Lattice Field Theory

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1 Introduction

When considering a field theory in regimes where couping constants are small, the use of perturbation theory can yield analytical results that agree with experiment. However, in situations when coupling constants are large, such as QCD at low energies, perturbation theory breaks down. In such cases, new methods are needed that do not involve a Taylor series expansion about in the coupling constant. One such method is lattice field theory. Quantities of interest are calculated using field defined on a lattice. These calculations are repeated with various lattice spacings to yield a trend line that is extrapolated to a lattice with infinitely small spacing, which should give the continuum behaviour, so long as the trend line is well behaved at small lattice spacings.

The key ingredient in the lattice method is the path integral, which dictates that the expectation value of an operator $\hat{O}(\phi)$ that is a function of the fields ϕ can be found by summing over all paths weighted by $\exp(iS(\phi, \partial_\mu \phi))$, where S is the action for the fields ϕ. The vacuum expectation value is given by

$$\langle 0|\hat{O}(\phi)|0\rangle = \frac{\int \mathcal{D}\phi O(\phi) \exp(iS(\phi, \partial_\mu \phi))}{\int \mathcal{D}\phi \exp(iS(\phi, \partial_\mu \phi))} \tag{1}$$

This is a natural place to start for the lattice method. When deriving the path integral method, one usually first considers the propagation of a particle at position x_i at time t_i to position x_f at time t_f. The expression for the path integral can be found by breaking up the integral into a finite number of 'time slices' and later taking the limit where the time slices are arbitrarily close together. This procedure will be very similar to what is done in the lattice method, except in most cases the continuum limit cannot easily be reached analytically and numerical methods must be used instead.

In the expression for the path integral given in (1), the action S appears in the term $\exp(iS)$, which can oscillate rapidly with S, making it difficult to integrate. For this reason, it is useful to use imaginary time τ, which is related to real time t by $\tau = it$ (which is a Wick rotation by $\pi/2$ in the complex t plane). With this time coordinate, the Minkowski metric tensor $\eta_{\mu\nu}$ becomes $\eta_{\mu\nu} = \delta_{\mu\nu}$, where $\mu, \nu = 1, \ldots, 4$ and $x^4 = \tau$, which is the four-dimension Euclidean metric tensor. To see why switching to imaginary time is useful, consider the action of a scalar field ϕ using real time

$$S = \int d^3x dt \left[\frac{1}{2}\partial_\mu \phi \partial^\mu \phi - V(\phi)\right] \tag{2}$$

where $\mu = 0, \ldots, 3$. If we now switch to imaginary time,(2) becomes

$$S = i \int d^3x d\tau \left[\frac{1}{2}\delta^{\mu\nu}\partial_\mu \phi \partial_\nu \phi + V(\phi)\right] \tag{3}$$

where $\mu = 1, \ldots, 4$. With this change of variables, $\exp(iS)$ becomes $\exp(-S)$, which does not oscillate with S and instead becomes small for large S. When using imaginary time, the metric is Euclidean, so there is no difference between upper and lower indices, so we can write terms like $\delta^{\mu\nu}\partial_\mu\phi\partial_\nu\phi$ as $\partial_\mu\phi\partial_\mu\phi$, which helps to remind us that we are using imaginary time.

2 Matter Fields

2.1 Scalar Fields

We consider a lattice where the lattice sites are the vertices of a hypercube with side length a, so that the continuous coordinate x_μ becomes

$$x_n = a(n_1\hat{e}_1 + n_2\hat{e}_2 + n_3\hat{e}_3 + n_4\hat{e}_4) \tag{4}$$

where x_4 is the imaginary time coordinate, $n = (n_1, \ldots, n_4)$ are integers, and $\hat{e}_1, \ldots, \hat{e}_4$ are unit vectors. We will define matter fields at each point on the lattice. Since we will be using path integrals in our lattice calculations, it will be important to know the form of the discretized propagators of our fields, which enters into the generating functional Z.

We begin by examining scalar fields. The Klein-Gordon equation for a scalar field $\phi(x)$ with mass m in Euclidean space is

$$(\partial_\mu\partial_\mu - m^2)\phi(x) = 0 \tag{5}$$

We can easily discretize this equation by using the three-point formula for the second derivative

$$\frac{1}{a^2}\sum_{\hat{e}_\mu}(\phi(x_n - a\hat{e}_\mu) - 2\phi(x_n) + \phi(x_n + a\hat{e}_\mu)) - m^2\phi(x_n) = 0 \tag{6}$$

We can write the Klein-Gordon equation in matrix form by

$$K_{nm}\phi_m = 0 \tag{7}$$

where K_{nm} is the inverse propagator in Euclidean space of the field ϕ, given by

$$K_{nm} = \frac{1}{a^2}\left[\sum_{\hat{e}_\mu}(\delta_{n-\hat{e}_\mu,m} + \delta_{n+\hat{e}_\mu,m}) - (8 + (ma)^2)\delta_{n,m}\right] \tag{8}$$

It is also useful to have the momentum space propagator. We can define the Fourier transform of a function $f(x_n)$ defined on the lattice by

$$f(p) = a^4\sum_{n=-\infty}^{\infty}\exp(-ip_\mu(x_n)_\mu) \tag{9}$$

$f(p)$ is periodic and therefore we can restrict p_μ to the first Brillouin zone $-\pi/a < p_\mu \leq \pi/a$. The inverse of this transformation is

$$f(x_n) = \int_{-\pi/a}^{\pi/a}\frac{d^4p}{(2\pi)^4}f(p)\exp(ip_\mu(x_n)_\mu) \tag{10}$$

so that the Kronecker delta can be expressed as

$$\delta_{nm} = \frac{a^4}{(2\pi)^4}\int_{-\pi/a}^{\pi/a} d^4p \exp(ip_\mu(x_n - x_m)_\mu) \tag{11}$$

By taking the Fourier transform of K_{nm} and using (11), one finds

$$\begin{aligned} K(p) &= a^4 \sum_{n,m} K_{nm} \exp(-ip_\mu(x_n - x_m)_\mu) \\ &= a^2 \left[4 \sum_\mu \sin^2\left(\frac{p_\mu a}{2}\right) + (ma)^2 \right] \end{aligned} \tag{12}$$

The propagator K^{-1}_{nm} in spacetime, which can be found from the relation $K_{nl}K^{-1}_{lm} = \delta_{nm}$, is then

$$K^{-1}_{nm} = a^2 \int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4} \frac{\exp(ip_\nu(x_n - x_m)_\nu)}{4\sum_\mu \sin^2\left(\frac{p_\mu a}{2}\right) + (ma)^2} \tag{13}$$

