A gentle introduction to lattice QCD

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The present article is intended to be a gentle introduction to lattice methods, particularly focusing on lattice QCD, for last year undergraduate students with enough background in statistical physics and quantum mechanics who would like to delve deeper into the most computational side of modern particle physics. The article begins by briefly presenting QFT and then explains in some detail how and why to introduce the lattice (as formulated by Wilson in 1974) as a regulator. It then goes on to cover to some extent the properties of the lattice and the difficulties arising from it which are not present in the typical continuum formulation. A small project is also included at the end of the article to apply the concepts explained.

***Index Terms*—QFT, QCD, Lattice, Wilson, Monte Carlo**

I. Introduction

With the advent of Quantum Mechanics in the early 20th century, a new way of understanding the mechanics of bodies was born. One that, unlike its classical counterpart (more precisely, its classical limit), rejected determinism altogether (at least in the Copenhagen interpretation) and instead explained the behaviour of systems through concepts typically associated with waves. In fact, a particle would now be associated a wavefunction, which would be a solution of Schrödinger's equation, whose modulus squared would give the probability density of the particle being found in some region of space (at some time). Nonetheless, this formulation of Quantum Mechanics has the same limitation as its classical counterpart, Hamiltonian mechanics: it is nonrelativistic.

In 1905, during Einstein's golden year, he published his theory of special relativity, where he proposed ideas such as time being relative to the observer (i.e: each inertial frame of reference has its own "internal clock", which measures the system's "proper time"). This was in direct conflict with Newton's formulation of Mechanics, where time is postulated time to be absolute (i.e: there is one universal clock and time passes equally for every observer), and since Hamilton's and Newton's formulations of Classical Mechanics are equivalent (i.e: we can recover one from the other and viceversa), Hamiltonian Mechanics had the exact same problem as Newton's formulation: it did not abide relativity. Schrödinger's formulation, being the quantum counterpart of Hamiltonian Mechanics, also encountered the same problem. At the same time, particles were being observed which were clearly relativistic (such as muons coming from particle showers in the atmosphere). What is more, in order to explore the (at the time, theoretical) internal structure of particles which at the time were believed to be fundamental, such as the proton and the neutron, a higher resolution was needed, and that translated to the need of using relativistic particle beams. These and many other reasons motivate us to formulate Quantum Mechanics in a way compatible with relativity, and that is how Quantum Field Theory (QFT) was born.

II. Brief introduction to QFT

The approach to Quantum Field Theory is rather different from the nonrelativistic approach. One no longer has a wavefunction associated to the particle in question, nor is the particle's state represented by a ket contained in a Hilbert space. Instead, the particle is now represented by a field, which can be vector, spinorial or scalar. What is more, the central problem of this formulation is not to diagonalize a Hamiltonian operator in order to know the energy spectrum of the system, as was the case in the nonrelativistic theory, but rather to calculate correlation functions and vacuum expectation values of some time-ordered operator, the probability amplitude of some process (this is widely used in scattering theory) and the decay rates of unstable particles. This can be done in several ways depending on which formulation of QFT one is using, but the most common one by far is Feynman's path integral formulation.

A. Lagrangian density and scalar fields

There may be two shocking realizations for the student who has not had previous contact with QFT as to the differences between the approach in QFT and in nonrelativistic QM: firstly, the Lagrangian (density) is typically employed instead of the Hamiltonian; secondly, the Lagrangian, which is now built using field operators, is taken *a priori*. That is to say, whilst in nonrelativistic QM one builds the Hamiltonian by taking into account the potential the particle is subjected to (which can usually be inferred or at least modeled to a great extent), the Lagrangian in QFT is the starting point.

Firstly, it is more interesting to use the Lagrangian than the Hamiltonian when building a relativistic theory due to the fact that the former is a Lorentz scalar, whilst the Hamiltonian is associated to the system's energy, which is just one of the components in the momentum four-vector and is therefore not Lorentz invariant.

Secondly, since the Lagrangian density is now used, and since it is a Lorentz invariant, we can try to construct it by using the simplest Lorentz invariant "building blocks" we can think of: scalar fields (ϕ) and, for instance, the lowest order

derivative of said field, $\partial_\mu\phi$, which shall of course be in the form: $\partial_\mu\phi^*\partial^\mu\phi$ so as to be a scalar magnitude. Therefore, one could have a Lagrangian density for a free scalar field as follows:

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi^*\partial^\mu\phi - \frac{1}{2}m\phi^*\phi \tag{1}$$

Note that we have not yet introduced the notion of potential. This Lagrangian only takes into consideration a free particle which can be represented by a scalar field (for instance, Higgs' boson; the rest of the known fundamental particles all have nonzero spin). It is precisely when one considers the interaction of these particles with some potential that gauge theories become relevant.

B. Gauge theories

There are several ways to define a gauge theory, but two of the most relevant ones can be found in [1]. The first definition offers the typical explanation of what a gauge theory is, whilst the second one, whilst being somewhat more abstract, is crucial for understanding Wilson's formulation of the lattice.

1) Gauge theories and local symmetry transformations

A gauge theory is simply a quantum field theory in which the Lagrangian (although some lattice texts prefer to speak in terms of the action) is left invariant under the effect of the members of some local transformation group, called the "gauge group". It is important to notice the symmetry is *imposed*: we ask the Lagrangian to remain invariant under the symmetry transformations we have come up with and then we define a covariant derivative D_μ, which takes the place of the partial derivative in (1). It is also crucial to remember the symmetry must be local, which is a nontrivial step. Let us formulate the simplest gauge theory that comes to mind, which is the invariance under a (local) phase.

We shall begin with the free scalar field in (1). We see that, if we do the transformation:

$$\phi \to e^{i\alpha}\phi; \quad \alpha \in \mathbb{R}$$

then the Lagrangian is left invariant, since the phases cancel out each other. Therefore, the Lagrangian is said to be invariant under the $U(1)$ transformation group (unitary matrices in one dimension, which is equivalent to a phase). Nonetheless, the Lagrangian is still not gauge invariant under $U(1)$ because, by definition, a gauge symmetry group needs to be local. Let us study how the Lagrangian transforms when we allow the phase α to be a function of the spacetime coordinates. In the mass term, we see the phases still cancel out. Nonetheless, in the first term the partial derivative extracts one additional factor:

$$\partial_\mu(\phi^* e^{-i\alpha(x)}) = \partial_\mu\phi^* e^{-i\alpha(x)} - i\partial_\mu\alpha(x)\phi^* e^{i\alpha(x)}$$

