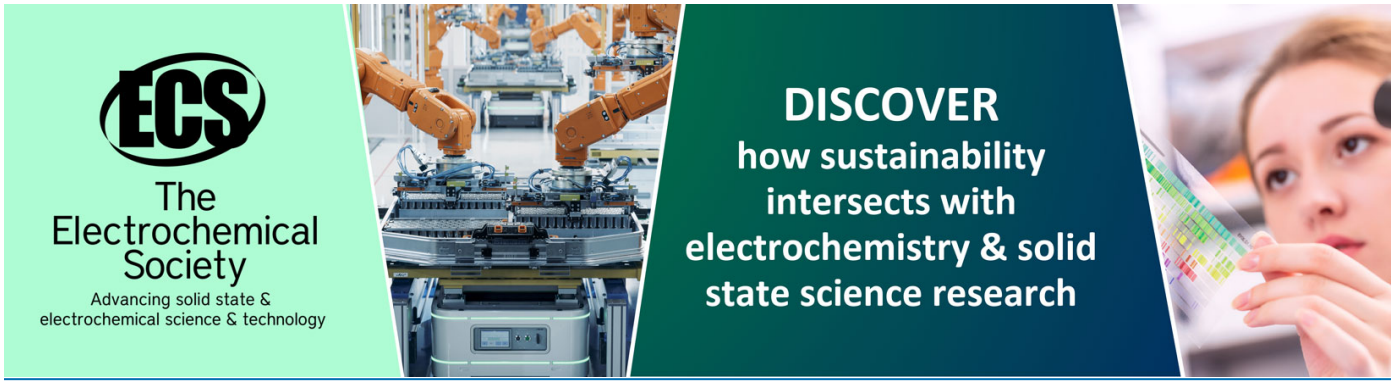
Lattice Gauge Theory for Nuclear Physics



Journal of Physics: Conference Series **403** (2012) 012043 doi:10.1088/1742-6596/403/1/012043

Lattice Gauge Theory for Nuclear Physics

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Abstract. Quantum Chromodynamcs (QCD) is now established as the theory of strong interactions. A plethora of hadronic physics phenomena can be explained and described by QCD. From the early days of QCD, it was clear that low energy phenomena require a non-perturbative approach. Lattice QCD is a non-perturbative formulation of QCD that is particularly suited for numerical calculations. Today, supercomputers have achieved performance capable of performing calculations that allow us to understand complex phenomena that arise from QCD. In this talk I will review the most recent results, relevant to nuclear physics. In particular, I will focus on results relevant to the structure and interactions of hadrons. Finally, I will comment on the opportunities opening up as we approach the era of exaflop computing.

1. Introduction

From the subatomic scales to the Universe itself, nuclear physics plays an important role in our understanding of the world around us. This is especially evident in this conference by the breadth of the presentations, which spanned across many different topics, ranging from the spectrum, structure and interaction of hadrons, to nuclear structure, and astrophysics. A common feature of all these topics is the enormous complexity of the problems we attempt to tackle. Often, numerical calculations with the aid of world class supercomputers are necessary to achieve the desired results.

At the core of nuclear physics, however, lies a very simple theory: Quantum Chromodynamics (QCD). The interactions of hadrons originate from this theory resulting the complex emergent phenomena we observe at low energies. Nuclear physics is a direct consequence of QCD and in principle all properties of atomic nuclei can be calculated from QCD. One of the major motivations of studying the interactions of hadrons in lattice QCD is precisely that: Understand how nuclear physics emerges from QCD, as well as compute from first principles some fundamental properties of nuclear matter. However, the large separation of the characteristic scales of QCD ($\sim$ 1 GeV) and the low nuclear scales of a few MeV or even KeV makes such calculations a daunting task. For this reason only recently lattice QCD calculations directly targeting nuclear physics have started to be undertaken.

From the very early times of lattice Quantum Chromodynamics, the importance of calculating properties of interacting hadrons had been recognized. However, the difficulty associated with such calculations on Euclidean space was also quickly recognized and solutions were proposed [1, 2, 3]. Pioneering work focusing on toy problems started also quite early [4] and since then significant work has been done in calculating elastic scattering phase shifts, investigating

the existence of bound states and resonances, as well as studying the properties of multi-hadron systems.