This is our first result from our lattice formulation. It is important to check that this result approaches the propagator in the continuum formulation when the continuum limit $a \to 0$ is taken. Using the small argument approximation of the sine function, it can readily be seen that the continuum limit of K^{-1}_{nm} is

$$\lim_{a\to 0} K^{-1}_{nm} = \int \frac{d^4p}{(2\pi)^4} \frac{\exp(ip_\nu(x_n - x_m)_\nu)}{p_\mu p_\mu + m^2} \tag{14}$$

This equation is written in terms of the Euclidean formulation, where the real time momentum p^r_μ is related to the Euclidean momentum p^E_μ by the relationship $p^r_\mu p^{r\mu} = p^0p^0 - \delta_{ij}p^ip^j = -p^4p^4 - \delta_{ij}p^ip^j = -p^E_\mu p^E_\mu$. Therefore, in the limit $a \to 0$, K^{-1}_{nm} approaches the propagator of scalar field theory in the continuum, which has a pole at $p_\mu p_\mu = -m^2$ (or at $(p^r)^2 = m^2$ using real time).

2.2 Fermion Fields

We now consider fermion fields, so our task will be to discretize the Dirac equation

$$(i\gamma^\mu \partial_\mu - m)\psi = 0 \tag{15}$$

For a metric $g_{\mu\nu}$, the γ-matrices for that space satisfy the Dirac algebra

$$\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu}\mathbb{1} \tag{16}$$

In the Euclidean formulation $g_{\mu\nu} = \delta_{\mu\nu}$. This algebra can be satisfied by choosing $\gamma^E_i = -i\gamma_i$ and $\gamma^E_4 = \gamma_0$, where γ and γ^E are the real time and Euclidean time γ-matrices, respectively, and $i = 1, \ldots, 3$. The Euclidean time Dirac equation is then

$$(\gamma^E_\mu \partial_\mu + m)\psi = 0 \tag{17}$$

Since we will be using the Euclidean formulation unless stated otherwise, we will now drop the superscript E. We will now try to discretize 17 by

$$\sum_{\hat{e}_\mu} \gamma_\mu \frac{1}{2a}[\psi(x_n + a\hat{e}_\mu) - \psi(x_n - a\hat{e}_\mu)] + m\psi(x_n) = 0 \tag{18}$$

so that discretized inverse propagator $K_{n,m}$ which satisfies $K_{n,m}\psi_m = 0$ is

$$(K_{n,m})_{\alpha\beta} = \frac{1}{2a}\sum_{\hat{e}_\mu}(\gamma_\mu)_{\alpha\beta}[\delta_{n,m+\hat{e}_\mu} - \delta_{n,m-\hat{e}_\mu}] + m\delta_{n,m}\delta_{\alpha,\beta} \tag{19}$$

Using (11), the Fourier transform of $K_{n,m}$ is

$$K(p)_{\alpha\beta} = \left[\frac{i}{a}\sum_\mu \sin(p_\mu a)\gamma_\mu + m\right]\delta_{\alpha\beta} \tag{20}$$

and the propagator K^{-1}_{nm} is

$$(K^{-1}_{nm})_{\alpha\beta} = \int_{-\pi/a}^{\pi/a}\frac{d^4p}{(2\pi)^4}\frac{(i\gamma_\mu p_\mu + m)_{\alpha\beta}}{\sum_\mu \sin^2(p_\mu a)/a^2 + m^2}\exp(ip_\nu(x_n - x_m)_\nu) \tag{21}$$

We now want to confirm that the propagator K^{-1}_{nm} in the limit $a \to 0$ approaches the continuum propagator. Taking this limit, the denominator in (21) approaches

$$\lim_{a\to 0}\sum_\mu \sin^2(p_\mu a)/a^2 + m^2 = p_\mu p_\mu + m^2 \tag{22}$$

Again, we see that the limit $a \to 0$ yields the expected continuum limit, and that the continuum version of the propagator K^{-1}_{nm} has a pole at $p_\mu p_\mu = -m^2$, as seen from the right hand side of (22).

While everything at this point seems well, a problem arises on closer inspection of the left hand side of (22). For simplicity, consider a masses fermion. For finite lattice spacing a, p_μ is restricted to the first Brillouin zone (BZ) $-\pi/a < p_\mu \leq \pi/a$. At the origin of the BZ, $p_\mu = 0$, so K^{-1}_{nm} has a pole at this point in the BZ, corresponding to an on-shell fermion. However, $p_\mu = \pi/a$ is also in the BZ, in which case $\sin^2(p_\mu a) = 0$, therefore we get another pole at the point $p_\mu = \pi/a$ and another on-shell fermion. This is referred to as fermion doubling. Because p_μ has four components, each of which can equal 0 or π/a, we actually get $2^4 = 16$ on-shell fermions, 15 of which we do not want! This problem did not arise in the case of the scalar field since the p_μ dependent part of the denominator of the scalar field propagator involved the term $\sin^2(p_\mu a/2)$, which because of the division by 2 in the sine function only allows one pole in the BZ. Because of the linearity of the Dirac equation, the denominator of the fermion propagator does not have the same form as the scalar case, causing the doubling problem.

There are two popular methods for dealing with the fermion doubling problem, one of which was proposed by Wilson, which we will examine, and one proposed by J. Kogut and L. Susskind referred to as the staggered fermions method, which we omit. The main idea of Wilson's method is to introduce the extra term $(r/2)\partial_\mu\partial_\mu\psi$ into the Dirac equation, where r is referred to as the Wilson parameter. This term (without the factor of $r/2$) is present in the Klein-Gordon equation and stops particle doubling in the scalar case and can stop the fermion doubling when introduced into the Dirac equation. It will be seen that this term vanishes as $a \to 0$ to preserve the correct continuum limit. We will then perform lattice calculations for various values of r to find a trend line and then extrapolate to $r = 0$ to find physical values.

