Using QCDLAB2 to Define Lattice Parameter

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Abstract: - Lattice Quantum Chromodynamics (LQCD) may be studied in low-energy regimes where non-perturbative approaches are useful because of their computational methods. Determining the lattice parameter, sometimes referred to as the lattice scale or lattice parameter, is a crucial objective in LQCD computations. The best way to get this parameter is to examine the quark-antiquark potential's behavior, which in LQCD simulations may be obtained by first computing the Wilson loops. We used an improved version of QCDLAB 2.0, a program specifically designed for lattice QCD simulations, in this paper. We concentrated on computing planar Wilson loops to extract the interquark potential. SU (3) gauge field configurations were used as the background field in the simulations. In contrast to the earlier work, we present it for larger lattice volumes of 16^4, 32^4, 48^4, and 64^4 in this publication. These simulations are configured with four distinct values of the coupling constant, which correspond to different background field configurations. One-hundred-gauge field configurations that were statistically independent were created and examined for every example. To derive the lattice scale for different lattice volumes, we used Python. It is feasible to translate physical values measured in lattice units into ordinary physical units once the lattice scale is defined. In our previous study, we used the FermiQCD program. With Artan Borici's help, we then switched to the more effective and user-friendly QCDLAB version 2.0, which greatly increased the efficacy of our simulations. In this study, we introduce an upgraded version of QCDLAB2 that uses Python to compute, even for dense lattices.

Key-Words: - algorithms, computational techniques, lattice Quantum Chromodynamics (QCD), lattice scale, QCDLAB version 2.0, numerical simulations, Python, Wilson loop calculations.

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1 Introduction

Quantum Chromodynamics (QCD) is the theoretical framework that describes the strong interactions between particles such as quarks and gluons. QCD, a quantum field theory, governs these interactions and exhibits two distinct behaviors: asymptotic freedom at high energy or short distances, and confinement at low energy or long distances, where quarks and gluons are bound into composite particles called hadrons. The quark model, first proposed in 1964 introduced the concept that hadrons are composed of more fundamental particles known as quarks, [1]. Experimentally, quarks were first observed in particle accelerators during the 1970s. Notably, quarks are never isolated but are always confined within hadrons or in neutral-colored groupings.

Lattice QCD (LQCD), which is the formulation of QCD on a lattice, is one of its main uses, [2]. Other important phenomena covered by QCD include the study of asymptotic freedom, perturbative techniques in gauge theories, and other applications described in [3]. One method for resolving the theory in low-energy or non-

perturbative regimes is the lattice formulation of QCD. Lattice QCD discretizes the theory on a four-dimensional grid with N points in each direction, consisting of three spatial dimensions and one temporal dimension. The sites on this lattice are quark fields, while the linkages between the sites are gluon fields. A cutoff momentum proportional to a^{-1} is introduced by this discretization, where a stands for the lattice spacing. The theory approaches the continuum formulation of QCD as the lattice spacing gets closer to zero. Lattice QCD makes it possible to precisely define QCD mathematically and quantify physical quantities accurately through numerical simulations by using non-perturbative techniques. To maintain the theory's clarity and computational manageability, the lattice spacing acts as an ultraviolet regulator. The energy transported by the gauge fields over a distance R is represented by the potential between two static quarks, [4]. Physical quantities cannot be calculated using perturbative methods since the energy grows as R does. The theory of quark confinement holds that quarks cannot exist independently and are constantly confined by hadrons. It is especially crucial to study the quark-antiquark potential at tiny distances because non-perturbative techniques may be used since lattice QCD simulations yield accurate findings in this range. Quarks are trapped in hadrons and cannot be seen in isolation, as proved by [5], [6] on the potential between static quarks in the 1970s. The quark-antiquark potential grows linearly at great distances, according to his studies, [4]. This linear behavior of the potential at intermediate distances has been confirmed by further research and more recent investigations, proving that quarks are uniformly contained within hadrons in all SU(3) representations, [5], [6], [7]. It is crucial to use a quantity that can be accurately measured experimentally and calculated in simulations to derive physical quantities from lattice QCD.

