Hadron Structure and Spectrum from the Lattice

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Abstract. Lattice calculations for hadrons are now entering the domain of resonances and scattering, necessitating a better understanding of the observed discrete energy spectrum. This is a reviewing survey about recent lattice QCD results, with some emphasis on spectrum and scattering.

INTRODUCTION

Quantum field theories in four dimensions are not well defined without some regularization. Wilson’s [1] formulation on a Euclidean space-time lattice is such a regularization with the advantage of maintaining gauge invariance and straightforward accessibility by computer. The path integrals become finite dimensional integrals, however of very high dimensions. The continuum limit is obtained by keeping the physical volume fixed while letting the lattice spacing \( a \) approaching zero. The scale parameter is determined by comparing a physical observable (e.g., a mass \( m \)) with the measured dimensionless lattice observable (e.g., the product \( a m \)). Once \( a \) is determined, all further lattice observables can then be translated to physical values. Since one has to fix also the quark mass parameters one has to trade \( n_f + 1 \) physical quantities for the lattice scale and quark mass parameters. In the continuum limit the lattice parameters are tuned such that \( a \rightarrow 0 \) while keeping the physical quantities fixed.

There are several concerns on the way to continuum results. The physical volume is limited to a few fermi, unless the lattice is very coarse. Typical calculation have lattice spacings between 0.05 fm and 0.2 fm. The leading finite size effect is due to the lightest hadron, the pion, thus one wants lattice sizes \( L \) where \( L m_{\pi} \) is large; typical values are larger than 4. Below that value boundary effects may be sizeable. This gives \( L > 6 \) fm and leads to lattices of demanding \( 10^4 \) sites. Bringing the quark masses and, equivalently the pion mass, down to physical values necessitates large volumes or good control on the finite size dependence and of the scaling behaviour in \( a \).

The main object of lattice simulations are correlation functions, the Euclidean equivalent of n-point functions. Masses or better: energies are obtained from the exponential decay of hadron propagators. However, in a quantum channels there will be contribution of (formally: infinitely) many states: \( C_{ij}(t) \equiv \langle X_i(t) \bar{X}_j(0) \rangle = \sum_n \langle X_i|n \rangle e^{-E_n t} \langle n| \bar{X}_j \rangle \).

Due to the finiteness of the lattice volume the energies are discrete even in the situation of open scattering channels. Asymptotically, for large \( t \) the ground state dominates. However, the statistical errors increasingly obscure the signal with increasing \( t \) and most often one has to work at not so large \( t \).

Depending on the type of calculation the excited states may be a nuisance or an advantage. In case one is interested in hadronic ground state parameters (there are not many such hadrons: the pseudoscalars and the nucleon with its strange, charmed, beautiful and maybe topped cousins) or in 3-point functions (like form factors or other matrix elements) the excited states are a “contamination” and one fights to get rid of their influence. If, on the other hand, one is interested in excited hadrons and decay properties one needs the excitation energies as precise as possible.

HADRON STRUCTURE

Obviously I have to concentrate here on a few highlights and the choice is subjective. Recent more complete reviews on the topic are [2, 3]. Also I am considering only information available at the time of this conference (Sept. 2015) with emphasis on results in the recent two years.
Hadron structure calculations are based on studying 3-point functions. A current is inserted between an incoming and an outgoing hadron $\langle H|\Gamma|H'\rangle$. In terms of lattice operators $O$ (also called interpolators) we have

$$\langle O(t, \vec{p})|\Gamma(\tau)|\bar{O}(0, \vec{r})\rangle.$$  

(1)

Fig. 1 shows the situation (and the concerns). Assuming that the temporal distances $|\tau|$ and $|t-\tau|$ are large enough that the ground state hadron dominates the intermediate state,

$$G_3 = \langle O(t, \vec{p})|H(\vec{p})\rangle e^{-E_p(t-\tau)} \langle H(\vec{p})|\Gamma(\tau)|H(\vec{r})\rangle e^{-E_r\tau} \langle H(\vec{r})|\bar{O}(0, \vec{r})\rangle$$  

(2)

the components factorize. One also determines the 2-point function

$$G_2 = \langle O(t, \vec{q})\bar{O}(0, \vec{p})\rangle = \langle O(t, \vec{p})|H(\vec{p})\rangle e^{-E_p t} \langle H(\vec{p})|\bar{O}(0, \vec{r})\rangle.$$  

(3)

and retrieves the wanted matrix element $\langle H|\Gamma|H\rangle$ from a plateau behavior of suitable ratios of $G_3$ and $G_2$.