We return to the Dirac equation (17), but add the additional term

$$\left(\gamma_\mu\partial_\mu + m - \frac{r}{2}\partial_\mu\partial_\mu\right)\psi = 0 \tag{23}$$

Repeating the same procedure as above with the modified Dirac equation yields the discretized inverse propagator

$$(K_{n,m})_{\alpha\beta} = \frac{1}{2a}\sum_{\hat{e}_\mu}[((\gamma_\mu)_{\alpha\beta} - r\delta_{\alpha\beta})\delta_{n,m+\hat{e}_\mu} - ((\gamma_\mu)_{\alpha\beta} + r\delta_{\alpha\beta})\delta_{n,m-\hat{e}_\mu}] + (m + 4r/a)\delta_{n,m}\delta_{\alpha,\beta} \tag{24}$$

which in momentum space is

$$K(p)_{\alpha\beta} = \left[\frac{i}{a}\sum_\mu \sin(p_\mu a)\gamma_\mu + m + \frac{2r}{a}\sum_\mu \sin^2\left(\frac{p_\mu a}{2}\right)\right]\delta_{\alpha\beta} \tag{25}$$

From the small argument approximation of the sine function, we can see that the additional term in (25) vanishes like a^1 as $a \to 0$, so the correct continuum limit is preserved. With the extra term, when $p_\mu = \pi/a$, $K(p)$ contains a term $2r/a$, preventing a pole at the edge of the BZ.

Unlike scalar fields, that take on c-number values, fermion fields are comprised of Grassmann numbers, which anticommute. In a full lattice calculation, we will eventually have to resort to a numerical calculation, such as the numerical evaluation of an integral, usually done by using Monte Carlo methods. Since these calculations only deal with c-numbers, we will need to simplify the integration over the fermion fields. This can easily be done by using the rule for integration over Grassmann variables ψ

$$\int d\psi = 0 \qquad \int \psi d\psi = 1 \tag{26}$$

We would like to calculated the discretized fermionic generating functional Z_f

$$Z_f[\eta,\bar{\eta}] = \int \prod_i \psi(x_i)\prod_j \psi(\bar{x}_j)\exp\left(-\sum_{nm}[\bar{\psi}(x_n)K_{nm}\psi(x_n) + \bar{\eta}(x_n)\psi(x_n) + \bar{\psi}(x_n)\eta(x_n)]\right) \tag{27}$$

where η is a Grassmann-valued source field and Dirac indices have now been suppressed. Neglecting the source field for the moment, the exponential in Z_f can be simplified greatly by writing it in its power series form where only linear terms in ψ survive the integration over ψ. The source terms can be dealt with by introducing shift fields, which gives[1]

$$Z_f[\eta,\bar{\eta}] = \det(K)\exp\left(\sum_{nm}\bar{\eta}(x_n)K^{-1}_{nm}\eta(x_m)\right) \tag{28}$$

Therefore, to include the effect of fermion fields in a lattice calculation, one simply has to calculate the determinant of the matrix K. However, in most lattice calculations, the matrix K is extremely large. Until recently, this task was too computationally expensive and the approximation that neglected the effects of off-shell fermions was used, known as the *quenched approximation*, which set $\det(K) = 1$. The quenched approximation was not motivated by a physical argument and was made simply to make lattice calculations easier to do. However, with recent advances in computing power and new algorithms, this determinant can be computed without too much trouble and the quenched approximation is used less often.

[1] See [7] p.26 for details of the calculation.

3 Lattice Gauge Theories

A central interest of lattice field theory are gauge theories, such as QCD. To find the most suitable way to incorporate gauge theories into the lattice formulation, we begin by reviewing gauge theories in the continuum. Assume the Lagrangian of interest is invariant under the gauge group G, where the fermion fields $\psi(x)$ transform under a representation of the group $\Omega(x)$ as $\psi(x) \to \Omega(x)\psi(x)$. It is not hard to form gauge invariant terms in the Lagrangian that do not involve derivatives, such as a mass term $\bar{\psi}(x)\psi(x)$, since each field is evaluated at the same point. On the other hand, a term with a derivative compares a field at two neighboring points. The derivative of $\psi(x)$ in the direction of the unit vector n^μ is given by

$$n^\mu \partial_\mu \psi = \lim_{\epsilon \to 0} \frac{\psi(x + \epsilon n) - \psi(x)}{\epsilon} \tag{29}$$

which subtracts field ψ at two different points in space. However, since we can apply a different transformation of the gauge symmetry G at each of these points, we need a way to compare the fields that takes this into account. This is very similar to what is encountered in general relativity when one tries to take a derivative. In GR, the concept of a covariant derivative is introduced, which compares the spacetime coordinates of two different points by making use of parallel transport. We will use the same concept here, but will compare the transformation of the fields ψ at two different points. We introduce the link variable $U(y, x)$ that accomplishes this task by having the transformation property

$$U(y, x) \to \Omega(y) U(y, x) \Omega(x)^\dagger \tag{30}$$

It is easy to check that $\psi(x + \epsilon n)$ and $U(x + \epsilon n, x)\psi(x)$ transform in the same way, so that the difference between these two quantities is meaningful. We can then construct the covariant derivative D_μ as

$$n^\mu D_\mu \psi = \lim_{\epsilon \to 0} \frac{\psi(x + \epsilon n) - U(x + \epsilon n, x)\psi(x)}{\epsilon} \tag{31}$$

In the continuum formulation, the derivative compares a field at two infinitely close points with separation ϵ, so we can expand $U(x + \epsilon n, x)$ in ϵ as

$$U(x + \epsilon n, x) = \mathbb{1} - ig\epsilon n^\mu A_{r\mu}(x) + \mathcal{O}(\epsilon^2) \tag{32}$$

so that the covariant derivative becomes $D_\mu = \partial_\mu + igA_{r\mu}$ and we recognize the appearance of the gauge fields $A_{r\mu}$. The gauge fields are analogous to the Christoffel symbol in GR.

We now turn our attention toward the same procedure on the lattice. The main difference between taking a derivative in a continuous space and on the lattice is that on the lattice, the separation between two point on the lattice will not necessarily be small and therefore we should reexamine the expansion of the link variable in (32). To find the form of the link variable on the lattice, we can simply divide the path from one lattice point to another into infinitely many infinitesimal paths, applying (32) at each segment, which for the path between the lattice points x and $x + a\hat{e}_\mu$ yields the product

$$\begin{aligned} U_\mu(x) &\equiv \lim_{N \to \infty} \prod_{n=0}^{N-1} \left[\mathbf{I} - ig \frac{a\hat{e}_\mu}{N} A_{r\mu}(x + an/N) \right] A_{r\mu} \\ &= P\text{exp} \left[ig \int_x^{x + a\hat{e}_\mu} dx_\mu A_{r\mu}(x) \right] \qquad \text{(no sum on } \mu \text{ for both lines)} \end{aligned} \tag{33}$$

The last line of (33) contains a line integral, where P denotes the path ordering of the multiplication of the gauge fields. We can see that the link variable $U_\mu(x)$ 'transports' the gauge transformation from the point x to the point $x + a\hat{e}_\mu$. Notice that $U_\mu(x)$ depends only on the gauge field $A_{r\mu}$. In the continuum formulation, $A_{r\mu}$ is usually used as the basic variable to describe the gauge particles, which are defined at each point in the space-time. In the lattice formulation, derivatives compare points that are separated by finite distances, therefore it is more natural to use the link variables $U_\mu(x)$ as the basic variable to describe the gauge particles. This choice of variables will simplify calculations when we construct the action for the gauge field. In summery, in the lattice formulation, we define scalar and fermion fields at lattice sites and describe the gauge fields with the link variables that connect adjacent lattice sites. It is also important to notice that from (33), it is clear that the link variable are elements of the representation r of the gauge group G. Finally, notice that the gauge field $A_{r\mu}$ has four degrees of freedom at each point in spacetime, which is paralleled by the four 'forward' link variables attached to each lattice point (where 'forward' denotes the link variable that connects a point to the adjacent point in the positively defined direction, so that each link is paired with a unique lattice point).