This need is met by the string tension σ, which is the energy per unit length along the line joining two static color quarks. The lattice spacing a may be computed using σ as a reference. Dimensionless values derived from lattice simulations may be transformed into physical units thanks to this parameter. Wilson loops in lattice QCD may also be used to determine the string tension σ, a technique that has been investigated in previous research, [8], [9], [10], [11]. Using the QCDLAB software program, version 2.0, [12], [13], this study presents a novel technique for measuring the quark-antiquark potential, building on these fundamental references, [14], [15], [16], [17]. For small to medium-scale lattice QCD issues, QCDLAB provides moderate scalability, making it ideal for academics looking for quick prototyping and ease of use. However, specialized frameworks such as Chroma or QUDA are more effective for large-scale production-level calculations.

By utilizing the advancements in this research, we want to maximize the accuracy and efficiency of lattice QCD simulations by improving the quark-antiquark potential computation. We bring here an updated version of QCDLAB2, and we are testing it for larger lattice volumes using Python, [17], [18], [19], [20], [21], [22].

2 Problem Formulation

In lattice QCD calculations, obtaining dimensional results is crucial. To achieve this, we calculated the lattice spacing a. This was achieved by utilizing the QCDLAB2 software program and Python to calculate the effective quark potential produced from Wilson loops with planar geometry, assessed for various lattice volumes: 16^4, 32^4, 48^4, and 64^4. Here, we suggest a brand-new technique for figuring out the potential between two quarks. By examining the Wilson loops' long-time behavior, this possibility can be discovered.

With a rectangular geometry, we first create a closed route C (R, T), where T is the time dimension. A mathematical definition of the Wilson loops W (R, T) is the trace of the route-ordered products of the link variables U_μ (n) directed along the path C (R, T). We build these loops from this path. The links between a quark-antiquark pair at rest, separated by a distance R, and changing over time T are represented by the resultant loop.

In the context of Euclidean space-time geometry, the observable derived from these loops provides the ground state energy for large T values. By calculating the energy, we evaluated the correlation function of two static quark operators over various time intervals. This approach allows us to compute the quark-antiquark potential with improved precision and efficiency.

$$W(R,T) = \langle 0|O_R(0)O_R(T)^*|0\rangle \\ \langle O_R(0)O_R(T)^*\rangle \qquad (1)$$

The gauge-invariant operator, $O_R(t)$, may be found as follows:

$$O_R(t) = \bar{q}(t,0)U\big((t,0)\to(t,R)\big)q(t,R) \qquad (2)$$

The gauge field between two static quarks from site (t, 0) to site (t, R) is represented by the link $U\big((t,0)\to(t,R)\big)$. Consequently, the Wilson loops have been established from the expression:

$$W(R,T) = \langle tr\, U\big((0,0) \to (0,R)\big)U\big((0,R) \to (T,R)\big)U\big((T,0) \to (T,R)\big)^{*}U\big((0,0) \to (T,0)\big)^{*}\rangle \quad (3)$$

Additionally, these loops can be expressed as:

$$W(R,T) = \sum_{n\geq 1} c_n e^{-V_n(R)T} \quad (4)$$

In this case, the state with the lowest energy is indicated by the formula V1(R) ≡ V(R), whereas the remaining states for n > 1 represent the potentials in the excited states.

3 Jackknife Method to Calculate Statistical Errors

Discrete gauge fields and quark fields must be simulated using Monte Carlo methods across a wide range of statistically independent configurations to measure observables in lattice QCD. Analyzing statistical errors is essential for accurately interpreting these findings. One of the most straightforward and popular methods for estimating uncertainty and correlations in lattice QCD computations is the jackknife method.

To calculate the errors of the derived sizes as in our concrete case with the potential, lattice distance, etc., the most used methods are the non-parametric ones such as Bootstrapping and Jackknife. In determining the errors, we used the Jackknife method, which follows these steps:

Step 1: Create new case choices for i = 1, 2 … n by choosing the initial case x_i for i = 1, 2…n according to the equation:

$$X_i = \bar{x} - \frac{x_i - \bar{x}}{n-1} \quad (5)$$

Step 2: Computes the magnitudes derived as a function of the new choices according to:

$$y_i = f_i(X_1, \ldots, X_n) \quad (6)$$

Step 3: Estimate standard deviation of the mean y according to the expression, [3], [4], [5]:

$$\sigma_{\bar{y}} = \frac{n-1}{n}\sum_i (y_i - \bar{y})^2 \quad (7)$$

Since lattice QCD has limited temporal and spatial extents, correlations between data points are prevalent and readily considered by the Jackknife approach. Because it eliminates the need to create fresh data as the bootstrap approach does, it is especially helpful when there are a small number of independent setups, [3], [4].

