

TEORETIČNI IZRAČUN MAS NUKLEONOV

ANDREJ KOLAR - POŽUN

Fakulteta za matematiko in fiziko
Univerza v Ljubljani

Prepričljiva potrditev pravilnosti kvantne kromodinamike (QCD) je natančna določitev nukleonskih mas. Članek se začne z opisom osnov kvantne teorije polja in z diskretizacijo QCD akcije. Predstavljene so metode za izračun Evklidskih korelatorjev ter njihova uporaba pri določitvi mas nukleonov. Tako pridobljeni rezultati so primerjani z eksperimentom.

THEORETICAL CALCULATION OF THE NUCLEON MASS

A convincing confirmation of the quantum chromodynamics (QCD) is an accurate prediction of the nucleon masses. The article begins by introducing the basic concepts of quantum field theory and discretizing the QCD action. The techniques for evaluation of Euclidean correlators and how they can be used to extract the nucleon masses are then discussed. The results are compared with the measured values of nucleon masses.

1. Introduction

It is well known that the two main composites of nuclei - proton and neutron have approximate masses of 938 MeV and 940 MeV, respectively. We would like to understand the origin of those values within the quantum theory. A nucleon is composed of three valence quarks, those being 2 up quarks and a down quark in a proton and vice versa in a neutron. The Standard Model of particle physics tells us a complete structure of a nucleon is more complex than just that: it is also made of gluons and the quark sea consisting of quark-antiquark pairs. Up quark masses have been determined to be approximately 1.8 – 2.9 MeV, while down quarks' mass is 4.4 – 5.2 MeV [1]. Obviously, simply adding the valence quark masses is wrong, since the sum is far below the measured nucleon mass. The missing component is exactly the contribution of gluons and the quark sea, which add up to the majority of the nucleon's rest energy. It is this additional energy that we will be accounting for in this article. Before we are able to perform this calculation, we will introduce in Section 2 basic features of quantum field theory (QFT), namely, quantum chromodynamics and its path integral formulation along with correlators and how they can be used to extract nucleon (or more generally any hadron) masses. In sections 3 and 4 we continue by introducing numerical techniques for evaluation of those correlators. We apply the presented information and calculate the masses in Section 5, comparing them with the experiment.

2. Summary of the necessary QFT elements

In this article we will be working in natural units: $\hbar = c = 1$. Consequentially the dimensions of quantities used will be some powers of eV. For example, from $1 = \hbar c \approx 200 \text{ MeV fm}$ we can see that $1 \text{ fm} \approx 0.005 \text{ MeV}^{-1}$. For reference, $1 \text{ MeV}/c^2$ corresponds to $1.78 \cdot 10^{-30} \text{ kg}$.

Also, we will perform a transformation of real time into imaginary time $t \rightarrow -it_E$. Such transformation is called a Wick rotation and it transforms the Minkowski metric $ds^2 = dt^2 - dx^2 - dy^2 - dz^2$ into an Euclidean metric $ds^2 = -dt_E^2 - dx^2 - dy^2 - dz^2$. We will refer to quantities calculated after a Wick rotation as Euclidean quantities as opposed to the usual Minkowski quantities. Validity of such transformation will not be discussed. For further explanation see [2]. There are several advantages to be gained from working with imaginary time. Due to the metric being Euclidean we no longer have to differentiate between covariant and contravariant tensors. In addition to this, quantities such as time evolution operators transform in the following way: $e^{-iHt} \rightarrow e^{-Ht_E}$. Such

form of a time evolution operator allows us to make simple approximations by neglecting certain exponentially small quantities as will be seen in Section 2.2. Disadvantages of using the Euclidean metric are having to slightly modify several known objects, such as gamma matrices and the Dirac equation [2].

2.1 Quantum chromodynamics Lagrangian

In SM the quarks interact under strong interaction, which is carried by massless particles - gluons. As is common practice in particle physics, we begin by writing the (Minkowski) Lagrangian, which we will not derive. Derivation and further interpretation can be found in [3]. The Lagrangian reads

$$\mathcal{L} = \bar{\psi}_f^a (iD_{ab}^\mu \gamma_\mu - \delta_{ab} m_f) \psi_f^b - \frac{1}{4} F^{\mu\nu C} F_{\mu\nu}^C \quad (1)$$

$$D_{ab}^\mu = \delta_{ab} \partial^\mu - ig \mathcal{A}^{\mu C} t_{ab}^C \quad (2)$$

$$F_{\mu\nu}^C = \partial_\mu \mathcal{A}_\nu^C - \partial_\nu \mathcal{A}_\mu^C - f_{ABC} \mathcal{A}_\mu^A \mathcal{A}_\nu^B. \quad (3)$$