In this talk I am reviewing recent results from lattice QCD calculations of properties of interacting hadrons. Emphasis is given to results relevant to nuclear physics.

2. Hadron Interactions in Euclidean Space

Computing the properties of an interacting hadronic system in Euclidean space requires a special treatment. In principle, one should calculate in Euclidean space appropriate correlation functions which after rotation to Minkowski they correspond to the desired scattering amplitude. However, analytic continuation cannot be simply performed using the Euclidean correlation functions on a discrete set of points. For this reason, it is desirable to extract the required information directly from Euclidean correlation functions. The simplest example where this is achieved is the calculation of the the spectrum of energy levels in a finite box, by observing the exponential decay of Euclidean correlation functions. Significant work has been performed nearly from the beginning of Lattice QCD formulation on understanding how properties of interacting hadrons can be calculated directly from Euclidean correlation functions. Pioneering work can be found in [1, 2, 3, 5]. The basic principle behind this work is the fact that all the information about the interactions of hadrons is encoded in the energy spectrum of the hadronic system in a box. Hence a calculation of this spectrum from Euclidean correlation functions can result in the calculation of the desired scattering amplitude. However, this is only possible where the analytic connection of the finite box spectrum to the desired scattering amplitude can be made.

2.1. Scattering and Bound States

The simplest example where the idea described above can be applied is the calculation of the elastic s-wave scattering phase shift of two hadrons. The formalism described here was developed in [1, 3]. In this case the scattering amplitude is described by a single phase (the scattering phase shift) $\delta(k)$.

$$\mathcal{A}(k) = \frac{4\pi}{\mu}\frac{1}{k\,\cot\delta(k) - ik} \tag{1}$$

where k is the magnitude of the center of mass scattering momentum and μ is the reduced mass of the two body system. The relation of this phase to the energy levels in a finite box can be easily worked out resulting for the case of equal mass particles of mass μ.

$$E_n = 2\sqrt{k_n^2 + \mu^2} \tag{2}$$

with E_n being the energy spectrum of the two body system in a finite box, and k_n the corresponding scattering momentum and,

$$k\cot\delta(k) = \frac{1}{\pi L}S(\frac{kL}{2\pi})\,, \qquad S(\eta) = \lim_{\Lambda\to\infty}\left[\sum_{\vec{n}}^{|\vec{n}|<\Lambda}\frac{1}{|\vec{n}|^2-\eta^2} - 4\pi\Lambda\right] \tag{3}$$

where $\vec{n}$ is a 3-vector with integer components. Thus in Euclidean space one calculates the energy levels E_n using normal spectroscopic methods and extracts the scattering phase shift using the above formula. At small enough scattering momentum, where the effective range expansion is valid, the scattering length $\mathtt{a}$ can be identified through

$$k\,\cot\delta(k) = \frac{1}{\mathtt{a}} + \frac{1}{2}\mathtt{r}^2k^2 + \cdots \tag{4}$$

with $\mathtt{r}$ being the effective range of the interaction. Expanding at small k one obtains the shift ΔE_0 of the lowest two particle energy level in a box of size L from the non-interacting two particle lowest energy level in the same box:

$$\Delta E_0 = -\frac{4\pi \mathtt{a}}{mL^3}\left[1 + c_1\frac{\mathtt{a}}{L} + c_1\frac{\mathtt{a}^2}{L^2}\right] + \cdots \tag{5}$$

This formula has been extended to more than two bosons in a box in [6, 7].

Generalization of to higher partial waves was also done in [3]. In this case complications arise due to breaking of rotational symmetry causing partial waves to mix. For s-wave scattering (angular momentum $l = 0$) the lowest wave that mixes in is $l = 4$ and its effects can be ignored in most cases. In general, these mixing effects cannot be ignored, and the scattering phase shifts δ_l can be determined as the zeros of a characteristic polynomial defined by

$$\det\left[e^{2i\delta} - \mathbf{U}\right] = 0 \tag{6}$$

with $\mathbf{U}$ an appropriately constructed matrix for each symmetry sector of the cubic group, and δ a diagonal matrix with entries the phase shifts of each partial wave contributing to the cubic symmetry sector at hand. In general, there are infinitely many partial waves contributing to each cubic symmetry sector, however, in practice the matrix is truncated to a small number of partial waves. For details of this formalism see [3] and the more recent [8].