4 Problem Solution

Based on the equation (4) we derived the potential under the assumption that:

$$W(R,T) \cong c_1 e^{-V(R)T} \quad (8)$$

The effective potentials have been established by us using:

$$V(R)_{eff} = -\log\frac{W(R,T+1)}{W(R,T)} \quad (9)$$

Furthermore, we used the theoretical physical model to fit the effective potential for a range of R values.

$$V(R)_{eff} = C + \sigma R + \frac{\alpha}{R} \quad (10)$$

The string tension is indicated by σ in equation (10), while the coefficient of the Coulomb term is represented by the constant parameter α. A modified variant of equation (10) stated in lattice units can be obtained by multiplying it by the lattice spacing.

$$\hat{V}(R)_{eff} = \hat{C} + \hat{\sigma}\frac{R}{\mathrm{a}} + \frac{\mathrm{a}}{R}\hat{\alpha} \quad (11)$$

As stated earlier, the QCDLAB2 software was used for all simulations. The first program created especially for four-dimensional lattice QCD simulations is QCDLAB version 2.0. Because it is organized as a tiny package with many little programs and algorithms, it makes it possible to examine QCD features without the requirement for specialized algorithm creation or high-performance computer hardware. The software was developed by Professor Artan Borici, who sadly passed away during the COVID-19 pandemic. The integration of QCDLAB2's linear operators with the GNU Octave language's linear operators is a significant benefit over comparable applications. This unique feature facilitates the development and testing of efficient coding programs while significantly reducing the time required to execute these simulations.

In our study, we calculated the string tension σ by performing simulations for 100 independent configurations across lattice sizes 16^4, 32^4, 48^4, and 64^4. The results were fitted to the equation (11), with the fitting range for R chosen with these interval values $R = 0.5$ to $R = 6$. The lattice physical volume L^4 with side length L in each direction corresponds to the lattice volume N^4 with N points per direction, following the relationship $L = aN$, where a is the lattice spacing.

Figure 1, Figure 2, Figure 3 and Figure 4 illustrate the graphical representation of the potential between two static quarks for different lattice volumes. The potential exhibits a Coulomb-

like behavior at short distances as described by the expression, and increases linearly at large distances, following the expression. Markers with error bars represent the simulated data points and the dashed line shows the fitted potential curve.

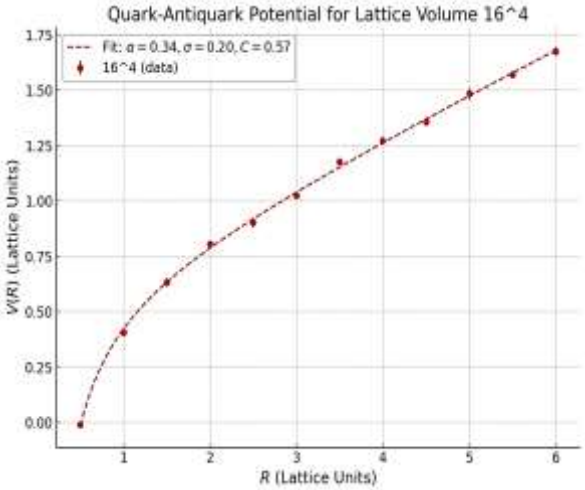

Fig. 1: The potential between two static quarks on a 16^4 lattice, shown in dimensionless units (lattice units)

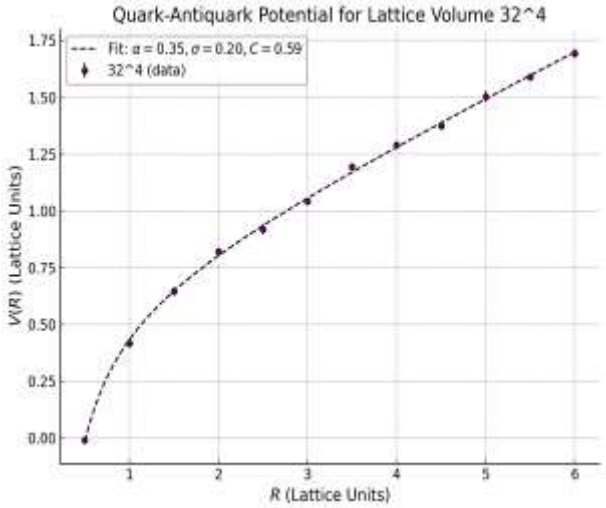

Fig. 2: The potential between two static quarks on a 32^4 lattice, shown in dimensionless units (lattice units)