In the above expressions we perform a summation over repeated Lorentz indices μ, ν , quark flavour indices f and color indices a, b, c taking the values of 3 colors. \mathcal{A}_μ^C represent gauge fields of the theory, where C runs from 1 to 8 (8 gluon fields). ψ are spinors representing quarks and D^μ is also called a gauge covariant derivative. t^C are SU(3) group generators and f_{ABC} are the group structure constants, i.e. quantities appearing in the commutator $[t^A, t^B] = if_{ABC} t^C$. An important property of the QCD Lagrangian is its invariance under local (spacetime dependent) SU(3) transformations (also called SU(3) gauge transformations) of the quark and gauge fields. Details will not be discussed, we only mention that also in the discrete version of the Lagrangian we will still demand SU(3) gauge invariance. The corresponding action is defined as the integral of the Lagrangian over spacetime $S = \int d^4x \mathcal{L}$.

As mentioned before, in Euclidean metric our Lagrangian is slightly modified [4] and becomes

$$\mathcal{L}_E = \sum_f \bar{\psi}^{(f)} (\gamma_\mu (\partial^\mu + g A^\mu) + m^{(f)}) \psi^{(f)} + \mathcal{L}_G(A). \quad (4)$$

In the above equation color indices have been absorbed into a now 12 component vector ψ and a 3×3 matrix $A^\mu = \mathcal{A}^{\mu C} t^C$. The last term is only dependent on the gauge fields A and its precise form will not be important for the purposes of this seminar.

Having the Lagrangian we can compute an expectation value of an observable O . We can do that using the following formula [2]

$$\langle O \rangle \propto \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A e^{iS[\psi(x), \bar{\psi}(x), A(x)]} O[\psi(x), \bar{\psi}(x)]. \quad (5)$$

In the above we integrate over all possible functions $\psi, \bar{\psi}$ and A . Each configuration is weighted by a factor e^{iS} , where S is the (Minkowski) action. This method of computation of expectation values is called the Feynman path integral formalism. The average looks very similar to the canonical ensemble in which we also sum over all possible configurations, weighed by a Boltzmann factor $e^{-\beta E}$. The operators appearing in the expectation value on the left-hand side become functions in the integral on the right. In Euclidean metric a similar formula holds with e^{iS} replaced by e^{-S_E} , where S_E denotes Euclidean action [2].

2.2 Correlators

We would like to compute Euclidean correlators, from which we can extract hadron masses as will be shown in this Section. The Euclidean correlator of two observables is defined as [2]

$$\langle O_2(t_E) O_1(0) \rangle_T \propto \text{Tr} \left(e^{-(T-t_E)\hat{H}} \hat{O}_2 e^{-t_E \hat{H}} \hat{O}_1 \right). \quad (6)$$

Here T represents the maximum possible time and would normally be sent to infinity. We will, however, eventually be working with discretized spacetime in which case, T will take the value of the temporal extent of our finite discretized lattice.

Introducing a set of a complete states n with $\hat{H}|n\rangle = E_n|n\rangle$, setting the vacuum energy E_0 to zero and using the well known identities $\text{Tr}A = \sum_n \langle n|A|n\rangle$ and $1 = \sum_n |n\rangle\langle n|$ we get

$$\langle O_2(t_E)O_1(0)\rangle_T \propto \sum_{m,n} \langle m|O_2|n\rangle\langle n|O_1|m\rangle e^{-t_E E_n} e^{-(T-t_E)E_m} \quad (7)$$

$$\lim_{T \rightarrow \infty} \langle O_2(t_E)O_1(0)\rangle_T = \sum_n \langle 0|\hat{O}_2|n\rangle\langle n|\hat{O}_1|0\rangle e^{-t_E E_n}. \quad (8)$$

The limiting process in the last line is to be taken with a grain of salt - as mentioned earlier T is merely the temporal extent of our discretized lattice. The limit in this case simply means that T will have to be much larger than a typical t_E we are interested in.

The next step is choosing the right operators \hat{O}_2 and \hat{O}_1 for our purpose of hadron mass calculation. We choose our operators in a way that makes the scalar products in (8) vanish for n that does not represent the state of a hadron we are interested in. We achieve that by choosing \hat{O}_1 as a field operator that creates a desired hadron from the vacuum, while \hat{O}_2 annihilates it. The resulting right-hand side of equation (8) will then only contain terms that are relevant for our hadron and will therefore provide us with its energies, which we now denote by E_k with $E_1 < E_2 < \dots$. The different energies correspond to numerous excited hadron states and a ground state. Those energies appear in the equation in the form of

$$\sum_k c_k e^{-t_E E_k} \propto e^{-t_E E_1} + \mathcal{O}(e^{-t_E E_2}). \quad (9)$$

The ground state energy is by definition lower than of any excited states' energy meaning the corresponding term decays exponentially slower than the other terms. For large enough t_E the other terms are much smaller and can be neglected. This is a big simplification we gain from working in Euclidean metric. The ground state energy is related to nucleon mass by the formula $E_1^2 = p^2 + m^2$.