Generalizations of the above formalism to non-center of mass frames can be found in [9, 10, 11, 12]. In addition, the extension to non-cubic boxes can be found at [13]. Finally, extensions to multi-channel scattering have been worked out in [14].

When two particles interact attractively, the possibility of the formation of a bound state arises. In this case the energy splitting ΔE_0 is negative resulting in an imaginary scattering momentum $k = i\kappa$,

$$\Delta E_0 = 2\sqrt{k^2 + \mu^2} - 2\mu \approx \frac{k^2}{2\mu} = -\frac{\kappa^2}{2\mu}\ . \tag{7}$$

It has been shown [15] that in the case of bound states the volume dependence of ΔE_0 is exponential rather than the power law found for scattering states. Recently, in [16] the finite volume energy shift $\delta(\Delta E_0)$ of the bound state energy ΔE_0 for angular momentum $l > 0$ was computed:

$$\delta(\Delta E_0) \sim \alpha(\frac{1}{\kappa L})\frac{e^{-\kappa L}}{\mu L} + \mathcal{O}(e^{-\sqrt{2}\kappa L})\ . \tag{8}$$

where the function $\alpha(x)$ depends on the partial wave as well as the lattice symmetry sector this partial wave is embedded. A notable result of this work is the fact that while s-wave bound states become more deeply bound in finite volume, p-wave bound states are less bound in small volume.

3. Signal to Noise ratio for baryons

Following the formalism described in the previous section the calculation of elastic scattering phase shifts from lattice QCD is reduced to the calculation of the energy spectrum of two bodies in a finite box. This is in principle straight forward to do. Methods for extracting not only the ground state but several low lying energy levels exist [4, 17]. In the case of baryons, however, the extraction of the spectrum of the multi-body system in a box is quite difficult. Here the problem is two fold. First, the energy gaps in the two (or multi) baryon systems are small requiring large Euclidean time to project out the ground state (or a set of few low-lying states). The cost of quark contractions is such that it makes it very difficult to build a sufficiently large basis of

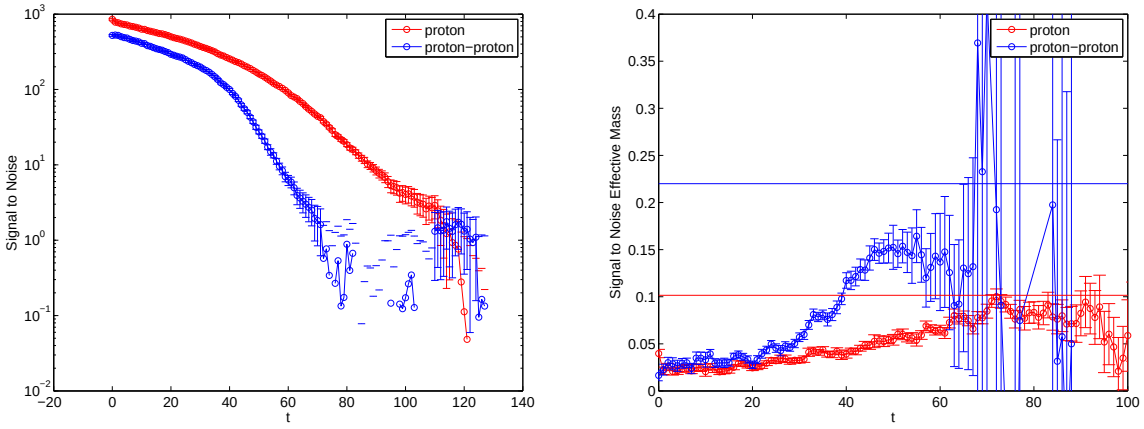

Figure 1. Signal to noise ratio for a single proton and a two proton system. Left, the signal to noise ratio. Right, the logarithmic derivative of the signal to noise ratio.

operators (as is now done for single baryon spectroscopy [18, 19, 20]). Secondly, the statistical noise in the correlators due to Monte Carlo sampling grows exponentially with Euclidean time.