And so we see the Lagrangian would no longer remain invariant, since the partial derivative picks up an extra term due to the chain rule. We are therefore compelled to define a new operator to plug into the Lagrangian, such that it is indeed left invariant under local gauge transformations (i.e: we ask for this operator to transform covariantly under the transformations of the gauge group). Let us propose the following covariant derivative:

$$D_\mu \equiv \partial_\mu - iqA_\mu \tag{2}$$

Where the factor q measures the coupling of the matter field to the gauge field (i.e: how strongly it feels the potential) and A_μ is a vector potential. Our new Lagrangian, which is indeed (rather by definition) invariant under this local gauge group, is:

$$\mathcal{L} = \frac{1}{2}(D_\mu\phi^*)(D^\mu\phi) - \frac{1}{2}m\phi^*\phi \tag{3}$$

And indeed, it is left invariant under the transformation $\phi \to \phi e^{i\alpha(x)}$, because since the new operator transforms covariantly, its contraction with itself is a scalar. Nonetheless, the work is not finished: we must now understand *what* the introduced vector potential represents. In order to do that, let us see how the action of D_μ transforms and then impose it to be equal to $e^{-i\alpha(x)}D_\mu\phi^*$. That way, we shall obtain a transformation rule for the vector potential and, hopefully, identify it with some known potential.

$$\begin{aligned} D_\mu\phi^* \to D'_\mu(\phi^* e^{-i\alpha(x)}) &= (\partial_\mu - iqA'_\mu)\phi^* e^{-i\alpha(x)} \\ &= e^{-i\alpha(x)}\left[\partial_\mu\phi^* - i\partial_\mu\alpha(x)\phi^* - iqA'_\mu\phi^*\right] \end{aligned}$$

We now impose the aforementioned equality to hold, and so the expression above must fulfill:

$$e^{-i\alpha(x)}\left[\partial_\mu\phi^* - i\partial_\mu\alpha(x)\phi^* - iqA'_\mu\phi^*\right] = e^{-i\alpha(x)}D_\mu\phi^*$$

Expanding the term on the right and canceling out common factors, we soon reach the conclusion that:

$$A'_\mu = A_\mu - \frac{1}{q}\partial_\mu\alpha \tag{4}$$

And this is just how the electromagnetic vector potential transforms, so that must be it. Indeed, the $U(1)$ local symmetry is associated to the electromagnetic interaction.

One could think once the covariant derivative is found, then one can rewrite the Lagrangian as in (3) and the whole dynamics of the system is captured. However, there is still one term missing, which is that referring to the behaviour of the gauge field itself. So far, we have focused exclusively on the matter field (i.e: the formerly free scalar field), but if one wants the full Lagrangian of the system (this is called the full interacting gauge theory), then one is compelled to introduce an additional term that accounts for the kinetic part of the photon's dynamics. This is accounted for by the field strength tensor $F_{\mu\nu}$, which can be expressed as a generalized curl of the vector potential:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \tag{5}$$

Therefore, the full Lagrangian of our "mock QED theory" would be:

$$\mathcal{L} = \frac{1}{2}(D_\mu \phi^*)(D^\mu \phi) - \frac{1}{2} m \phi^* \phi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \tag{6}$$

This is indeed a "mock" Lagrangian since, in order to keep the explanation simple, scalar fields have been used, which are solutions of the Klein-Gordon equation. Nonetheless, the (fundamental) charged particles (except for the $W^\pm$ bosons) are all spin $1/2$ fermions, and therefore one must use solutions to the Dirac equation. Hence, the real full QED Lagrangian is:

$$\mathcal{L} = \bar{\Psi}(i\not{D} - m)\Psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \tag{7}$$

Where Ψ is a Dirac spinor and $\not{D} = \gamma_\mu D^\mu$, but an explanation of Dirac's equation is not in order, since the reasoning of gauge invariance is the same for all kinds of particles, and the slightly more complex spinor formalism would only opaque the objective of this section.

2) Gauge theories and the path-dependent phase

The second definition of a gauge theory is due to Mandelstam (1962) and Mills (1975). The essence of said definition is brilliantly summarized by Creutz in a single sentence: "the interaction of a particle with a gauge field involves a phase factor associated with any possible world line that the particle might traverse." [1]. Originally, Mandelstam proposed this approach for QED, where the matter field, upon interaction with the photonic field, would pick up a path-dependent phase such that:

$$\Psi \to \Psi \exp\left(i g_0 \int_P A_\mu dx_\mu \right) = U(P)\Psi \tag{8}$$

The last equality simply states we can relate the original field to the field after the interaction through some unitary path-dependent operator $U(P)$. In a non-Abelian theory, as is QCD, the potential is still a four-vector, but its components are matrices, and so in taking their exponentials we find the phase factor becomes a matrix. Therefore, $U(P)$ will in general be a matrix operator. This is a key idea when it comes to understanding Wilson's formulation of the lattice, since it is precisely this second definition of gauge theories that he uses in order to explain how the particles in the lattice interact with each other.

C. Perturbation theory and the need for nonperturbative methods

When working in QFT, one finds it is often the case that the theory, elegant as it may be, is somewhat limited as for the calculations that can be done in an exact manner. So much so that one often resorts to perturbation theory, expanding the amplitude of the process of interest or whichever magnitude one is interested in calculating in terms of some coupling constant. In QED, this is the fine structure constant, $\alpha \sim 1/137$. This perturbative approach, based on Feynman diagrams, was crucial in the development of QED and is still the most used tool nowadays in quantum field theories.

In QCD one can also apply perturbation theory and the corresponding Feynman diagrams, the catch being that this is only possible in the weak coupling limit. QCD predicts quarks are asymptotically free at short distances (i.e: high energies), and therefore the theory behaves similarly to QED. We call this regime "weak coupling", since the coupling constant at these energies is small enough for the perturbative expansion to converge, and to do so reasonably quickly. Nonetheless, at greater distances (i.e: lower energies), the quarks experience a linear potential, so we say they are "confined" (i.e: it would take an infinite amount of energy to separate them an infinite distance). This regime is called "strong coupling", and as one might guess, perturbation theory does not apply in said regime. Therefore, one must resort to other nonperturbative methods, such as dispersion relations (there are some fantastic lectures on this topic. A good beginning would be [2]) or lattice QCD.

III. From the continuum to the lattice

It is now clear why and when one must resort to nonperturbative methods when working with the strong interaction (of course, less complex theories such as QED do not present this need, or at least not for the same reason as QCD, since they do not exhibit strong coupling). Let us now study *how* the lattice is introduced as a regulator in our theory. The construction of the lattice from the ordinary spacetime continuum formulation can be done in three steps: using Feynman's path integral formulation, we can make the problem of calculating vacuum expectation values and correlation functions resemble a statistical mechanics problem in the canonical ensemble. Nonetheless, we will find the analogous to the Boltzmann measure, now given by the system's action, has an imaginary unit, and so we will have to perform a Wick rotation in time to transition to Euclidean spacetime. Finally, we shall reduce the dimensionality of the phase space to a finite number of degrees of freedom. This will effectively turn our problem entirely into one of statistical mechanics, and indeed the connection between the two problems could not be any closer.