What is the appropriate choice for the operator \hat{O}_1 that creates a desired hadron from the vacuum? Let us take a proton as an example. We have to make sure the known proton properties are accounted for in that operator. We know its flavour structure is 2 up quarks and a down quark. The operator will therefore have to contain 2 up quark creation operators and a down quark one. In case of our functional integral approach, those operators reduce to up and down quark spinors [2]. We can easily check that such choice also gives the charge of e_0 and spin and isospin of $1/2$, with the isospin z component being $+1/2$, all of which are correct for the case of a proton. Before discussing the rest of proton properties further let us, for the readers' convenience, state the correct operator first [2]

$$O_1(n) = \epsilon_{abc} 1/2(1 + \gamma_4)u(n)_a(u(n)_b^T C \gamma_5 d(n)_c). \quad (10)$$

The spinor indices correspond to quark colors and are summed over. Completely antisymmetric Levi-Civita symbol ϵ_{ijk} thus guarantees our operator is antisymmetric in colour, which is a known property of all baryons. The product appearing in the parentheses on the right-hand side is a so called di-quark, which transforms as a Lorentz (pseudo) scalar, meaning our operator will transform as a u quark (and therefore a spinor), which is precisely what we want since a proton (being a fermion) can itself be represented by a spinor. What is left to check is parity, which should be 1 for the proton. That is taken care of by the operator $P_+ = 1/2(1 + \gamma_4)$ which is a projector on positive parity. γ_4 matrix in this case is the Euclidean version of what we would normally write as γ_0 . For more information see [2].

In order to get annihilation operator \widehat{O}_2 from our creation operator, we simply complex conjugate the latter. In the case of a neutron it can be checked that simply interchanging $u \leftrightarrow d$ gives rise to the correct operator.

3. Discretization

So far we have been assuming our spacetime is continuous and performed usual integration (in the case of action) and differentiation of our functions. Very often, however, path integrals cannot be solved analytically and we have to resort to numerical approximations. In order to do that, we have to discretize our spacetime turning it into a finite lattice. We slice each spatial dimension and the time dimension into N parts. Our whole lattice then has N^4 lattice points, which are defined by a 4 dimensional vector

$$\mathbf{n} = (n_t, n_x, n_y, n_z), \tag{11}$$

with each of the components going from 0 to $N - 1$. Our position/time vector (remember that in natural units distance and time have the same units) is given by $a\mathbf{n}$, where a is our lattice spacing. We can imagine that $N \rightarrow \infty$ and therefore $a \rightarrow 0$ corresponds to the continuum limit. In our discretization process we choose a small a (typically the lattice spacings are chosen to be around 0.1 fm) and calculate the quantities we are interested in at several values of it. We then extrapolate them to $a \rightarrow 0$. The boundary conditions of the lattice are usually taken to be periodic [2].

Naturally, our field functions like $\psi(r, t)$ will now only have definite values at points of the lattice $\psi(\mathbf{n})$. Other natural discretizations we are making are

$$\mathcal{D}\Psi \rightarrow \prod_{\mathbf{n}} d\Psi(\mathbf{n}), \tag{12}$$

$$\int d^4x f(x) \rightarrow a^4 \sum_{\mathbf{n}} f(\mathbf{n}), \tag{13}$$

$$\partial_\mu f \rightarrow \frac{f(\mathbf{n} + \boldsymbol{\mu}) - f(\mathbf{n} - \boldsymbol{\mu})}{2a}. \tag{14}$$

Integration and differentiation have simply been replaced by finite sums and differences. As for the integration over all possible functions the discretization is also intuitive: Integration over all possible functions defined on lattice points is equal to integration over all possible values of the function at those points.

During the discretization an issue arises that should be discussed. Remember that one of the important properties of QCD is its gauge invariance. In discretized lattice a gauge transformation would look something like

$$\psi(\mathbf{n}) \rightarrow \Omega(\mathbf{n})\psi(\mathbf{n}) \tag{15}$$

$$\bar{\psi}(\mathbf{n}) \rightarrow \bar{\psi}(\mathbf{n})\Omega(\mathbf{n})^\dagger, \tag{16}$$

where Ω is the element of the SU(3) group. The Lagrangian contains terms proportional to $\bar{\psi}\partial_\mu\psi$. After discretizing the derivative we get terms such as, for example, $\bar{\psi}(\mathbf{n})\psi(\mathbf{n} + \boldsymbol{\mu})$. This term transforms as

