. Masses are given in lattice units. Data from Table 2. For these data, $m_{\text{eff}} \sim (m_u + m_d)^{0.26}$ with $r^2 = 0.98$.

is clearly highly inaccurate, meaning we were unable to verify the GMOR relation for quenched lattice QCD simulations. The cause of this significant error is likely our use of the quenched approximation which is known to yield large error when applied to calculating effective masses [6]. Smaller contributions to this error could also come from our use of a relatively small $8^3 \times 16$ lattice. In checking for convergence, we were able to try lattices with fewer points, but due to the dimensionality of the system, scaling up would significantly increase run times.

Although we were unable to verify the GMOR relation between pion masses and simulated quark masses, in this paper, we gained valuable insights into improvements that can be made to accurately verify the GMOR in future simulations. Most notably, we demonstrated that the quenched approximation results in large errors when calculating effective masses. Therefore, in future works, our results could be improved by simulating dynamical quarks rather than quenched quarks. This would take much more computational resources, however, due to the difficulty of calculating large determinants. As a result, a more powerful computer would

be needed to perform such simulations. Moreover, in the future, improved actions other than the basic Wilson action can be applied to extend our results into the domain of smaller and more physical quark masses.

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