A. Feynman's path integral

In nonrelativistic Quantum Mechanics, the central problem of the theory is to diagonalize some Hamiltonian operator in order to study the energy spectrum of the system. In QFT, the approach is somewhat different, and one is chiefly interested in calculating correlation functions, vacuum expectation values and amplitudes, from which the Physics of the system can be extracted. In fact, the typical expectation value of some time ordered observable F (again, for the simplicity of this presentation, we shall stick to using scalar fields) takes the form:

$$\langle F \rangle = \frac{\int \mathcal{D}[\phi] F e^{iS[\phi]}}{\int \mathcal{D}[\phi] e^{iS[\phi]}} \tag{9}$$

where the denominator usually receives the name of "Feynman integral", and is denoted by the letter Z just as the partition function in the canonical ensemble of statistical mechanics. The integration measure, $D[\phi]$, implies one must integrate over all possible field configurations. That is to say,

the scalar field $\phi(x_\mu)$ has some amplitude in every point of the spacetime continuum, and so one must consider all the infinite possible amplitudes at each point in spacetime, for the whole region of spacetime for which the field is defined. Let us notice that, since the degrees of freedom are now the amplitude of the field at each point in spacetime, the action of the system is now constructed as:

$$S = \int \mathcal{L} d^4x \tag{10}$$

Let us observe the close resemblance of expression (9) with the ensemble average of some dynamical function f defined in the phase space in statistical mechanics:

$$\langle f \rangle = \frac{\int d\Gamma f e^{-\beta H}}{\int d\Gamma e^{-\beta H}} = \frac{\int dq_1 \dots dq_N dp_1 \dots dp_N f e^{-\beta H}}{\int dq_1 \dots dq_N dp_1 \dots dp_N e^{-\beta H}} \tag{11}$$

where Γ denotes the phase space. Nonetheless, we observe the Boltzmann measure in (9) is quickly oscillating due to the imaginary unit in the exponential. To solve this issue, we introduce a Wick rotation.

B. Wick rotation and Euclidean spacetime

Up until now, we have been implicitly working in the Minkowski spacetime metric, which is the typical choice when working with special relativity. Nonetheless, one can absorb the imaginary unit in the exponential (which is equivalent to rotating the imaginary time in the Minkowski metric and make it it coincide with the real axis). That way, for the price of working in Euclidean spacetime, one finds that the Boltzmann measure is now a real decaying exponential. Effectively, what one is doing is:

$$\tau \to -it \tag{12}$$

and thus the expectation value (9) can be written as:

$$\langle F \rangle = \frac{\int \mathcal{D}[\phi] F e^{-S[\phi]}}{\int \mathcal{D}[\phi] e^{-S[\phi]}} \tag{13}$$

where the action is still defined as in (10), except for the fact that we are now in Euclidean spacetime, and so the spacetime coordinate has now absorbed that imaginary unit. Strictly speaking, one would have to change the symbol used for the action, but since for the rest of the article we shall be working in Euclidean spacetime, we shall stick to the usual S. One must beware, however, of the fact that the action in (9) and (13) are different in the way explained. This new spacetime, the Boltzmann measure behaves like an ordinary real exponential and therefore is no longer rapidly oscillating: we are now able to do some serious importance sampling without the importance factor oscillating. Nonetheless, we find it that the analogy between the QFT problem and the statistical mechanics problem is not complete: in the latter, the number of degrees of freedom is finite, whilst in the former we are presently still considering an infinite number of field configurations (and therefore the dimensionality of our "phase space" is still infinite). This is elegantly solved by introducing the lattice as a regulator.

C. Introducing the lattice

At its core, the idea of a lattice is simply performing a discretization of spacetime. That is to say, we take spacetime to be comprised of a crystal-like structure instead of a continuum. That way, we only probe the field in a finite number of points, thus considering a finite number of degrees of freedom. Therefore, in our scalar field example, we would now have the vacuum expectation value of the observable F is:

$$\langle F \rangle \approx \frac{\int \prod_x d\phi(x) F e^{-S(\{\phi(x)\})}}{\int \prod_x d\phi(x) e^{-S(\{\phi(x)\})}} \tag{14}$$

and the analogy between the QFT problem and the mechanical statistical problem is now complete. What is more, the integration measure is now well-defined, since we are not integrating over an infinite number of field configurations. If we take the scalar fields to be real, then we are integrating over all the possible values of the amplitude of said fields (which need not be bounded). The reader must bear in mind that the amplitude of the original field in each point of our lattice is now an independent degree of freedom. Therefore, equation (14) may be written as:

$$\langle F \rangle \approx \frac{\int_{-\infty}^{\infty} d\phi_1 \dots \int_{-\infty}^{\infty} d\phi_M F e^{-S(\{\phi_i\})}}{\int_{-\infty}^{\infty} d\phi_1 \dots \int_{-\infty}^{\infty} d\phi_M e^{-S(\{\phi_i\})}} \tag{15}$$

In complete analogy with (11). We must keep in mind that, since our lattice is four-dimensional, the total number of lattice sites (and therefore the number of degrees of freedom) is:

$$M = N_X \times N_y \times N_z \times N_t \tag{16}$$

One of the main advantages of introducing the lattice as a regulator is computational: in order to calculate vacuum expectation values and correlation functions, one must essentially compute two integrals in a high-dimensional "phase space" and take their quotient. In order to do this, it is almost a requirement to employ Monte Carlo methods for two main reasons: firstly, they allow us to do importance sampling using the our analogous Boltzmann measure with the action (we can see which field configurations in the lattice offer a significant value in the action and consider only those when integrating to a very good approximation). Secondly, one must notice that if we were to employ some typical "deterministic" integration algorithm, we would need to discretize the phase space (of field amplitudes) uniformly, and so if we have M degrees of freedom, then the number of points we need to use is:

$$N_{pts} \sim n^M \tag{17}$$

where n is the number of points we intend to use for each dimension (i.e: if we only had two degrees of freedom and we discretized each dimension in 10 steps, then we would need to evaluate 100 points). The fact that the number of points to be considered when using a deterministic integration tool escalates exponentially with the dimensionality of the integration region often receives the name "curse of

dimensionality." [3].