$$\bar{\psi}(\mathbf{n})\psi(\mathbf{n} + \boldsymbol{\mu}) \rightarrow \bar{\psi}(\mathbf{n})\Omega(\mathbf{n})^\dagger\Omega(\mathbf{n} + \boldsymbol{\mu})\psi(\mathbf{n} + \boldsymbol{\mu}), \tag{17}$$

which is not gauge invariant. A solution is to introduce the so-called link variables $U_\mu(\mathbf{n})$ [3, 2], which transform as

$$U_\mu(\mathbf{n}) \rightarrow \Omega(\mathbf{n})U_\mu(\mathbf{n})\Omega(\mathbf{n} + \boldsymbol{\mu})^\dagger. \tag{18}$$

The quantity $\bar{\psi}(\mathbf{n})U_\mu(\mathbf{n})\psi(\mathbf{n} + \boldsymbol{\mu})$ is then gauge invariant since $\Omega(\mathbf{n})^\dagger\Omega(\mathbf{n}) = 1$.

Applying discretization rules 12, 13 and 14 to the Euclidean Lagrangian and plugging in link variables where necessary, our discretized action looks like [2]

$$S = S_F + S_G \tag{19}$$

$$S_F = a^4 \sum_f \sum_{\mathbf{n}} \bar{\psi}^f(\mathbf{n}) \sum_{\mu=1}^4 \gamma_\mu \frac{U_\mu(\mathbf{n})\psi^f(\mathbf{n} + \boldsymbol{\mu}) - U_{-\mu}(\mathbf{n})\psi^f(\mathbf{n} - \boldsymbol{\mu})}{2a} + m^{(f)}\bar{\psi}^f(\mathbf{n})\psi^f(\mathbf{n}) \tag{20}$$

$$S_G = S_G(U_\mu). \tag{21}$$

Following a similar notation as in Section 2, we have split our action into terms containing fermions and link variables S_F and the term containing just the link variables S_G .

The recently introduced link variables can be pictured as not living on the lattice sites as all the functions do, but instead living on the links between the sites, connecting them. A link variable $U_\mu(\mathbf{n})$ connects a site \mathbf{n} to a neighbouring site in a direction $\boldsymbol{\mu}$, that is the site $\mathbf{n} + \boldsymbol{\mu}$, as seen on Figure 1 [2]. The expression for the oppositely oriented link variables can be obtained from the definition (18) and is $U_{-\mu}(\mathbf{n}) = U_\mu(\mathbf{n} - \boldsymbol{\mu})^\dagger$. Link variables allow us to maintain gauge invariance even in discretized Lagrangian and their introduction can be further justified: A known quantity in gauge field theory satisfying transformation properties given in (18) is a gauge transporter [2] defined in a discrete sense as

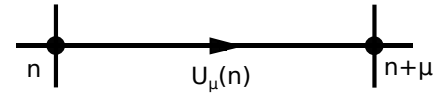


Figure 1. Link variables live on links between lattice sites

$$U_\mu(\mathbf{n}) = \exp(igaA_\mu(\mathbf{n})). \tag{22}$$

Plugging this definition into (20) we can, in the continuum limit, recover our familiar Lagrangian we have seen in (4). Let us do that. First we expand our link variables in powers of the lattice spacing a

$$U_\mu(\mathbf{n}) = 1 + igaA_\mu(\mathbf{n}) + \mathcal{O}(a^2) \tag{23}$$

$$U_{-\mu}(\mathbf{n}) = 1 - igaA_\mu(\mathbf{n} - \boldsymbol{\mu}) + \mathcal{O}(a^2). \tag{24}$$

Plugging this into the part of (20) not containing mass (since the mass term has no link variables) we get

$$\begin{aligned} & a^4 \sum_f \sum_{\mathbf{n}} \bar{\psi}^f(\mathbf{n}) \sum_{\mu=1}^4 \gamma_\mu \left(\frac{\psi^f(\mathbf{n} + \boldsymbol{\mu}) - \psi^f(\mathbf{n} - \boldsymbol{\mu})}{2a} + \right. \\ & \left. + \frac{1}{2}(gA_\mu(\mathbf{n})\psi^f(\mathbf{n} + \boldsymbol{\mu}) + gA_\mu(\mathbf{n} - \boldsymbol{\mu})\psi^f(\mathbf{n} - \boldsymbol{\mu})) + \mathcal{O}(a) \right) = \\ & = a^4 \sum_f \sum_{\mathbf{n}} \bar{\psi}^f(\mathbf{n}) \sum_{\mu=1}^4 \gamma_\mu \left(\frac{\psi^f(\mathbf{n} + \boldsymbol{\mu}) - \psi^f(\mathbf{n} - \boldsymbol{\mu})}{2a} + gA_\mu(\mathbf{n})\psi^f(\mathbf{n}) + \mathcal{O}(a) \right), \end{aligned} \tag{25}$$

which is a discrete version of the Lagrangian in (4).