We can graphically represent a link $U_\mu(x)$ by an arrow from the lattice point x to $x+a\hat{e}_\mu$, shown in Fig.1. Since $U^\dagger_\mu(x) = U_{-\mu}(x+a\hat{e}_\mu)$ (where the minus sign in $U_{-\mu}$ simply denotes that the path integral in (33) is to be taken in the opposite direction), we can represent $U^\dagger_\mu(x)$ by an arrow connecting the same points as $U_\mu(x)$, but pointing in the opposite direction.

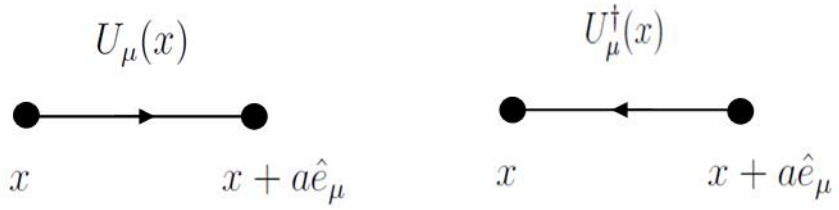

Figure 1: Link variable in the μ direction.

Using the link variable to rewrite the Wilson fermion discretized Green's function K_{nm} to be gauge invariant yields

$$(K_{n,m})_{\alpha\beta}[U] = \frac{1}{2a}\sum_{\hat{e}_\mu}[((\gamma_\mu)_{\alpha\beta} - r\delta_{\alpha\beta})U_\mu(x_n)\delta_{n,m+\hat{e}_\mu} - ((\gamma_\mu)_{\alpha\beta} + r\delta_{\alpha\beta})U_{-\mu}(x_n)\delta_{n,m-\hat{e}_\mu}] + (m + 4r/a)\delta_{n,m}\delta_{\alpha,\beta} \tag{34}$$

We now would like to find the lattice version of the pure gauge part of the action, which approaches the appropriate continuum action as the lattice spacing tends to zero. This can be written in the Euclidean formalism as

$$S_G = \frac{1}{4T_2(r)}\int d^4x \mathrm{tr}(F_{\mu\nu}F_{\mu\nu}) \tag{35}$$

where the field strength $F_{\mu\nu}$ is matrix valued ($F_{\mu\nu} = F^a_{\mu\nu}t^a_r$). Since we are using the link variables as the basic variables for the gauge field, we will need to build a gauge invariant combination of the link variables. The simplest non-trivial object of this type is the plaquette $U_{\mu\nu}(x)$, which is defined as

$$U_{\mu\nu}(x) \equiv U_\mu(x)U_\nu(x + a\hat{e}_\mu)U^\dagger_\mu(x + a\hat{e}_\nu)U^\dagger_\nu(x) \tag{36}$$

Using the gauge transformation of the link variables on the lattice, $U_\mu(x) \to \Omega(x)U_{mu}(x)\Omega^\dagger_\mu(x + a\hat{e}_\mu)$, which is the discretized version of (30), it is easy to show that $\mathrm{tr}(U_{\mu\nu}(x))$ is gauge invariant. The link

variables in the plaquette 'transports' the gauge transformation around a square of side length a in the $\mu\nu$-plane, as shown in Fig.2.

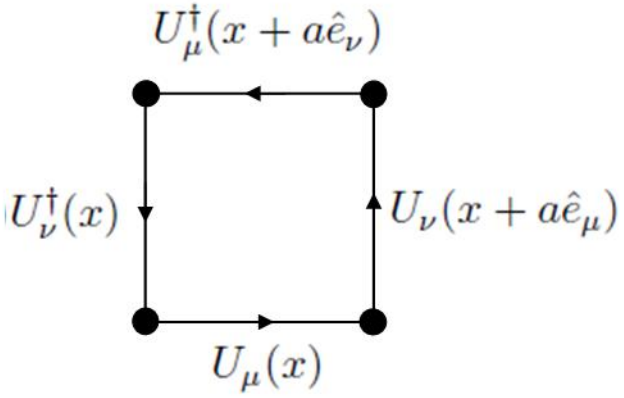

Figure 2: Plaquette in μ-ν plane.

We will now show that a gauge invariant action on the lattice can be built from the plaquette that in the limit $a \to 0$ approaches the continuum pure gauge action (35). To accomplish this task, we must first find the form of the plaquette in the limit $a \to 0$. In this limit, the link variable $U_\mu(x)$ can be approximated by replacing the line integral in (33) by the value of $A_{r\mu}(x)$ evaluated in the middle of the line, $U_\mu(x) \approx \exp(igaA_{r\mu}(x + a\hat{e}_\mu/2))$ (no sum on μ). $A_{r\mu}(x + a\hat{e}_\mu/2)$ can then be expanded in a to yield

$$U_\mu(x) \approx \exp[iga(A_{r\mu}(x) + \frac{a}{2}\partial_\mu A_{r\mu}(x))] \qquad \text{(no sum on } \mu\text{)} \tag{37}$$

We can approximate the other link variables in the plaquette in the same manner

$$\begin{aligned} U_\nu(x + a\hat{e}_\mu) &\approx \exp[iga(A_{r\nu}(x) + \frac{a}{2}\partial_\nu A_{r\nu}(x) + a\partial_\mu A_\nu(x))] \\ U_\mu^\dagger(x + a\hat{e}_\nu) &\approx \exp[-iga(A_{r\mu}(x) + \frac{a}{2}\partial_\mu A_{r\mu}(x) + a\partial_\nu A_{r\mu}(x))] \\ U_\nu^\dagger(x) &\approx \exp[-iga(A_{r\nu}(x) + \frac{a}{2}\partial_\nu A_{r\nu}(x))] \qquad \text{(no sum on } \mu,\nu \text{ for all lines)} \end{aligned} \tag{38}$$