The second reason for which it is interesting to use Monte Carlo methods when working in the lattice is precisely because said methods completely avoid the curse of dimensionality: one can prove the error in Monte Carlo integrals scales as the inverse of the square root of the points that one uses. That is to say:

$$\sigma \propto \frac{1}{\sqrt{N}} \tag{18}$$

Which means one can perform integrals in higher dimensions without worrying about having to use a great number of points.

IV. Properties of the lattice

So far, we have successfully managed to discretize Euclidean spacetime and introduce the lattice as a regulator, which, at the lowest level, has allowed us to perform calculations computationally. Nonetheless, the lattice is much more than just a mathematical trick: it is a scaffolding of spacetime, and as such it has some interesting properties which we shall explore in this section.

A. Lattice sites and links

Upon discretizing spacetime, we are left with a finite-volume crystal with three spatial dimensions and one time dimension. This volume encloses a total of M points as per (16), which receive the name of "lattice sites". The separation between two contiguous lattice sites ("nearest neighbours") is measured by the lattice parameter a. Each pair of lattice sites is said to be connected by a link. Recalling our second definition for a gauge theory, it is only natural that the link from the lattice site i to j is represented by an operator U_{ij} (since we are working in QCD, this is a 3x3 matrix). In fact, these operators are members of some gauge group G:

$$U_{ij} \in G \tag{19}$$

Following Mandelstam's and Mills' phase factor expression in (8) and taking into account the lattice parameter, we can approximate the integral and the lattice link operators now take the form:

$$U_{ij} = e^{ig_0 A_\mu a} \tag{20}$$

Of course, since the vector potential is now a matrix (as it can be conveniently expressed in terms of the generators of $SU(3)$ as shown in (21) [1]), the link operators are also bound to be matrices.

$$A_\mu = A_\mu^\alpha \lambda^\alpha \tag{21}$$

B. The continuum limit

In statistical mechanics one invariably works with systems large enough for them to be in the thermodynamic limit. Said limit is taken when both the number of particles and the volume in the system are infinite, whilst keeping the density finite:

$$\begin{aligned} N &\to \infty \\ V &\to \infty \\ \frac{N}{V} &= \text{const.} < \infty \end{aligned}$$

In the lattice formulation we proceed in an analogous fashion. We cannot make the number of lattice points to be infinite because that would reintroduce the problem of an infinite phase space, which is what we were trying to solve by using the lattice in the first place. Instead, since we have discretized spacetime, we may simply recover the spacetime continuum by making the separation between adjacent lattice sites arbitrarily small. That is to say, we take:

$$a \to 0 \tag{22}$$

In addition to the analogous thermodynamic limit in our system. In practice, however, one cannot fine tune the lattice parameter, but instead one needs to ensure β is adequate such that the lattice parameter is small enough. In a rough first estimate, it is clear that this parameter should at least be of the order of magnitude of the proton's radius, since that is the typical reach of the strong interaction. Nonetheless, since we are interested in studying quarks, it is perhaps more interesting to use an even smaller lattice parameter (it is typically one tenth of the proton's radius).

C. The plaquette action

Let us now construct the action in the lattice formulation. Of course, we now expect it to be expressed in terms of our new degrees of freedom, which are the link operators. We also expect it to have a contribution corresponding to the pure gauge theory and another part associated with the quark degrees of freedom. Finally, we would also like our action in the lattice to reduce to its continuum counterpart as per the Yang-Mills theory [1], since otherwise the lattice formulation would be inconsistent with gauge theories in the continuum. We shall see that this is indeed the case. Let us begin by calculating the action associated to the gauge fields.

As is detailed in [1], since the dynamics of the aforementioned fields are given by the field strength tensor, and since this tensor is the generalized curl of a vector potential (5), Wilson intuited the gauge fields' contribution to the action should be a summation over all the smallest elementary squares in the lattice. These squares receive the name of "plaquette" and the contribution to the action of an individual plaquette is as follows:

$$S_\square = \beta \left[1 - \frac{1}{n} \text{ReTr}(U_{ij} U_{jk} U_{kl} U_{li}) \right] \tag{23}$$

where the sites i, j, j, k, k, l and l, i are nearest neighbours to each other, thus forming a square. For future reference, we shall lighten the notation by referring to the product of the four link operators of the plaquette as $U_\square$. Of course, after calculating the action of one individual plaquette, one must then sum over all the plaquettes comprising the lattice, so the action is:

$$S = \sum_{\square} S_\square \tag{24}$$

if we now take the continuum limit, we find that the lattice action reduces to:

$$S = \frac{\beta g_0^2}{2n} \int \frac{1}{2} \mathrm{Tr}(F_{\mu\nu})^2 d^4x + O(a^6) \tag{25}$$

which coincides with the ordinary Yang-Mills action if we do the identification:

$$\beta = \frac{2n}{g_0^2} \tag{26}$$

where n is the dimension of the matrices of the gauge transformation group (in our case, $n = 3$). Most evidently, we need not worry about the higher order terms in the lattice parameter, as they will vanish in the continuum limit.

If we now introduce the quark degrees of freedom in order to build the action of the full interacting theory, we can introduce the fermion action in our expression, "inserting a factor U_{ij} on the fermi field whenever a quark hops from lattice site i to site j" [1]:

$$\begin{aligned} S = &\sum_{\square} \beta \left[1 - \frac{1}{n} \mathrm{ReTr}(U_\square) \right] \\ &+ \frac{1}{2} i a^3 \sum_{\{i,j\}} \bar{\Psi}_i (1 + \not{e}) U_{ij} \Psi_j \\ &+ (a^4 m_0 + 4a^3) \sum_i \bar{\Psi}_i \Psi_i \end{aligned}$$

D. Phase transitions

If one only considers the pure gauge theory instead of the full interacting picture, then it is possible to do an analogy between a magnetic system and our lattice [1]. We know a magnetic sample is ferromagnetic if, in the absence of an external magnetic field, said sample exhibits a nonzero magnetic moment (assuming it is indeed magnetized) for a temperature below its critical temperature. Therefore, just by evaluating whether a single parameter is vanishing or not, one can know what phase the ferromagnetic sample is in. These magnitudes are often referred to as "order parameters". Taking into account our present theory also allows for the existence of two phases (confined and unconfined), it would be interesting to look for an order parameter in it.

1) Discontinuities in the average plaquette

The simplest gauge invariant magnitude we can evaluate is the average plaquette P:

$$P = \langle 1 - \frac{1}{n} \mathrm{Tr} U_\square \rangle = \frac{1}{6} \frac{\partial}{\partial \beta} \log Z \tag{27}$$

Which, as we can see, is proportional to the action of the system without including the quark degrees of freedom (24) (this is what one would expect, since we are currently focusing exclusively in the gauge theory, not the full interacting theory). It is interesting to note the close parallel between the average plaquette in lattice theory and the ensemble average of the Hamiltonian in statistical mechanics. In a more extended version, a digression on this topic would be in order.