The part of the action S_G corresponds to a kinetic term of our gauge fields. As in section 2 its precise form will not be important and we again just say that it only depends on the link variables U_μ and that in the continuum limit we also recover (4).

4. Evaluation of the correlation functions

After proper discretization we want to calculate correlation functions of certain operators

$$\langle O_2(t_E)O_1(0) \rangle \propto \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}U e^{-S_E[\psi(x), \bar{\psi}(x), U(x)]} O_2[\psi(x), \bar{\psi}(x)](t_E) O_1[\psi(x), \bar{\psi}(x)](0). \tag{26}$$

Note that, while we only write time argument of those operators, they are also calculated at a certain point of space, which will soon become relevant. We can imagine numerical evaluation of this will be difficult. Even for a small lattice such as $N = 10$, it seems like we have to integrate over a number of variables propotional to $N^4 = 10000$.

However, there is a useful formula, which we can use to quickly integrate over all our fermionic fields

$$\int d\psi_N d\bar{\psi}_N \dots d\psi_1 d\bar{\psi}_1 \exp\left(\sum_{i,j=1}^N \bar{\psi}_i D_{ij} \psi_j\right) = \det(D). \tag{27}$$

The right-hand side of above equation is known as fermion determinant and we notice that the left-hand side is of the same form as some functional integrals with our action S_F where D is our discretized Dirac operator. Comparing the above equation with (20), we can see that diagonal elements of D are proportional to quark masses, while the first upper/lower diagonals are proportional to the appropriate link variables. The kind of functional integrals we will encounter can be calculated using the Wick's theorem

$$\begin{aligned} & \int d\psi_N d\bar{\psi}_N \dots d\psi_1 d\bar{\psi}_1 \psi_{i_1} \bar{\psi}_{j_1} \dots \psi_{i_n} \bar{\psi}_{j_n} \exp\left(\sum_{i,j=1}^N \bar{\psi}_i D_{ij} \psi_j\right) = \\ & = \det(D) (-1)^n \sum_{P(1,2,\dots,n)} \text{sgn}(P) (D^{-1})_{i_1,j_{P1}} \dots (D^{-1})_{i_n,j_{Pn}}. \end{aligned} \tag{28}$$

We will now apply Wick's theorem to calculate the nucleon masses in the next section.

5. Extracting nucleon masses

Let us remind ourselves of the quantity we are trying to calculate

$$\langle O_2(t_E) O_1(0) \rangle \propto \int \mathcal{D}U e^{-S_G[U]} \mathcal{D}[u, \bar{u}] \mathcal{D}[d, \bar{d}] e^{-S_F[U, u, \bar{u}, d, \bar{d}]} O_2(n_t) O_1(0). \tag{29}$$

Inserting the previously determined expressions for our operators we end up with

$$\begin{aligned} C(\mathbf{n}, \mathbf{m}) = \langle O_N(\mathbf{n}) \bar{O}_N(\mathbf{m}) \rangle & \propto \int \mathcal{D}[U] e^{-S_G[U]} \mathcal{D}[u, \bar{u}] \mathcal{D}[d, \bar{d}] e^{-S_F[U, u, \bar{u}, d, \bar{d}]} \times \\ & \times \epsilon_{abc} \epsilon_{a'b'c'} (\bar{u}(\mathbf{m})_a C \gamma_5 \bar{d}(\mathbf{m})_b^T) \bar{u}(\mathbf{m})_c P_+ u(\mathbf{n})_{c'} (u(\mathbf{n})_{a'}^T C \gamma_5 d(\mathbf{n})_{b'}). \end{aligned} \tag{30}$$

This time we have written all operators' spacetime arguments. The time component of \mathbf{n} corresponds to t_E , while the time component of \mathbf{m} is zero. Our operators are in essence just products of spinors, meaning we can use Wick's theorem to integrate over them resulting in the following

$$\begin{aligned} \langle O_N(\mathbf{n}) \bar{O}_N(\mathbf{m}) \rangle & \propto \int \mathcal{D}[U] e^{-S_G[U]} \det(D) \epsilon_{abc} \epsilon_{a'b'c'} (C \gamma_5)_{\alpha'\beta'} (C \gamma_5)_{\alpha\beta} (P_+)_{\gamma\gamma'} D_d^{-1}(\mathbf{n}|\mathbf{m})_{\beta'\beta} \times \\ & \times (D_u^{-1}(\mathbf{n}|\mathbf{m})_{\alpha'\alpha} D_u^{-1}(\mathbf{n}|\mathbf{m})_{\gamma'\gamma} - D_u^{-1}(\mathbf{n}|\mathbf{m})_{\alpha'\gamma} D_u^{-1}(\mathbf{n}|\mathbf{m})_{\gamma'\alpha}). \end{aligned} \tag{31}$$