Substituting these approximations for the link variables into the plaquette (36) and using the Baker-Campbell-Hausdorff formula $e^A e^B = e^{A+B+[A,B]/2+\cdots}$ yields to lowest lower in a

$$\begin{aligned} U_{\mu\nu}(x) &\approx \exp\left(iga^2[\partial_\mu A_{r\nu}(x) - \partial_\nu A_{r\mu}(x)] - ga^2[A_{r\mu}(x), A_{r\nu}(x)]\right) \\ &= \exp(iga^2 F_{\mu\nu}(x)) \end{aligned} \tag{39}$$

We have now related the plaquette $U_{\mu\nu}(x)$ to the field strength $F_{\mu\nu}$ in the continuum limit, so we would now like to find the combination of plaquettes that approaches (35) in the continuum limit. In this limit, expanding (39) in powers of a yields

$$U_{\mu\nu} \approx \mathbb{1} + iga^2 F_{\mu\nu} - \frac{1}{2}g^2 a^4 F_{\mu\nu}F_{\mu\nu} + \mathcal{O}(a^6) \qquad \text{(no sum on } \mu,\nu\text{)} \tag{40}$$

so that to lowest power in a

$$\sum_n \sum_{\mu<\nu} \sum_\nu \text{tr}\left[\mathbb{1} - \frac{1}{2}(U_{\mu\nu}(x_n) + U_{\mu\nu}^\dagger(x_n))\right] \approx \sum_n \sum_{\mu,\nu} \frac{1}{4}g^2 a^4 F_{\mu\nu}(x_n)F_{\mu\nu}(x_n) \tag{41}$$

where in the right hand side we sum over the plaquette in each orientation (clockwise and counter-clockwise), and so introduce a factor of 1/2. We can now form the lattice version of the pure gauge action S_G

$$S_G = \beta \sum_P \text{tr}\left[\mathbf{I} - \frac{1}{2}(U_P + U_P^\dagger)\right] \tag{42}$$

where $U_P = U_{\mu\nu}$ is shorthand notation for the plaquette variable, Σ_P is the sum over all plaquettes of both orientations, and $\beta = 4T_2(r)/g^2$. Using (41) and $a^4\Sigma_n \overset{a\to 0}{=} \int d^4x$, it is evident that the lattice version of the pure gauge action in (42) approaches the continuum version in (35) in the limit $a \to 0$.

4 Running Coupling and the Continuum Limit

The previous section dealt with a gauge theory with coupling constant g, which is a bare coupling. We now raise the question of what the value of this bare coupling should be? We first remark that the lattice introduces a UV cutoff $\Lambda = \pi/a$ that increases for decreasing lattice spacing a. This UV cutoff introduces a running in the bare coupling constant that can be examined with the renormalization group. The β-function for the bare coupling g is given by

$$\tilde{\beta}(g) \equiv -\frac{\partial g}{\partial \ln a} \tag{43}$$

where we put a tilde above the β-function to distinguish it from the inverse coupling squared. The β-function gives the relationship between the bare coupling g and the lattice spacing a. It can be shown [3] that for $SU(N)$ gauge groups, $g \to 0$ as $a \to 0$. Therefore, the continuum limit can be reached by taking $\beta \propto 1/g^2 \to \infty$.

While taking the limit $a \to 0$, we have to be mindful of the physical size of our lattice. Suppose our lattice has N_L lattice point along each spatial dimension and N_T lattice points along the temporal dimension. The physical length and time extensions of the lattice, L and T respectively, is then $L = aN_L$ and $T = aN_T$. We can see that if we keep the number of lattice points constant as we decrease a, we shrink the physical extensions of our lattice, which will approach zero as $a \to 0$. To avoid this, we increase the number of lattice points as we decrease a such that the physical extensions of the lattice remain constant.

In summery, to perform our lattice calculations, we choose a number of lattice point and find a such that the physical extensions of are lattice match some constant values. We then use the β-function to determine $g(a)$ and perform the lattice calculation to determine the value of some parameter that is an observable in the continuum limit. We then repeat this process with an increased number of lattice points to form a trend line in the parameter, which is then extrapolated to $a = 0$.

We now have the basic ingredients for our formulation of field theory on the lattice and now investigate some uses of lattice field theory.

5 The Quark-Antiquark Potential

An essential feature of QCD at low energies is confinement, i.e. that quarks and antiquarks are only observed as bound, colour-neutral states. We were unable to use perturbation theory in this regime, which makes it an important study of lattice QCD. We can demonstrate confinement by examining the potential between a non-relativistic quark and antiquark (a similar but more difficult calculation is required for the three quarks in a baryon).

We will make a number of approximations to make the lattice calculation easier. The first is that we will assume that the quark and antiquark are very heavy and can be treated non-relativistically, so that the notion of a potential is meaningful. We will use the limit that the mass of the quark/antiquark approaches an infinte mass, so that we can treat them as sationary. Although we will treat the on-shell quark and antiquark as very heavy, we expect that virtual quarks will enter into the calculation. Since these quarks will in general be off-shell, we cannot use the same non-relativistic approximation. While in reality we cannot isolate a particular quark and label it as a finite or infinte mass quark, for the purpose of our lattice calculation we will make this distinction to make the calculation easier. We label the heavy quark/antiquark with the spinors ψ^Q and $\bar{\psi}^Q$ and label the light quarks with the spinors ψ and $\bar{\psi}$

We would like the study the gauge invariant state consisting of a quark and antiquark at (Euclidean) time T

$$|\Psi(\vec{x},\vec{y},T)\rangle = \bar{\psi}^Q(\vec{x},T)U(\vec{x},T;\vec{y},T)\psi^Q(\vec{y},T)\,|0\rangle \tag{44}$$

where $U(\vec{x},T,\vec{y},T) = \prod_l n_l^\mu U_\mu(T)$ is the product of link variables along a straight path connecting the quark and antiquark at positions $\vec{x}$ and $\vec{y}$, n_l^μ is a unit vector along this path, and $|0\rangle$ is the ground state of the system. Since the two spinors in (44) are spatially separated, $U(\vec{x},T,\vec{y},T)$ is required in the expression to allow a comparison between the gauge transformations at each point.