As Lepage showed [21], the signal to noise ratio $\mathcal{R}$ of hadronic correlation functions drops exponentially with Euclidean time with an exponent related to the gap between the mass of the pion and the mass of the the lowest hadronic state contributing to the correlator. In particular, for a system with A nucleons we have,

$$\mathcal{R} \approx e^{-A(m_N - \frac{3}{2}m_\pi)t} \tag{9}$$

where m_N is the nucleon mass and m_π the pion mass and assuming weak interaction between nucleons. Fortunately, as it was shown in [22, 23] this asymptotic bound does not set in at early times leaving some region where reasonable accuracy can be achieved with sufficiently high statistics. In Fig. 1, I show the drop of the signal to noise ratio for the case of a single proton as well as the case of a two proton system in the singlet spin state. In both cases after a region of a mild drop the exponential rapid decay sets in. In the case of the proton, we can follow the signal at sufficiently large time to observe the saturation of the Lepage bound, as it is seen in the right panel of Fig. 1. For the two proton system the correlator becomes too noisy as the Lepage bound is approached, never quite saturating the bound. The data I present here are from NPLQCD collaboration for an ensemble with dynamical anisotropic clover fermions with a 390 MeV pion mass with anisotropy of about 3.5 and volume of $32^3 \times 256$ and a spacial lattice spacing of about 0.125fm.

The issue of the rapid growth of the noise as well as the dense two body spectrum in a box present a major challenge that needs to be overcome, for reaching precision calculations of properties of systems with interacting baryons.

4. Baryon-Baryon Interactions

Pioneering calculations of baryon-baryon scattering lengths have been performed many years ago with the work of Fukugita et al. [24] in the quenched approximation (where quark vacuum polarization effects are ignored). It took ten years for the first calculation for quark vacuum polarization effects to be included. This pioneering work was performed by NPLQCD collaboration [25]. The state of nucleon-nucleon elastic scattering length calculations is summarized in a recent review by Beane *et al* [23]. In addition, HALQCD has been reporting

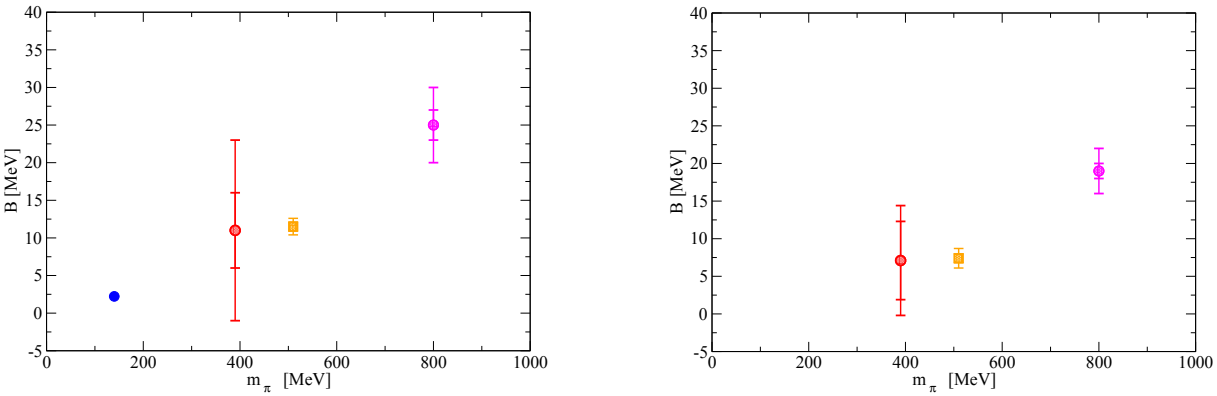

Figure 2. The binding energies of the deuteron (left) and the di-neutron (right) computed by NPLQCD (390 and 800 MeV points) and Yamazaki *et al* (510 MeV point).

results on two-baryon scattering phase shifts in the recent years. Most recently in Ref. [26] results on nucleon-nucleon as well as hyper-nucleon and hyper-hyperon elastic scattering phase shifts were presented.

The issues related to the noise and the complexity of the spectrum of two baryon systems in a box outlined in Sec. 3 are the prime reasons for the sparsity of results in the baryon sector in contrast to the meson sector. As a result, systematic effects due to excited state contamination, heavy quark masses, and lattice spacing effects, are far from being well under control. The fine tuned nature of nuclear physics close to the physical point might be one of the reasons of the clear disagreement between lattice and experimental results. On the other hand, these pioneering results represent the first solid step in the direction of obtaining reliable calculations of these important to Nuclear physics quantities. Clearly, in order to make progress improved methodology, as well as availability of significant computational resources are required.