The above result can be physically interpreted. The inverse of the Dirac operator $D^{-1}(\mathbf{n}|\mathbf{m})$ is actually a quark propagator, representing the propagation of our quark from point \mathbf{m} to point \mathbf{n} . Wick's theorem can be understood graphically as all the possible ways of drawing a Feynmann diagram for our proton as seen on

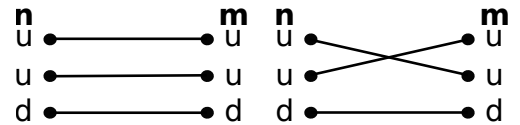


Figure 2. The corresponding Feynmann diagrams.

Figure 2. We can connect the 2 up quarks in two different ways, resulting in two terms under our integral.

We are left with having to compute the following

$$\int \mathcal{D}U e^{-S_G(U)} \det(D) f(U), \quad (32)$$

where f is a function only depending on link variables. For such high dimensional integrals the only viable method is Monte Carlo integration. Say we would like to compute a volume integral over some domain V of a function f , we can do that in the following way

$$\int_V f(r) dV \propto \frac{1}{N} \sum_{n=1}^N f(r_n). \quad (33)$$

The points r_n are randomly chosen points from our domain V and as we increase N we get closer to the value of the integral we are trying to compute. Our case will be done in a similar way, with us randomly picking certain configurations of link variables. To increase the efficiency of the method, those points are not chosen uniformly. Their distribution is instead weighed by a factor of $e^{-S(U)} \det(D)$ to ensure we pick the configurations with bigger contribution to the integral more often. This method is called the Metropolis algorithm.

Remember that $C(\mathbf{n}, \mathbf{m}) \propto e^{-t_E E_1}$ for large enough t_E . We would like to now fit a decaying exponential to our correlator to extract the energy of our nucleon. However, there is one last thing that we need to do. Remember that E_1 on the right-hand side of the above equation depends on proton momentum p : $E_1 = \sqrt{p^2 + m^2}$. In order for E to really represent the proton mass we want to have $p = 0$. Until now we have not specified any momentum in our calculations - our correlators instead have definite position. What needs to be done is to Fourier transform them into Fourier space, where they will instead have well defined momentum. This is done by a discrete Fourier transformation

$$\langle O_2(\mathbf{p}, t_E) O_1(\mathbf{0}, 0) \rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{n}} e^{-i\mathbf{a}\mathbf{n}\mathbf{p}} \langle O_2(\mathbf{n}, t_E) O_1(\mathbf{0}, 0) \rangle, \quad (34)$$

where N is the total number of points in our lattice. We have placed the proton creation operator at the origin $\mathbf{n} = \mathbf{0}$ so we only have to Fourier transform the annihilation operator, that annihilates the particle at a definite position into an operator that annihilates a particle with definite momentum.

Choosing $\mathbf{p} = 0$, giving $E_1 = m$, we can now, as mentioned before, fit our calculations to

$$C(t_E) = \langle O_2(t_E) O_1(0) \rangle = \sum_k c_k e^{-t_E E_k} \propto e^{-t_E E_1} + \mathcal{O}(e^{-t_E E_2}). \quad (35)$$

An important thing to consider is how large must t_E get for us to be able to say that the first term in the above sum dominates? A simple way to determine that is to look at the quantity

$$m_{\text{eff}}(t_E + 1/2) = \ln \frac{C(t_E)}{C(t_E + 1)}, \quad (36)$$

which becomes approximately constant and equal to E_1 after this very time we are looking for as seen in Figure 3.