Consider now the Green's function for the propagation of the quark-antiquark state from the positions $\vec{x}$ and $\vec{y}$ at time $T=0$ to the positions $\vec{x}'$ and $\vec{y}'$ at time T, given by

$$G(\vec{x},\vec{y},\vec{x}',\vec{y}',T) = \langle 0|\mathcal{T}(\bar{\psi}^Q(\vec{y}',T)U(\vec{y}',T;\vec{x},T)\psi^Q(\vec{x}',T)\bar{\psi}^Q(\vec{x},0)U(\vec{x},0;\vec{y},0)\psi^Q(\vec{y},0))|0\rangle \tag{45}$$

where $\mathcal{T}$ denotes the time-ordering operator.

To extract the quark-antiquark potential, we will use a similar method as used in the Feynman-Kac formula to find the ground state energy of a non-relativistic particle of mass m moving in a potential $V(x)$. In this case, the propagator for the particle to move from position x to x' in real time t is given by

$$G(x,x',t) = \langle x'|e^{-iHt}|x\rangle \tag{46}$$

where $H = p^2/2m + V(x)$. By inserting a complete set of energy eigenstates $|n\rangle$ into (46) yields

$$G(x,x',t) = \sum_n \langle x'|n\rangle\,\langle n|x\rangle\, e^{-iE_nt} \tag{47}$$

Switching to Euclidean time T makes the replacement $e^{-iE_nt} \to e^{-E_nT}$, so that the exponential term now damps higher energy states more than lower ones. Taking the large Euclidean time limit $T\to\infty$ gives

$$\lim_{T\to\infty} G(x,x',t) \to \langle x'|0\rangle\,\langle 0|x\rangle\, e^{-E_0T} \tag{48}$$

We see that the ground state E_0 can be extracted from the propagator in the large Euclidean time limit.

With this in mind, we return to the quark-antiquark case, starting before the quantization onto the lattice. In the limit where the valence quark masses are infinite, their positions are static. Taking the same steps as above, the quark-antiquark Green's function $G(\vec{x},\vec{y},\vec{x}',\vec{y}',T)$ in the limit $T\to\infty$ is [2]

$$\lim_{T\to\infty}\left(\lim_{m_Q\to\infty} G(\vec{x},\vec{y},\vec{x}',\vec{y}',T)\right) \to \delta^{(3)}(\vec{x}'-\vec{x})\delta^{(3)}(\vec{y}'-\vec{y})e^{-E_0(R)T} \tag{49}$$

[2] See [7] p.99 for more details.

where $R = |\vec{x} - \vec{y}|$.

We will now compute this Green's function, which is given by

$$G(\vec{x}, \vec{y}, \vec{x}', \vec{y}', T) = \frac{1}{Z} \int \mathcal{D}A\mathcal{D}\psi\mathcal{D}\bar{\psi}\mathcal{D}\psi^Q\mathcal{D}\bar{\psi}^Q(\bar{\psi}^Q(\vec{y}', T)\dots\psi^Q(\vec{y}, 0))e^{-S} \tag{50}$$

Under our assumptions, the action S can be broken down as

$$S = S_G[A] + S_F[\psi, \bar{\psi}, A] + S_F[\psi^Q, \bar{\psi}^Q, A] \tag{51}$$

where S_G is the pure gauge part of the action and S_F is the fermionic part.

We first consider $S_F[\psi^Q, \bar{\psi}^Q, A]$ and separate the pure fermionic term from the fermion-guage field interaction term. Let K^Q_{mn}, given in (24), represent the pure fermionic Green's function for the heavy quarks. The heavy quark fields can be integrated over, as was done in (28), to give a coefficient of $\det(K^Q)$. Since we will take the limit $m_Q \to \infty$, from (24) we can see that $\det(K^Q)$ will approach an infinite constant that will be canceled by the same term in Z in the denominator of (50). Since we are considering these quarks to be non-relativistic, we will take the interaction action between the heavy quarks and the gauge field A_μ as $S_{int} = \int d^4x j_\mu(x)A_\mu(x)$, where j_μ is the current associated with the non-relativistic heavy quarks. Since the quark and antiquark are assumed to be stationary, we can take $j_i = 0$ and $j_4(z) = -ig\delta(\vec{z} - \vec{x}) + ig\delta(\vec{z} - \vec{y})$ so S_{int} becomes

$$S_{int} = -ig \int d\tau(A_4(x) - A_4(y)) \tag{52}$$

So far, the integration over τ has been from $-\infty$ to ∞. Consider now the approximation where we make the substitution $\int_{-\infty}^{\infty} d\tau \to \int_0^T d\tau$ for $T \gg R$, so that the integration in (52) can be approximated by the integral over a closed loop

$$\int_0^T d\tau(A_4(x) - A_4(y)) = \int_0^T d\tau A_4(x) + \int_T^0 A_4(y) \approx \oint_C dx_\mu A_\mu(x) + \mathcal{O}(R/T) \tag{53}$$

where C is the loop defined in Fig.3. With this approximation, $\exp(-S_{int})$ becomes

$$\exp(-S_{int}) \approx \exp(ig \oint_C dx_\mu A_\mu(x)) \tag{54}$$

By comparison to (33), $\exp(-S_{int})$ in this approximation is merely the path ordered product of link variables U_μ around the closed loop C (With $a \to 0$ in (33) since we are in the continuum limit). This is the Wilson loop W_C, given by [3]

$$W_C[U] = \prod_{l \in C} n_l^\mu U_\mu \tag{55}$$

When we put the theory on the lattice, the link variables will be the basic gauge field variables, so W_C will be (relatively) easy to calculate. We can also recognize that the plaquette is the Wilson loop around an elementary square on the lattice.

[3] See [6] p.491 for more details on the Wilson loop.

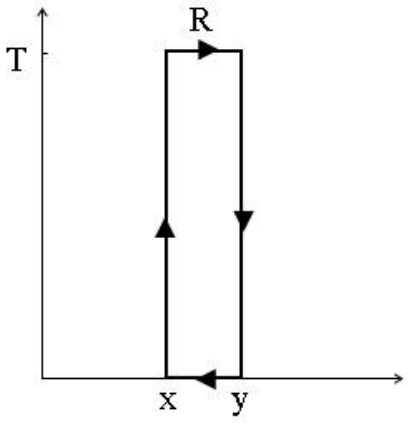

Figure 3: Wilson loop for quark-antiquark potential.