When plotting the average plaquette against the "inverse temperature" β, we may observe a discontinuity, just as is the case in ordinary thermodynamic phase transitions with the adequate magnitudes.

Nonetheless, the average plaquette's interest does not end here. In fact, it is oftentimes used to determine whether a simulation has thermalized. By plotting the average plaquette against the iteration number, we can study when this quantity has stabilized and therefore we can see in a graphical fashion how many of the first iterations are to be discarded. This is due to the fact that, for a given temperature (and of course in a given lattice), the average plaquette takes on a specific value. If we do not vary the inverse temperature parameter, then the average plaquette should always adopt the same value once the fluctuations previous to thermalization have attenuated.

2) String tension, area law and confinement

The idea of a plaquette can be extended to any arbitrary closed loop in the lattice. Its expectation value (perhaps now we should talk in terms of ensemble averages) receives the name of "Wilson loop" [1]:

$$W(C) = \langle \mathrm{Tr} \prod_{ij \in C} U_{ij} \rangle \tag{28}$$

where C is the closed loop of lattice sites to be followed. In Creutz's words, "If the loop is a rectangle of dimensions T by R, a transfer matrix argument suggests that for large T:"

$$W(C) \sim \exp\left(-E(R)T\right) \tag{29}$$

where $E(R)$ is "the gauge field energy associated with the static quark-antiquark sources separated by a distance R" [1]. This realization has very significant implications, the most important of which is the area law, which states that, for a large enough Wilson loop, its exponent only depends on the area enclosed by said loop up to a multiplicative factor called the "string tension" (σ). At this point, there are two approaches one can take: one can either take the strong coupling potential as linear *a priori* or derived from other arguments and therefore immediately demonstrate the area law, since:

$$V(R) \sim \sigma R \tag{30}$$

for long enough distances (where strong coupling is dominant), and inserting this into (29), we get:

$$W(C) \sim \exp\left(-\sigma R T\right) \tag{31}$$

for large enough R, T, and thus argue that confinement predicts the area law. One can also proceed inversely and take the area law as a given (perhaps from observations in the lattice), and thus argue that, for long enough distances, the potential felt by the quarks due to the strong interaction is linear. It may appear surprising at first that the lattice formalism predicts quark confinement with such ease, but the catch is it *could not* not predict it. Confinement is "hard-coded" into the very formulation of the lattice, and in fact Creutz challenges us in [1] to bring to terms the apparent contradiction between QED not exhibiting confinement in the continuum theory and our experience, and yet exhibiting it when formulated as a lattice theory. Personally, I believe one can formulate QED on the lattice even if it is showcases a strong coupling regime, provided that we can have this regime be comparable to the usual Coulombian potential (asymptotic freedom) only for an infinite distance. Nonetheless, this argument would still need some polishing, since when calculating, for instance, the electrostatic energy of two static charges (which should be equal to the sum of their self-energies), one would get an extra linear term that would introduce a divergence in the integral.

The string tension can be used as an order parameter, since it behaves just like the magnetization of a ferromagnetic sample: in the unconfined phase ("demagnetized sample") the string tension vanishes identically (since quarks are free, they no longer feel the linear potential previously binding them together), whilst being nonzero in the confined phase ("magnetized sample"). Nonetheless, the string tension is only a good order parameter whilst the linear potential between the two quarks holds, and, so it happens, reality is always richer than our models. So much so that the linear potential is not always enough to capture the whole picture: if one studies the fully interacting picture, where there are dynamical quarks, one observes that, upon separating two quarks, energy will build up in a so-called "tube" and eventually a quark-antiquark pair will be created, thus reducing the energy of the original system. Therefore, string tension is not a good order parameter when the quarks are too separated. There are other order parameters, such as Polyakov loops, which offer a better estimate of the phase the system is in.

E. Difficulties arising in the lattice formulation and proposed solutions

If the purely theoretical introduction to the lattice formulation were to end here, one could say the whole article is rather biased, since we have introduced the lattice as a regulator for the problems arising in QFT and yet we have not mentioned the difficulties arising in the lattice which do not appear in the continuum. The most significant is the phenomenon of "doubling", to which we shall devote this last section. The upcoming explanation is essentially a harmonization of the descriptions provided by [1] and [4] on the topic.

When working with a single free fermion, the Dirac Lagrangian is given by:

$$\mathcal{L} = \bar{\Psi}(\not{\partial} + m)\Psi \tag{32}$$

And therefore, according to our definition of the action (10), the so-called "Dirac action" for the free fermion in the continuum is:

$$S_D = \int \bar{\Psi}(\not{\partial} + m)\Psi \; d^4x_\mu \tag{33}$$

Provided that the lattice parameter is small enough (which we can assume will always be the case, as we are to take the continuum limit (22) in the end), we can expand the partial derivative in (33) in differences symmetrically to first order, thus having an expression for the action in the lattice:

$$S_D = \sum_{m,n} \bar{\Psi}_m M_{mn} \Psi_n \tag{34}$$

where:

$$M_{mn} = \frac{a^4}{2} \sum_{\mu}^{4} \gamma_\mu (\delta^4_{m_\nu + \delta_{\mu\nu}, n_\nu} - \delta^4_{m_\nu - \delta_{\mu\nu}, n_\nu}) + a^4 m \delta^4_{ij} \tag{35}$$

This is usually referred to as the "naive fermion discretization", since one is mindlessly substituting partial derivatives by differences to first order just because the lattice parameter is small. One would think that, since the Lagrangian describes a single free fermion in the continuum, then this naive action (34) also describes just one free fermion, this time in the lattice. Nonetheless, one surprisingly finds it actually describes 16 different fermions at the same time. This phenomenon, where one tries to discretize the action of one fermion and ends up describing multiple, receives the name of "doubling", and the extra fermions are often referred to as "doublers". Sometimes, we also say we get several "tastes" of fermions, as in the early days of this theory it was believed this was indeed a feature predicted by the lattice, and so the additional fermions were referred to with a term that reminds one of the flavour of quarks. Nonetheless, there are no doublers in reality, and this is an issue introduced by the lattice. In fact, the issue is inherent to the lattice, as in the continuum one need not substitute derivatives by differences. A somewhat convincing argument of why we get 16 fermions is given by Creutz in [1], where he explains that one can express the inverse of the matrix M in terms of some quantity $\bar{M}_k$, given by:

$$\bar{M}_k = m + \frac{i}{a} \sum_{\mu} \gamma_\mu \sin(a q_\mu) \tag{36}$$

One can then go on to expand the sine to first order since the lattice spacing is arbitrarily small in the continuum limit, and of course recovers the free fermion propagator:

$$\bar{M}_k \xrightarrow[a\to 0]{} m + i\not{q} + O(a^2) \tag{37}$$

This is indeed possible except for those values of the argument of the sine were it vanishes and $q_\mu \neq 0$. This is precisely what happens in $q_\mu = \pi/a$ which, not surprisingly, is the limit of the first Brillouin zone in the lattice. This region of the reciprocal lattice is quite known in solid state physics for giving raise to "strange" phenomena, like the concept of bands in band theory. In the case of the lattice, it gives place to doublers.