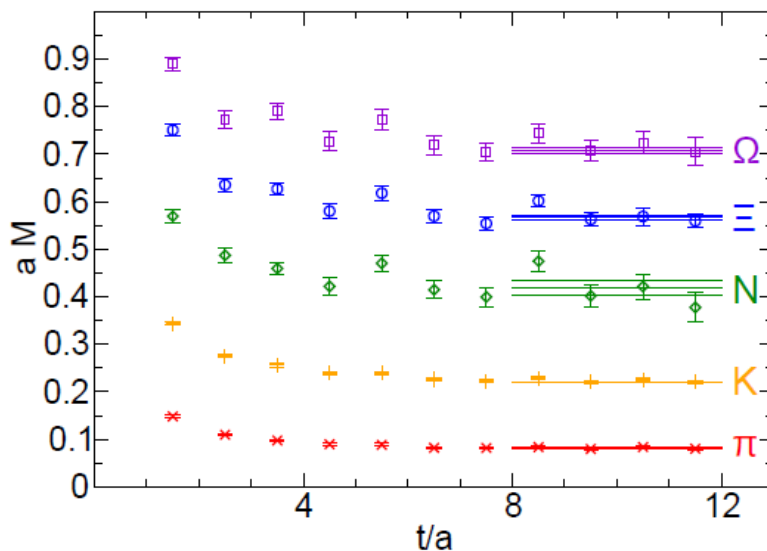


Figure 3. The plot shows Euclidean time dependence of the effective mass for a few different baryons including nucleons (N). We can see that it becomes constant after a time of approximately 8 lattice spacings [5]. Note that for different hadrons different operators appearing in (10) have to be used. For more information see [2].

The obtained mass is in dimensionless units am_N , where a is the lattice spacing. Usually, we extrapolate our results to $a \rightarrow 0$, so how can we extract the mass in the units we are familiar with? A solution to this problem is to calculate the ratio of the mass we are interested in and another known hadron's mass. The resulting quantity is still dimensionless, but it tells us how our nucleon's mass compares to another hadron's mass, which is known in conventional units. This is less trivial than it sounds, because we also use some known hadron masses to fix the parameters of the theory, namely the quark masses and the strong interaction coupling constant. For this reason the choice of our reference baryons is important. A common choice are Ξ and Ω baryons. The Ω baryon is convenient for it consists of 3 valence strange quarks, meaning it is not too influenced by our light quark (up and down) masses. The Ξ baryon is also often chosen for its high strange quark content (its flavour structure is 2 strange quarks and a light quark) and its experimentally better known mass, compared to an Ω baryon. The hadron we use to fix light quark masses with is a pion, which is a meson composed of light quark - antiquark pairs. Calculations are performed with larger than physical pion masses and then extrapolated to the physical one. The reason behind this lies in numerical computation: for small quark masses, the Dirac operator matrix D approaches a singular matrix and is harder to invert. The final results are shown in Figures 4 and 5.

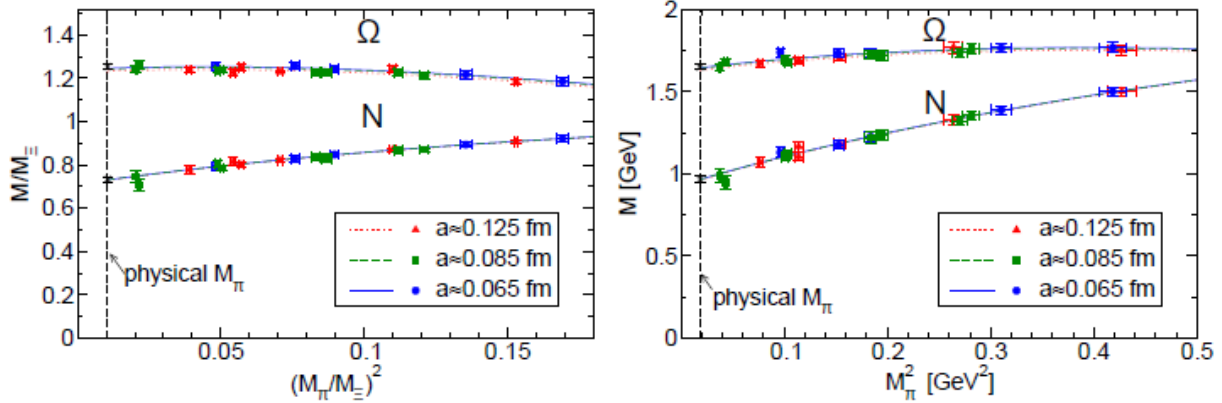


Figure 4. On the left graph, ratios with a well known Ξ baryon are plotted. On the right side we plot the masses in GeV. The pion mass is extrapolated to the physical point giving correct nucleon masses. We can also see that further shrinking the lattice spacing does not influence our results in a meaningful way [5].