All simulations were performed using the Wilson action on 16^4, 32^4, 48^4, and 64^4 lattices with various background gauge fields. Specifically, we utilized 100-gauge field configurations and tested three different coupling constants, using the QCDLAB2 software. The Jackknife method, which is especially useful for estimating the statistical uncertainties of derived quantities, [13], [23], [24], was used to evaluate the statistical errors for the parameters in equation (10).

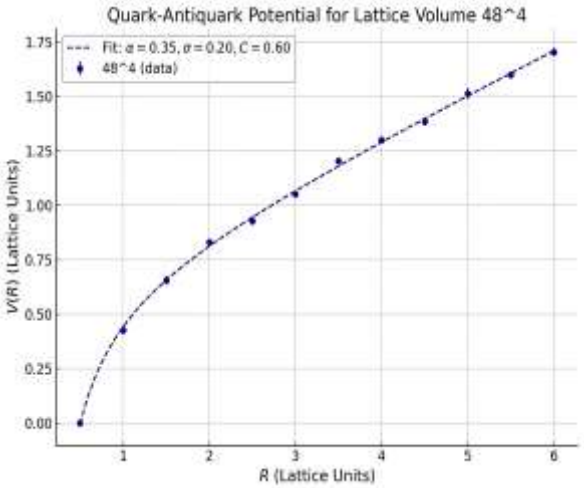

Fig. 3: The potential between two static quarks on a 48^4 lattice, shown in dimensionless units (lattice units)

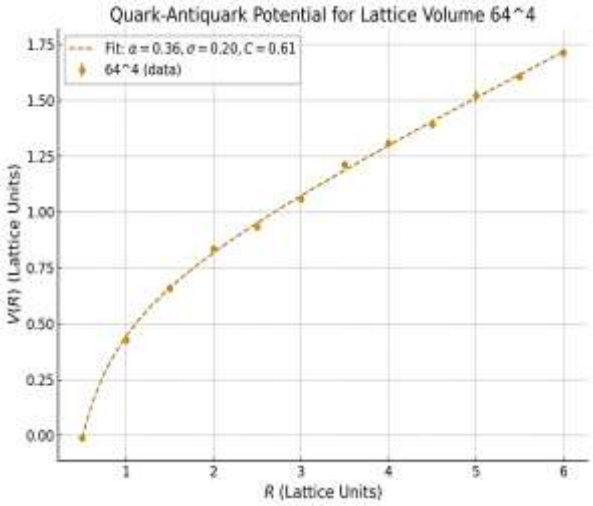

Fig. 4: The potential between two static quarks on a 48^4 lattice, shown in dimensionless units (lattice units)

Table 1. String tension $\hat{\sigma}$ the computed lattice space a, and the corresponding statistical errors for 16^4, 32^4, 48^4, and 64^4 lattice volumes

Lattice	Lattice space (fm)	The string tension parameter (lattice unit)	The error of lattice space	The error of string tension
16^4	0.1286(4)	0.1951(2)	1.091e-05	2.77e-04
32^4	0.1029(1)	0.1974(5)	1.034e-05	3.89e-05
48^4	0.0972(3)	0.2009(6)	1.006e-05	1.54e-05
64^4	0.0900(8)	0.2081(9)	1.001e-05	1.01e-05

Table 1 summarizes the numerical results and the statistical errors that go along with them. The numerical results presented in Table 1 include the values of the lattice spacing parameter and the string tension parameter for 16^4, 32^4, 48^4, and 64^4

lattices. Additionally, the table provides the statistical errors associated with these parameters, calculated using the Jackknife method.

As evident from the data, the values of the lattice spacing and string tension fall within the range of their respective statistical error margins, ensuring the reliability of the calculated results. Specifically, for lattice 16^4 the lattice space parameter is:

$$a = [0.1286(4) \pm 1.091\text{x}10^{-5}]\ (fm) \qquad (12)$$

And the string tension is:

$$\hat{\sigma} = [0.1951(2) \pm 2.77\text{x}10^{-4}]. \qquad (13)$$

After these calculations, we can make a continuum extrapolation to take the real value of string tension as it is shown in Figure 5.