Using our results in (50) gives

$$\lim_{T\to\infty}\left(\lim_{m_Q\to\infty} G(\vec{x},\vec{y},\vec{x}',\vec{y}',T)\right) = \lim_{T\to\infty} W(R,T) \equiv \frac{\int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi} W_C[U] e^{-S_G[U]-S_F[\psi,\bar{\psi},U]}}{\int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi} e^{-S_G[U]-S_F[\psi,\bar{\psi},U]}} \tag{56}$$

where we have now implicitly put in the form of Z. By comparison to (49), we can identify the interaction energy of the quark-antiquark pair in their ground state E_0, or in other words the quark-antiquark potential, as

$$E_0(R) = -\lim_{T\to\infty}\frac{1}{T}\ln W(R,T) \tag{57}$$

We now have our prescription for calculating the quark-antiquark potential. One caveat is that E_0 in (57) also contains contributions from R-independent quark self-energies that must be subtracted to find the potential.[4]

The last step needed before we perform the numerical calculation is to deal with the off-shell virtual quarks. We can perform the same integration over the Grassmann valued fields ψ and $\bar{\psi}$ as done in (28), but with K_{nm} now given by (34), to give

$$\lim_{T\to\infty} W(R,T) = \frac{\int \mathcal{D}U W_C[U] e^{-S_G[U]+\ln(\det(K[U]))}}{\int \mathcal{D}U e^{-S_G[U]+\ln(\det(K[U]))}} \tag{58}$$

While $\det(K[U])$ is difficult to calculate, it can be done with Monte Carlo methods. $W(R,T)$ in (58) is now only a function of the link variables U_μ and the integral can be performed by Monte Carlo Markov chains (taking T to be a finite large number with $T \gg R$). The result of such a calculation is shown in Fig. 4

[4]See [7] p.111 for details.

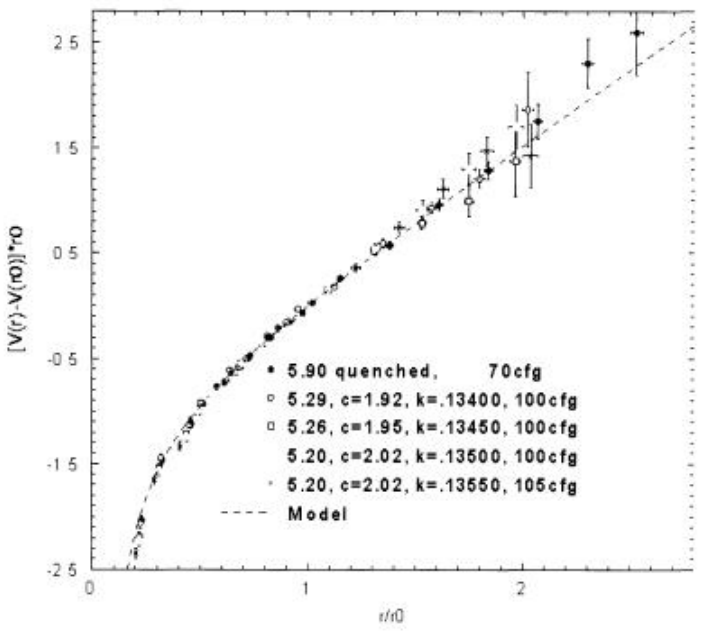

Figure 4: Static quark-antiquark potential calculated from lattice QCD with comparison to string model. From: J. Garden et al. (UKQCD collaboration) Nucl. Phys. Proc. Suppl. **83**, 165 (2000).

The points from the numerical lattice calculation agree reasonably well with the relation $E_0(R) = C + \sigma R - \alpha/R$, shown in Fig. 4, where C, σ and α are constants. From the plot, we can see that at small R the potential act like a Coulombic potential and at large R the potential increases approximately linearly with R. This implies that QCD predict that for large separations, the colour fields do not spread out and are confined to a tube or 'string' like region between quarks (accordingly, σ is known as the string tension). We expect that once R is increased to a point where the inter-quark energy is higher than the energy required to make another bound quark-antiquark state between the quarks, this quark-antiquark pair will be formed, thereby 'breaking' the string. The lattice calculation performed gives a quantitative prediction of confinement in QCD.

6 Hadron Masses

An important part of testing QCD is calculating the masses of hadrons and comparing these to measured values. This is a low-energy QCD calculation and thus is an important case to study with lattice QCD.

The method to calculate hadron masses is very similar to the quark-antiquark potential calculation. First, operators O and $O^\dagger$ will be constructed so that they annihilate and create the particle state we wish to examine. The correlation function $\langle 0|O(T)O^\dagger(0)|0\rangle$, where $|0\rangle$ is again the ground state of the system, will be calculated by inserting a complete set of energy eigenstates. The limit $T \to \infty$ is then taken, so that in this limit $\langle 0|O(T)O^\dagger(0)|0\rangle$ is given by (48), but with $|x\rangle \to |0\rangle$ and $\langle x'| \to \langle 0|$ in this situtation, so that

$$\lim_{T\to\infty} \langle 0|O(T)O^\dagger(0)|0\rangle \to Ce^{-E_0 T} \tag{59}$$

where C is a constant. Therefore, by studying the correlation function $\langle 0|O(T)O^\dagger(0)|0\rangle$ at large T, we can extract the ground state energy E_0

The first task is to construct the appropriate operators that create and annihilate the valence quarks that comprise the hadron whose mass we wish to calculate. To do this, we will construct Dirac bilinears $\bar{\psi}\Gamma\psi$ that have the same quantum numbers (parity, charge, spin) as the particle under consideration. The transformation properties of the Dirac bilinears $\bar{\psi}\Gamma\psi$ under C and P,[5] as well as its spin J, are listed in Table 1

Bilinear	Γ	J	P	C
Scalar	$\mathbb{1}$,γ_4	0	1	1
Vector	γ_i, $\gamma_4\gamma_i$	1	-1	-1
Tensor	$\gamma_i\gamma_j$	1	1	-1
Pseudo-vector	$\gamma_i\gamma_5$	1	1	1
Pseudo-scalar	γ_5, $\gamma_4\gamma_5$	0	-1	1

Table 1: Spin and transformation under P and C of Dirac bilinears.