The efforts to reduce the effects of doublers or remove them altogether in the lattice formulation have been many. In the present article, we shall only treat Wilson's fermion action, although the interested reader is encouraged to read about the staggered fermion action, which follows a radically different approach. Of course, regardless of which method we employ to correct the naive fermion action, we must ensure we still recover the Dirac action in the continuum when taking said limit.

In order to reduce the doublers in the lattice formulation, Wilson proposed introducing an additional term in the naive fermion action which vanishes when taking the continuum limit but suppresses the extra fermions while still in the lattice [1]. More precisely, he proposed to go from (36) to:

$$\bar{M}_k = m + \frac{i}{a}\sum_\mu \gamma_\mu \sin(aq_\mu) + \frac{r}{a}\sum_\mu (1-\cos(aq_\mu)) \tag{38}$$

As a side note, we must take into account simulations often prefer to work in the position representation rather than the momentum representation. In that case,the equivalent to (38) is:

$$M_{mn} = (a^4 m + 4a^3)\delta^4_{mn} + \frac{1}{2}a^3 \sum_\mu \left[(1+\gamma_\mu)\delta^4_{m_\nu+\delta_{\mu\nu},n_\nu} + (1-\gamma_\mu)\delta^4_{m_\nu-\delta_{\mu\nu},n_\nu}\right]$$

Notice that, in (38), the only addition is the last term, which vanishes in the continuum limit when $q_\mu \neq \pi/a$ but introduces a divergence in the limit of the first Brillouin zone. This is equivalent to adding an effective mass to the doublers which depends on their momentum and which diverges in the border of the first Brillouin zone. Therefore, the doublers are effectively uncoupled from the theory since they only appear when the momentum is close to π/a, and when they do appear they have an infinite mass anyway, so they do not contribute to the lower energy states, which are associated with our particles (in this case, with our only particle, since we were working with a single free fermion). Nonetheless, Wilson's solution is not perfect, as it completely mutilates chiral symmetry in our equations [1], but for the purposes of this article, it is more than sufficient.

V. Conclusion and final remarks

The aim of the present article is to convey a gentle introduction to the lattice formulation of theories which are typically only presented in their continuum representations in the undergraduate syllabus of the Physics degree. After introducing the continuum formulation of QFT, we have identified its weaker points (QCD becomes non-perturbative at low energies) and we have proposed the lattice as a regulator which allows us to do non-perturbative calculations. We have then explicitly built the lattice formulation beginning by the continuum using scalar fields (the reasoning is the same for other types of fields and these are the simplest). By introducing a Wick rotation we have rotated our time axis from the imaginary Minkowski time to the kinder Euclidean spacetime, and by discretizing this spacetime in a four-dimensional lattice we have been able to reduce to a finite (although typically very large) number the dimensionality of our phase space when using the Feynman integral. Therefore, we have effectively turned our problem of calculating expectation values and correlation functions into an equivalent statistical mechanical problem in the canonical ensemble, which we know how to solve computationally employing Monte Carlo simulations such as the Metropolis algorithm. We have concluded this article by presenting the characteristics inherent to the lattice formulation and, among them, the main weakness of the lattice approach when working with QCD, which is fermion doubling.

The theoretical work is essentially done with. For an application of the presented concepts, the interested reader is referred to the supplementary materials section.

Acknowledgements

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Finally, I wholeheartedly thank my *alma mater*, Universidad Complutense de Madrid (UCM), for granting me the opportunity to carry out this project in the first place with their generous scholarship.

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Supplementary Materials

August 18, 2025

1 Calculating the mass of the π meson with lattice QCD

1.1 Theoretical background

Outline of the project: our objective with this project is to measure the mass of the π meson emoploying lattice methods in order to exemplify how one works with the lattice in practice.

In order to extract the mass of the pion, we must measure the so-called "pion correlator", which is essentially the vacuum expectation value of the (time ordered) product of two pion interpolators, one at some time $t = 0$ and another one at some time t:

$$C(t) = \langle 0|\mathcal{O}_\pi(t)\mathcal{O}_\pi^\dagger(0)|0\rangle$$

where we are creating a pion state from the vacuum at some time $t = 0$ and annihilating said state at another time t, and then measuring the expectation value of this action.

Note: It is important to note that, since we are discretizing spacetime, if our time axis is discretized in N_t points, we should then expect to have N_t values of the correlator in each iteration, since it is being measured at all 24 considered instants of time in each iteration

In the Heisenberg picture, the interpolating operator evolves in time as:

$$\mathcal{O}(t) = e^{Ht}\mathcal{O}(0)e^{-Ht}$$

Where the time evolution operator lacks its characteristic imaginary unit since we are now in Euclidean spacetime. Introducing this expression in our correlator function:

$$C(t) = \langle 0|e^{Ht}\mathcal{O}_\pi(0)e^{-Ht}\mathcal{O}_\pi^\dagger(0)|0\rangle$$

Since the energy of the vacuum is taken to be zero ($H|0\rangle = 0|0\rangle$), acting said operator from the left we get the identity operator. If we now introduce a complete set of states (eigenkets of the system's Hamiltonian) between the second exponential and $\mathcal{O}_\pi^\dagger(0)$, we get:

$$C(t) = \sum_n \langle 0|\mathcal{O}_\pi(0)e^{-Ht}|n\rangle\langle n|\mathcal{O}_\pi^\dagger(0)|0\rangle$$

and now the exponential can operate immediately on the energy eigenket, so we are left with the expression:

$$C(t) = \sum_n \langle 0|\mathcal{O}_\pi(0)|n\rangle\langle n|\mathcal{O}_\pi^\dagger(0)|0\rangle e^{-E_n t}$$

Where E_n is the energy of the system's Hamiltonian corresponding to the eigenstate $|n\rangle$. Of course, the lowest energy of this Hamiltonian (aside from the vacuum state) will correspond to the rest mass of the pion, and since we are in Euclidean time, the exponentials are real, which means for long enough timet the only term left in the correlator shall be that corresponding to the pion's rest mass:

$$\boxed{C(t) \sim e^{-m_\pi t}}$$

Hence, if we manage to measure the correlator for long enough time and fit it logarithmically, we can extract the mass of the pion. That is what we shall do in the rest of this section.