In lattice calculations of matrix elements there are several concerns: volume (finite size effects), lattice hadron operators, contamination from excited states, disconnected contributions (depending on the insertion type), renormalization factors (and possible mixing with other operators), dependence on the pion (quark) mass and lattice spacing. Most studies are at higher pion mass and have to be extrapolated to the physical value. All these aspects have to be carefully considered for a reliable result.

**Axial Charge of the Nucleon**

That axial isovector coupling $g_A$ can be obtained from $\langle \bar{p}|\gamma_5\gamma_\mu\gamma_5d|n\rangle$. Fig. 1, right\(^1\) show results of recent years. All are slightly below the experimental value $g_A/g_V = 1.2723(23)$. The different numbers of dynamical quarks do not explain this. The dependence on lattice spacing or volume (recent results cover a range $3 < m_sL < 6$) also shows no trend (cf. plots in [2]).

The most likely suspect is the influence of excited states that may be still significant in the region of the insertion. Fitting the mentioned ratio at several values of $\tau$ to a plateau may lead to an underestimation of the value. Analysis variants are a summation method [4] or adding excited states to the fit function. Recent studies carefully analyse those approaches [5, 6]. From Fig. 2 of Ref. [6] one clearly sees that the nucleon has admixture from excitations up to about 0.6 fm; the source and sink are at $t = 0$ and $t = t_f \approx 1$ fm, so the center of the hoped-for plateau is at 0.5 fm, clearly in the contaminated region. In the ratio $g_A/F_F$ ($F_F$ is the pion decay constant) some of the finite volume influence seems to cancel [7] and extrapolation to physical pion masses gives a value close to experiment [6].

Further recent results include a study of the disconnected contribution to the isoscalar (S and A) matrix elements, which are $O(7\%)$ [8]. In [6, 5] also isovector couplings $g_S$ and $g_V$ have been determined and in a ChPT study the nucleon-pion-state contributions in the determination of the nucleon axial charge have been estimated to be a few percent [9].

\(^1\)Thanks to Martha Constantinou and Sara Collins for help.
The so-called Dirac ($F_1$) and Pauli ($F_2$) form factors are determined from the matrix element

$$\langle N(p)|V_\mu|\bar{N}(r)\rangle \sim \bar{u}_N(p) \left[ F_1(q^2)\gamma_\mu + F_2(q^2)\frac{i\gamma_\mu q_\nu}{2m_N} \right] u_N(r) \quad \text{with} \quad q^2 \equiv (p-r)^2 \equiv -Q^2.$$  

(4)

Here recent work has been already at close to physical pion masses [10, 11, 12, 13]. The results are generally consistent. They cover, however, only a very small range of $Q^2$ as compared to experiments. The reason is indigenous to the lattice approach. Due to the finite box size the momenta are quantized. (E.g., $q^2 \approx \vec{k}^2(2\pi/L)^2$ for the non-interacting case, where $\vec{k}$ is a vector with integer components.) This constrains both, the lowest and the highest achievable values. For small $q^2$ one need large volumes, for large $q^2$ the statistical noise increases. Already $\vec{k}^2 = 6$, which corresponds to $Q^2 \approx 1 \text{ GeV}^2$ for $L = 3 \text{ fm}$, is a problem in that regard. A recently proposed approach utilizing the Feynman-Hellmann relation between $\langle h|O|h\rangle$ and the derivative of a 2-point function may help in going to larger $Q^2$ [14, 15, 16]

Lower values of $Q^2$ are important for the charge radii which are obtained from extrapolating fits to the lattice data. As can be seen from Fig. 2 the bulk of the values is significantly smaller than both experimental values.