For example, the pions and η-meson have quantum numbers $J = 0$, $P = -1$, and $C = 1$, so their operators will be comprised of pseudo-scalar bilinears as

$$\begin{aligned} O_{\pi^+} &= \bar{d}\gamma_5 u \\ O_{\pi^-} &= \bar{u}\gamma_5 d \\ O_{\pi^0} &= \frac{1}{\sqrt{2}}(\bar{u}\gamma_5 u - \bar{d}\gamma_5 d) \\ O_{\eta} &= \frac{1}{\sqrt{2}}(\bar{u}\gamma_5 u + \bar{d}\gamma_5 d) \end{aligned} \tag{60}$$

where u and d are the spinors for the up and down quarks of the same colour, respectively, and we have neglected the contribution of the s-quark in the η-meson for this example. Baryon operators can be formed in a similar manner, but are slightly more complicated.[6]

We can compute the correlation function in (59) with a meson operator of the form $O_M = \bar{f}_1\Gamma f_2$, where f_1 and f_2 are the spinors for the two fermions comprising the meson, by first integrating over the Grassmann fields (denoted by $\langle\ldots\rangle_F$) by using Wick's theorem, which yields[7]

$$\langle 0|O_M(x_n)O_M^\dagger(x_m)|0\rangle_F = -\mathrm{tr}\left[\Gamma(K^{f_2}_{nm})^{-1}\Gamma(K^{f_1}_{mn})^{-1}\right] \tag{61}$$

where $(K^f_{nm})^{-1}$ is the propagator for the Wilson's fermion f (the inverse of (34)). From (61), we can see that the correlator in (59) will involve propagating the fermion f_1 from point x_n to x_m and fermion f_2 in the opposite direction, which is depicted schematically in Fig.5a. A term that propagates a fermion from one place in spacetime to another, as in (61), is referred to as a *connected piece*.

The correlator for a meson state with operator of the form $O_M = 1/\sqrt{2}(\bar{f}_1\Gamma f_1 \pm \bar{f}_2\Gamma f_2)$, such as the operator for neutral pion or the η-meson, can be found by using the same procedure as above, which yields

$$\begin{aligned} \langle 0|O_M(x_n)O_M^\dagger(x_m)|0\rangle_F = &-\frac{1}{2}\mathrm{tr}\left[\Gamma(K^{f_1}_{nm})^{-1}\Gamma(K^{f_1}_{mn})^{-1}\right] + \frac{1}{2}\mathrm{tr}\left[\Gamma(K^{f_1}_{nn})^{-1}\right]\mathrm{tr}\left[\Gamma(K^{f_1}_{mm})^{-1}\right] \\ &\pm \frac{1}{2}\mathrm{tr}\left[\Gamma(K^{f_1}_{nn})^{-1}\right]\mathrm{tr}\left[\Gamma(K^{f_2}_{mm})^{-1}\right] + f_1 \leftrightarrow f_2 \end{aligned} \tag{62}$$

[5]See [6] p.65 for derivation of transformations under C and P.

[6]See [3] p.129 for the formation of baryon operators.

[7]See [3] p.127 for details of the intergration.

This correlation function contains connected pieces as well as terms that propagate fermions from a point back to the same point, seen in Fig.5b, referred to as *disconnected pieces*. In the case where we take f_1 and f_2 to have the same mass, as when considering an exact isospin symmetry, $K^{f_1}_{mn} = K^{f_2}_{mn}$ since K^f_{mn} only differs between fermions by their mass. In this case, the disconnected terms in (62) cancel for a meson that has the operator $O_M = 1/\sqrt{2}(\bar{f}_1 \Gamma f_1 - \bar{f}_2 \Gamma f_2)$, like the neutral pion, which is the $I_z = 0$ component of the iso-triplet pion state.

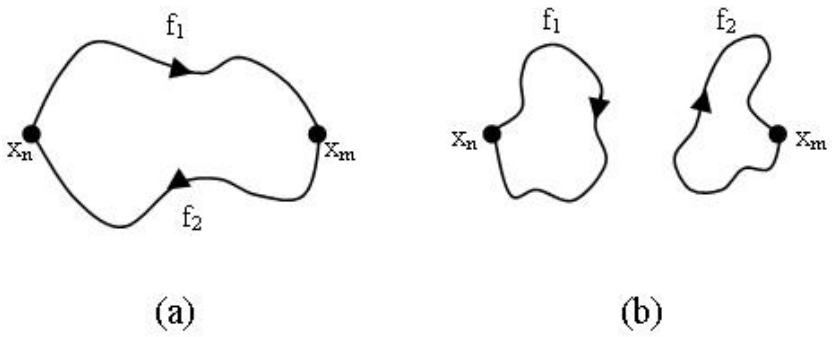

Figure 5: (a) Connected piece of a meson correlator (b) Disconnected piece of a meson correlator.

The final step in calculating the correlation function is to make the operators states of definite spatial momentum $\vec{p}$, which we can do by taking the spatial Fourier transform

$$O(\vec{p}, n_4) = \frac{1}{\sqrt{V_{sp}}} \sum_{\vec{n}} O(x_n) e^{-ia\vec{n}\cdot\vec{p}} \tag{63}$$

where V_{sp} is the spatial volume of the lattice. The final expression for the correlation function in (59) is then

$$\langle 0|O(\vec{p}, an_4)O^\dagger(\vec{0}, 0)|0\rangle = \frac{1}{\sqrt{V_{sp}}} \sum_{\vec{n}} e^{-ia\vec{n}\cdot\vec{p}} \langle 0|O(a\vec{n}, an_4)O^\dagger(\vec{0}, 0)|0\rangle \tag{64}$$

where

$$\langle 0|O(x_n)O^\dagger(x_m)|0\rangle = \langle \langle 0|O(x_n)O^\dagger(x_m)|0\rangle_F \rangle_G \tag{65}$$

where $\langle \ldots \rangle_G$ denotes the integration over the gauge fields (i.e. link variables). By setting $\vec{p} = 0$, one can use (64) to calculate the decay of this solution with increasing $T = an_4$ and can extract the ground state energy, in this case the mass of the particle, by comparison to (59). For example, the correlation function for the π^+ meson is

$$\langle 0|O(\vec{0}, an_4)O^\dagger(\vec{0}, 0)|0\rangle = \frac{1}{\sqrt{V_{sp}}} \sum_{\vec{n}} \left(-\frac{1}{Z} \int \mathcal{D}U e^{-S_G[U]} \det(K^u_{n0}) \det(K^d_{n0}) \mathrm{tr}\left[\gamma_5 (K^u_{n0})^{-1} \gamma_5 (K^d_{0n})^{-1}\right] \right) \tag{66}$$

where

$$Z = \int \mathcal{D}U e^{-S_G[U]} \det(K^u_{n0}) \det(K^d_{n0}) \tag{67}$$

Results of lattice calculations can be seen in Table 2 for various hadrons, which agree with experimental values.

Particle	Mass (lattice calculation), MeV	Mass (experiment), MeV
p	920±100	938
ρ	730±90	770
Σ^0	1176±22	1193
Δ^0	1257±36	1232

Table 2: Hadron masses from lattice calculations. p and ρ masses calculated in [8] and Σ^0 and Δ^0 masses calculated in [1].

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