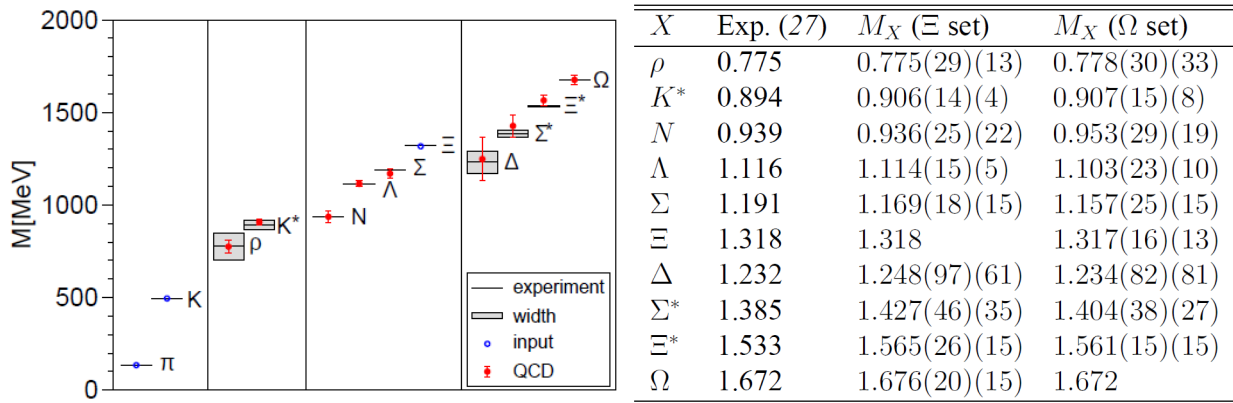


Figure 5. On the left we can see the comparison of our mass values with the experiment for the nucleon and other baryons, calculated in a similar way, with corresponding experimental decay widths. The 3 input hadrons shown are used to fix the parameters of the theory. The numbers on the right are baryon masses (in GeV) obtained by calculating mass ratios with two different baryons Ξ and Ω . An excellent matching with the experiment can be seen [5].

6. Conclusion

In this article we have introduced basic features of QCD and its path integral formalism. Performing a Wick rotation into an Euclidean metric we were then able to relate certain correlators to nucleon mass. We have shown how the choice of a proper correlator is motivated by what we know about nucleons. We have then discretized our spacetime, taking extra care to maintain gauge invariance of our QCD action by introducing the link variables. Making use of Wick's theorem and Metropolis algorithm, we were able to evaluate the needed correlators and calculated nucleon masses that agree well with the experiment. Our approach can be further generalized: including 4 quark masses and QED corrections allows us to accurately determine the mass difference between the two nucleons as seen below [4]. This all serves as a convincing confirmation of the validity of QCD. Having convinced ourselves that QCD gives correct results, we can now begin predicting bound state particles, that have not been observed in an experiment yet, including more mysterious handrons -tetra or even pentaquarks - composed of more than 3 valence quarks.

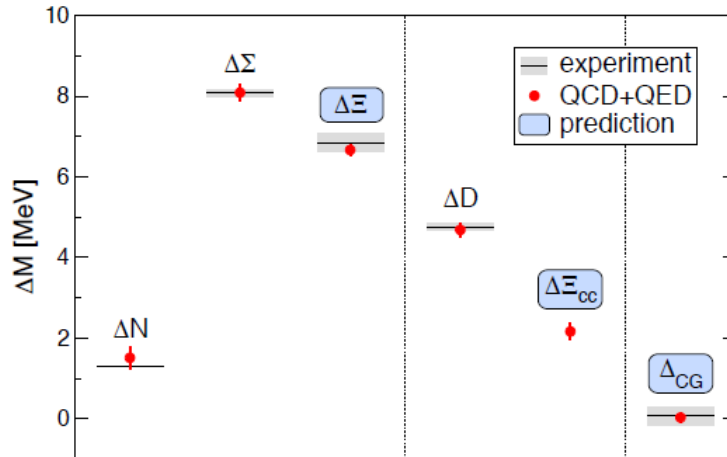


Figure 6. Including further corrections we can calculate more precise hadron mass differences that also agree with the experiment [4].

REFERENCES

- [1] M. Tanabashi et al. Review of particle physics. *Phys. Rev. D*, 98:030001, Aug 2018.
- [2] Christian B. Lang (auth.) Christof Gattringer. *Quantum chromodynamics on the lattice: an introductory presentation*. Lecture notes in physics 788. Springer-Verlag Berlin Heidelberg, 1 edition, 2010.
- [3] Dan V. Schroeder Michael E. Peskin. *An introduction to quantum field theory*. Frontiers in Physics. Addison-Wesley Pub. Co, 1995.
- [4] S. Borsanyi, S. Durr, Z. Fodor, C. Hoelbling, S. D. Katz, S. Krieg, L. Lellouch, T. Lippert, A. Portelli, K. K. Szabo, and B. C. Toth. Ab initio calculation of the neutron-proton mass difference. *Science*, 347:1452–1455, March 2015.
- [5] S. Dürr, Z. Fodor, J. Frison, C. Hoelbling, R. Hoffmann, S. D. Katz, S. Krieg, T. Kurth, L. Lellouch, T. Lippert, K. K. Szabo, and G. Vulvert. Ab Initio Determination of Light Hadron Masses. *Science*, 322:1224, November 2008.