Recently calculations of the binding energy of the deuteron were performed in the quenched approximation [27]. In the same calculation, a bound di-neutron was observed. The key features of these calculations were the big volumes (up to 12fm), the heavy pion masses (800MeV), and the use of a variational method with 2 operators with wavefunctions designed to have large overlap with the ground state of the system. The combination of these choices makes the noise problem tractable. Furthermore, the same authors preformed similar calculations of the binding energy of the helium nuclei (^3He and ^4He) in quenched approximation [28]. In work performed this year, Yamazaki *et al* [29] also presented results with dynamical quarks (allowing for vacuum polarization effects) for both the deuteron the di-neutron and the helium nuclei (^3He and ^4He). Their result for the ^4He nucleus is in remarkable agreement with experiment, in contrast with the rest of the binding energies which are found to be larger than those in nature. However, these calculations where performed at unphysical heavy quark masses (pions with mass about 500 MeV). Significant further work is required in order to achieve results that are free of systematic errors currently not controlled.

The NPLQCD collaboration has also performed calculations at the flavor SU(3) symmetric point as well as at a point with 390 MeV pion mass and broken SU(3) flavor symmetry. The two calculations, were done with different quark actions (finer grid in the Euclidean time direction). The lighter pion mass point calculations presented in Ref. [30] were performed using an anisotropic quark action that allowed better control of the fitting systematics for extracting binding energies. However, the cost of these calculations was such that statistical errors were substantial. In Ref. [31] the NPLQCD collaboration presented results with very high statistics

using an isotropic quark action that allowed better control of the statistical errors. The results with dynamical quarks are summarized in Fig. 2. In this figure it is clear that the lattice calculations by the two different collaborations are in agreement. In addition a general trend of decreasing binding energies with pion mass is observed. This trend is in the right direction for obtaining the experimental result for the deuteron binding energy at the physical pion mass. However, the calculation of the deuteron binding energy at the physical pion mass still remains a daunting task for lattice QCD.

4.1. Strange bound states: H-dibaryon

Two baryon bound states containing strange quarks were also studied in lattice QCD during recent years. Most notable was the work on the h-dibaryon by HALQCD and NPLQCD. The h-dibaryon as a possible six quark state (two of each of the three light flavors in the quark model picture) was proposed by Jaffe in 1977 [32]. This is a strangeness -2, baryon number 2, and angular momentum 0 state. Jaffe's argument was based on the MIT bag model and the perturbative attractive color-spin interactions that form di-quarks in his model. Since then there have been several experimental searches for the h-dibaryon. All this effort is comprehensively reviewed in [33]. Most recently, at RIHC [34] using some input from models, the region between 0 and 95 MeV was excluded for the binding energy of the h-dibaryon. In addition, the possibility of a near threshold resonance is still not excluded by experimental results [35].

Theoretically there have been significant activity attempting to understand the existence of the h-dibaryon within various models. A review of all this work can be found in [36, 33]. Model predictions vary in a wide range, from deeply bound h-dibaryon to a resonance significantly above threshold. In lattice QCD, efforts to address the possibility of existence of the h-dibaryon started early on [37, 38, 39, 40, 41], in the quenched approximation (i.e. ignoring quark vacuum polarization effects).

Recently the first unquenched calculations appeared. NPLQCD collaboration used anisotropic clover improved lattices with two light (up,down) quarks and one strange quark at a single pion mass of 390MeV and a single spacial lattice spacing of approximately 0.125fm. Details of these ensembles can be found in [42]. The calculation was performed on four volumes ranging between 2fm and 4fm and the infinite volume binding energy was calculated by extrapolation using the formalism outlined in Sec. 2. This calculation provides evidence that at 390MeV pion mass the h-dibaryon is bound with binding energy of $B = 13.2 \pm 1.8 \pm 4.0$ MeV where the first error is statistical and the second systematic. In addition to this number, NPLQCD has preliminary results at a lighter pion mass (220MeV). However the precision obtained at this mass is not sufficient to determine the sign of the binding energy. NPLQCD results as well as more details on their calculation can be found in [43, 44].