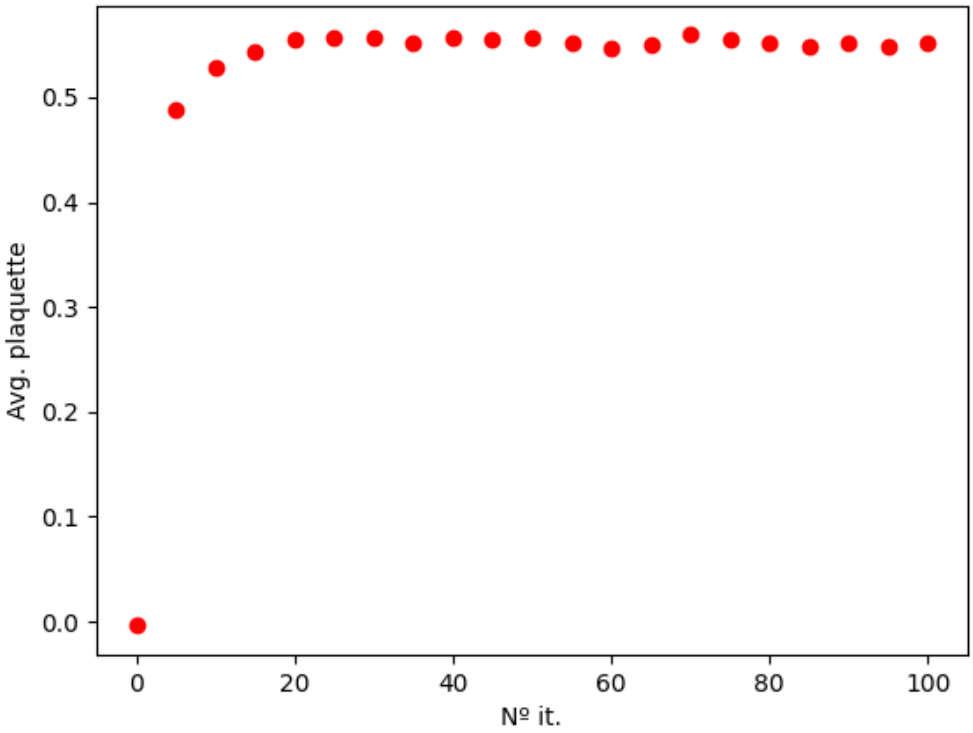
1.2 Generating the parameters of the simulation

Lattice simulations require a large amount of computational resources, and therefore they are usually carried out using supercomputers. Since this simulation will be done using a laptop, we will be forced to make some concessions (mainly affecting the volume of the lattice and the algorithm used in our simulation). We shall be using a lattice of dimensions $4^3 \times 24$ and we shall employ a quenched simulation, which is equivalent to ignoring the dynamical quarks in our theory. That is to say, we shall only focus on the valence quarks, not paying attention to the sea of quarks. We must also select the mass of the quarks we are going to use to "build" our pion, and since this particle is composed of the two lightest quarks, we want their masses to be quite low. There is a parameter, called "hopping parameter" (κ) which essentially determines the mass of our quarks, and therefore also influences the mass of the pion we will estimate with our simulation. As a rule of thumb:

$$m_\pi^2 \propto \frac{1}{\kappa} - \frac{1}{\kappa_c}$$

with κ_c some critical value for the hopping parameter (where the quarks are massless). We do not know the ideal κ value *a priori* and that is the reason why one might want to run several simulations with different hopping parameters. We shall be monitoring two magnitudes in our simulation: the average plaquette (to check when the simulation has thermalized and remove all the earlier data) and the pion correlator. All of this is conveniently managed by the LatticeQCD Julia package, to which one must only specify the parameters they want for their simulation.

After running the simulation, one obtains a text file for the average plaquette, which can be easily plotted:



And so we see the simulation has thermalized after approximately 20 iterations. Since we measured the pion correlator every 2 iterations, we can proceed to discard the first 10 rows of our document "Pion_correlator.txt" and work with the rest of the data. We have now produced the pion correlator data and therefore proceed to its analysis. The code and its corresponding explanation are added below:

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt

raw = np.loadtxt("Pion_correlator.txt")

# Eliminate first column (numpy automatically only loads numerical data so the␣
 ↪comment at the end of each line can be ignored)

data =  np.delete(raw, 0,1)

# Step 2: 2 <-> 24, 3<-> 23, ..., 13 (periodic boundary conditions) --> reduces␣
 ↪number of new columns to just 11

Ncols = np.shape(data)[1] # 23

# Average equivalent columns
for col in range(13):
```

```
    data[:,col] += data[:,-(col+1)]
    data[:,col] /= 2

# Remove the now residual columns after the 13th
while np.shape(data)[1] != 13:
    data = np.delete(data, -1, 1)

# Now we extract the effective mass in each time step for each iteration: m_eff␣
 ↪= -log(C(t+1)/C(t))

m_effs = np.zeros((np.shape(data)[0], np.shape(data)[1]-1))

for col in range(np.shape(m_effs)[1]):
    m_effs[:,col] = -np.log(data[:,col+1]/data[:,col])

# Take average in all iterations for a given time --> gives me a single mass␣
 ↪function of time, m(t)

mass_t = []

for i in range(np.shape(m_effs)[1]):
    mass_t.append(np.mean(m_effs[:,i]))

# Plot effective mass time function and see where it plateaus to average the␣
 ↪mass in the plateau and get the effective mass (in lattice units)
x = np.arange(0, len(mass_t))
plt.plot(x, mass_t, "ro")
plt.show()
input("Enter>")
am_pi = np.mean(mass_t[4:])