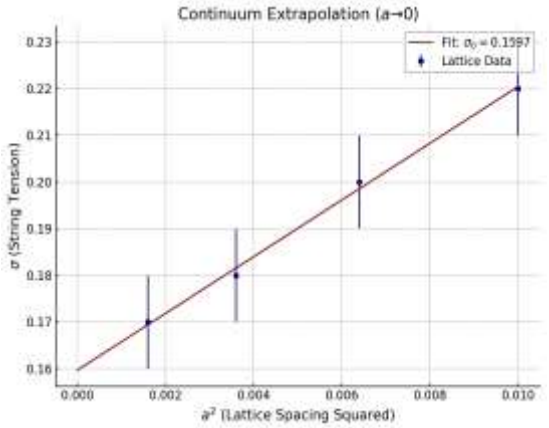

Fig. 5: The continuum limit (a→0) extrapolation of string tension parameter

On the other hand, we can provide it even by infinite volume extrapolation [23], [24], as it is shown in Figure 6.

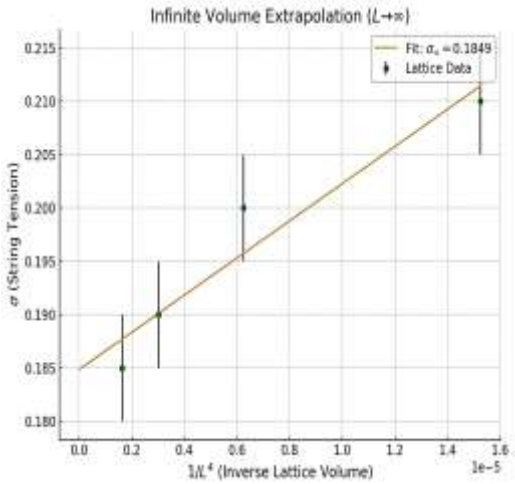

Fig. 6: The infinite volume extrapolation ($L\rightarrow\infty$) of string tension parameter

5 Conclusion

In lattice QCD simulations, Wilson loops may be used to calculate the lattice spacing for various lattice volumes and coupling constants. For a lattice volume of 16^4, the lattice spacing is = 0.128; for 32^4, it is a = 0.103; for 48^4, it is a = 0.097 and for 64^4, it is a = 0.09. Using simple yet highly effective software, we successfully determined the lattice spacing for various lattice volumes. Once the lattice spacing is established, all physical quantities can be derived from dimensionless values, expressed with their corresponding physical units.

The graphical results, shown in Figure 1, Figure 2, Figure 3 and Figure 4, demonstrate that the potential between two static quarks exhibits a key feature of QCD at low energy regimes: quark confinement. This expected outcome underscores the efficiency and utility of QCDLAB2 software, even for dense lattices. One of our group's future goals is to develop simulation and inversion algorithms that further optimize computation times. QCDLAB version 2.0, an advancement over version 1.0, is designed for four-dimensional simulations, making it suitable for lattice QCD simulations in SU (3) gauge fields. To achieve even greater accuracy in our results, future work will involve incorporating a larger number of Wilson loops into simulations and conducting analyses at larger R values. This will necessitate larger lattice volumes and extensive statistical computations.

In conclusion, the updated version of QCDLAB2 proves to be highly promising software for lattice QCD simulations and holds significant potential for further advancements in this field. For specifying lattice parameters in lattice QCD simulations, QCDLAB2 offers a robust framework. It works very well for different lattice volumes starting from small sizes to larger volumes. Researchers can benefit from its extensive feature set and user-friendly design. Subsequent advancements could concentrate on expanding its functionalities to include sophisticated mistake analysis and assistance with frameworks outside QCD.

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Declaration of Generative AI and AI-assisted Technologies in the Writing Process

During the preparation of this work the authors used Grammarly and DeepL Write in order to improve the readability and language of the manuscript and for grammatical accuracy, spelling corrections and readability enhancement. After using this tool/service, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

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Contribution of Individual Authors to the Creation of a Scientific Article (Ghostwriting Policy)

The authors equally contributed to the present research, at all stages from the formulation of the problem to the final findings and solution.

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Conflict of Interest

The authors have no conflicts of interest to declare.