HALQCD, using very different methodology, also presented results on the h-dibaryon binding energy [45, 46, 26]. Their work is at flavor SU(3) symmetric points and pion masses that range between 469MeV and 1.2 GeV. They also found evidence of a bound h-dibaryon with binding energies ranging from 26MeV up to 37MeV.

The results for the h-dibaryon binding energy discussed here are presented in Fig. 3. As it is evident, the binding energy is decreasing as the pion mass approaches the physical point. In addition, at lighter pion masses the calculations become harder providing less accurate results. For these reasons, although a bound h-dibaryon is observed at heavier pion masses, it is not clear what its fate is at the physical point. Apart from obtaining precision close to the physical point, lattice calculations will have to address and control other remaining systematic errors such as lattice spacing effects, isospin breaking and electromagnetic effects. Given the fact that the h-dibaryon may be a near threshold state (bound or resonance) all these effects have to be carefully addressed before a final result is obtained from lattice QCD. It is encouraging though, that during the last year significant progress has been made. In addition to lattice calculations,

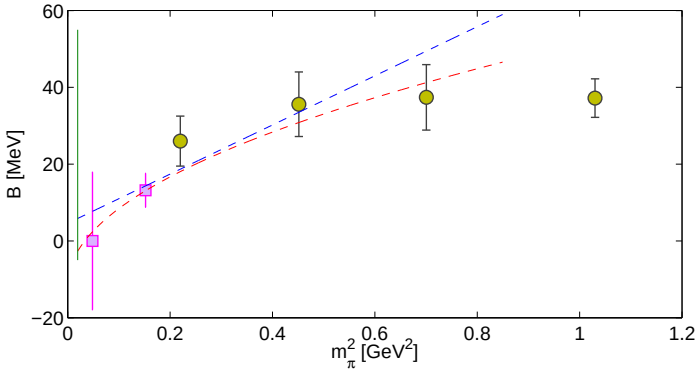

Figure 3. Summary of lattice results for the h-dibaryon binding energy. The squares are results from NPLQCD (Nuclear Physics Lattice QCD) collaboration [43, 44] and the circles are results from HAL QCD (in [45] and in this conference [46]). The solid vertical line marks the physical point. The two dashed lines are plotted to guide the eye (the blue is linear in m_π^2 while the red is linear in m_π).

in the literature recently appeared work that addresses the quark mass dependence of the binding energy of the h-dibaryon [47] using chiral symmetry constraints. In this case, the binding energy also seems to decrease with the pion mass.

5. Hypernuclear physics

The NPLQCD collaboration, using very high statistics and volumes up to 7 fm, recently calculated the spectrum of nuclei and hypernuclei up to atomic number A=4 [31], in lattice QCD. These calculations were performed at the flavor SU(3) symmetric point with pion mass of 800 MeV and a single lattice spacing of approximately $a = 0.145$ fm. The heavy pion masses allowed for good control of the statistical errors. The interpolating fields (quark and hadron level wave-functions) that were used in this work were constructed using an algebraic program. This program constructs both the wave-functions with the relevant quantum numbers, as well as finds the wave-functions with a tractably small number of terms. It is a well known problem that many body wave-functions contain a large number of terms growing exponentially with atomic number. Taking advantage of the underlying quark structure and the Fermi exclusion principle it turns out that particularly simple wave functions can be constructed as shown in [48] [1]. Although these first results look very encouraging, controlling all systematic errors, such as control of excited state contamination, continuum extrapolation, physical up and down quark masses, and large volume extrapolations, will require significant computational resources as well as new clever algorithms to deal with the exponential growth of statistical errors as the physical pion mass is approached.

6. Conclusions

There has been significant progress in the last few years in studies of multi-baryon systems in lattice QCD. The ultimate goal being understanding how nuclear physics emerges from QCD. The challenges in tackling this problem are quite difficult, however, the emergence of new methods, and the expected significant increase in computer cycles in the exaflop era, makes me optimistic that we will continue on this pace of steady progress in the years to come.

Acknowledgments

I would like to thank the organizers for inviting me to take part at this conference in honor of Jerry Draayer's 70th birthday. This work was supported in part by the DOE grants DE-AC05-06OR23177 (JSA) and DE-FG02-04ER41302.

[1] Similar methodology was also presented in [49]

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