### Passing to MeV / c^2

r0=0.5
a = lambda beta: r0*np.exp(-1.6805-1.7139*(beta -6) + 0.8155*(beta-6)**2-0.
 ↪6667*(beta-6)**3)

beta = 5.7
a_val = a(beta)

print(f"a = {a_val} (fm)")

a_inv = 197/a_val

print(f"Mass of the pion (Mev/c^2) = {am_pi*a_inv}")
```

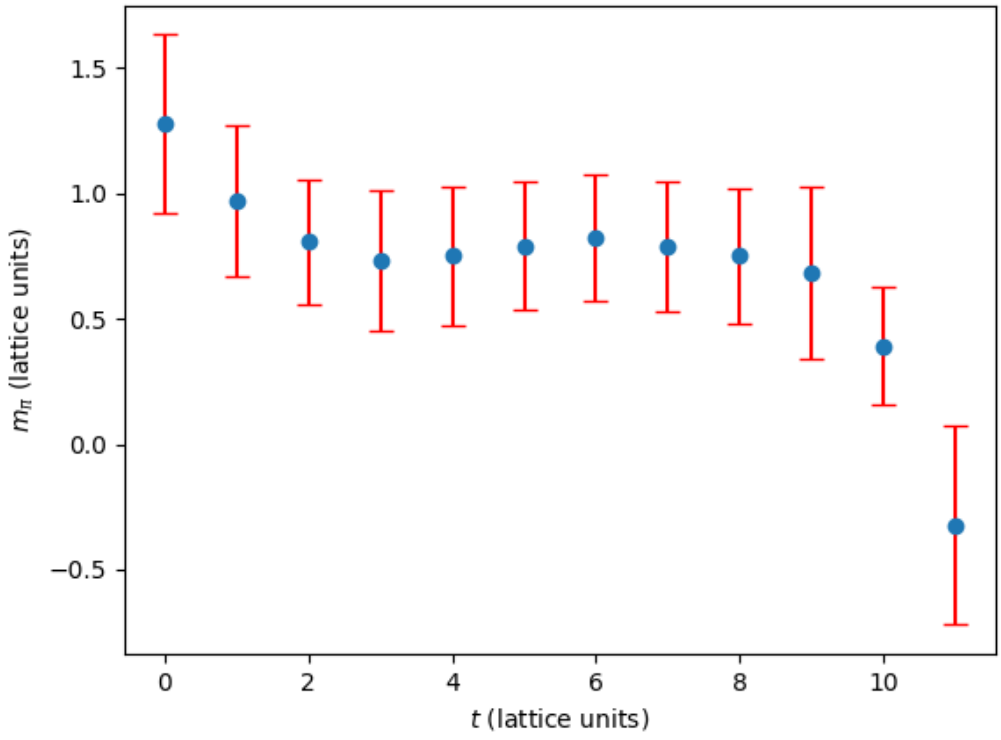
The explanation of this code is quite simple: we firstly extract the raw text from the

Pion_correlator.txt file and check it has indeed 24 columns of numerical data (this corresponds to the evaluation of the pion correlator in each point of the discretized Euclidean time). Since this specific package uses periodic boundary conditions (in solid state physics, Born-Von Kármán conditions), we identify column 2 to be the same as 24, 3 as 23, etc. all the way until 13. The first column does not correspond to any other one as is seen by the large discrepancy in the numerical values and hence we discard it altogether. We now "fold" the data averaging out the equivalent pairs of columns and so we have managed to find a correlator function in time for each iteration. Is is now of our interest to calculate the effective mass of the piuon as a function of time in each iteration. Since $C(t) \sim e^{-m_\pi t}$, and since the lattice parameter is a, we can advance one step in the correlator (of each iteration) to isolate a mass term: $C(t+a) = C(t)e^{-m_\pi a}$, and so we can now extract the pion's mass (in lattice units) from each correlator as follows:

$$m_\pi = -\log\left(\frac{C(t+a)}{C(t)}\right)$$

We are therefore left with a mass function for each iteration, and now we may simply average out the mass at a given instant for all the iterations (since the simulation has thermalized, this is valid, as the fluctuations in the calculated mass from one iteration to another should not be too great and therefore taking the average of each column is indeed statistically significant)

After doing so, we have a function for the mass at each instant, $m_\pi(t)$. We can now plot it to see where it plateaus, as is seen in the picture below:



We can then average out the mass in the plateau to get the mass of the pion in lattice units. In order to convert it to the ordinary units MeV/c^2, we use the appropriate formula to calculate

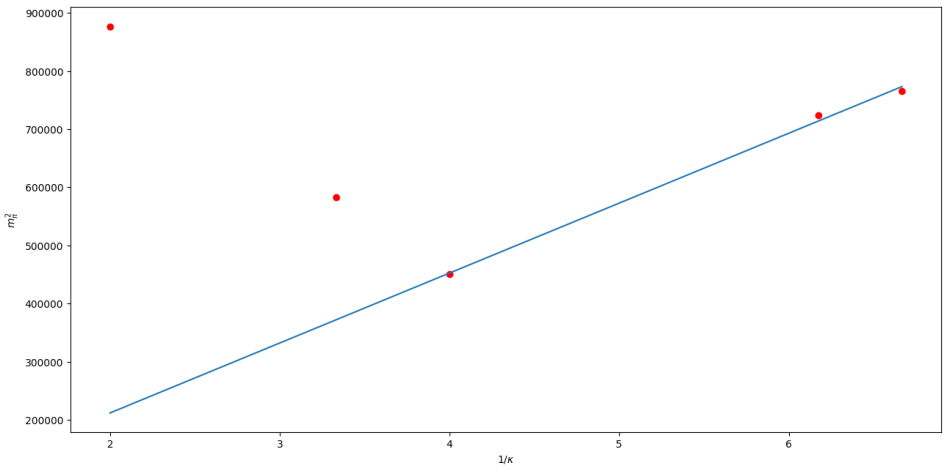
the lattice parameter of our lattice, kindly shared by professor Akio Tomiya, and we extract the physical mass of the pion by doing:

$$m_\pi = \frac{(a \times m_\pi)}{a}$$

Of course, this simulation is not expected to get a physically accurate value for the pion's mass. Paraprhasing professor Tomiya's diagnosis, the lattice volume is simply too small as to reach sensible results (as both professors Tomiya and Wingate point out, when taking the continuum limit, the pion's dimensions exceed those of the box, and therefore we encounter undesired effects which affect our results). In our case, we get $m_\pi = 671.4 MeV/c^2$, which is well off from the actual physical value, $m_\pi \sim 135 MeV/c^2$. Despite the value being far from the physical result, this mini project serves well to exemplify how one may work with the lattice formulation at the most hands-on, practical level.

1.3 Bonus: adjusting the hopping parameter

As we have mentioned earlier in this appendix, the pion's mass our simulation will estimate is closely related to the hopping parameter used. One can perform simulations with several hopping parameters in order to extrapolate the critical value κ_c. After running the exact same simulation with $\kappa \in \{0.15, 0.162, 0.25, 0.3, 0.5\}$, we get:



We therefore conclude it is no coincidence that the best value of the pion's mass is obtained for $\kappa = 0.25$, which coincides with the lowest mass for the quarks being used. The two first points are far off from the linear relation due to the fact that, for said values of the hopping parameter, the pion exceeds the boxe's dimensions and therefore our results are no longer sensible. We see that, for smaller hopping parameter's, the linear relation is indeed followed. From extrapolating this fit and calculating where it intersects the X axis, one would be able to directly extract $1/\kappa_c$ and thus study the critical hopping parameter of the system.