The proton spin has contributions from the quarks and the gluons: $\frac{1}{2} = \sum_q J_q + J_G$, where one may distinguish the quark orbital and spinor contributions $J_q = L_q + \frac{1}{2} \Delta \Sigma_q$, suggested in [19]. The quark contributions need computation of matrix elements like $\langle x\rangle^q$ and $\langle p'|T^{\mu\nu}\rangle^q$, involving derivative operators. To determine individual $\Delta \Sigma_q$ one needs to consider disconnected contributions which require high statistics and special methods (stochastic source methods).

All lattice calculations need to be extrapolated down to the physical pion mass. In [20] Heavy Baryon Chiral Perturbation Theory was used and the results are quite sensitive on the extrapolation leading to large systematic errors. For the light quarks the values have stabilized at $\Delta u + \Delta d = 0.35(6)$ [20, 21, 2]. For the strange quarks the contribution comes from gluonic coupling to vacuum loops. Several collaborations’ results [3] are barely dependent on $m_\pi$ giving a value $\Delta s = -0.02(1)$ [22]. This sums to $\Delta \Sigma = \Delta u + \Delta d + \Delta s = 0.33(7)$ in good agreement with the COMPASS(2007) value 0.33(3)(5).

The uncertainties are still large: the pion mass extrapolation introduces significant model dependence. For a recent more detailed review see [23].

Low energy parameters like leptonic and semileptonic decay constants, CKM matrix elements, quark masses, the quark condensate, $\alpha_s$, and others are collected in the compilation of the Flavor Lattice Averaging Group - FLAG (http://itpwiki.unibe.ch/flag) [24]. Heavy meson decay constants can be found in recent work by [25].
Radiative Decays

On the lattice on-shell decays are forbidden due to the Maiani-Testa theorem; however Lellouch and Lüscher [26] found a method to circumvent that problem. Recently Briceño [27] formulated a technique to address radiative decays like $\rho \rightarrow \pi \gamma$ (For alternative approaches see [28, 29]). In [30] the $\rho$ was assumed to be stable and basic tools for the analysis were formulated. The pion mass there is quite high of $O(700$ MeV). The CSSM collaboration presented results at almost physical pion mass (157 MeV)[31].

In the real process, however, the $\rho$ is a resonance: $\pi \gamma^{*} \rightarrow \rho \rightarrow \pi \pi$. This now has been studied in a lattice simulation [32]. The transition matrix element was computed and a parametrisation of the amplitude allows the analytic continuation to the $\rho$-pole in the unphysical sheet and extraction of the form factor $F_{\pi \rho}(E_{\pi \pi}^{*}, Q^{2})$ from the residue. The calculation still is for large pion mass of 400 MeV but compares favorable with phenomenological model calculations. For more information see Briceño’s contribution to this conference.

HADRON SPECTROSCOPY

Single Hadron Approximation

A recent highlight is the determination of the electromagnetic mass differences for $p$, $\Sigma$, $\Xi$ and others [33]. Four quark species $u$, $d$, $s$, and $c$ were taken into account and QED in its non-compact version was added to QCD, both non-perturbatively. QED needs special care: gauge fixing, finite volume corrections $O(1/L)$ and regularisation scheme make life hard (see also [34, 35]). The results obtained for $197$ MeV $\leq m_{\pi} \leq 440$ MeV were extrapolated to the physical point leading to high precision values in good agreement with experiment, in some cases predictions like for $\Delta \Sigma$.

Milestones in the determination of the hadronic states were [36, 37, 38]. In [36] prominent members of the $(u, d, d)$ family of hadrons were obtained, in [37, 38] meson and baryon excitations were determined for several spin-parity channels. This year has brought results on singly- and doubly charmed baryons with and without strangeness[39] for ground states and first excitations. The pion masses were between 260 and 460 MeV and the results could be extrapolated to the physical point. Ground state energies for baryons with up to three heavy quarks ($c$ and $b$) were computed by [40] at several pion masses and extrapolated to the physical point.

A challenging problem is the identification of spin, since different continuum spins couple to the same lattice operator. Comparing the overlap patterns the Hadron Spectrum Collaboration resolved spins up to 4 in the (excited) charmonium spectrum [41] and for charmed mesons [42]. Based on that experience, in [43] doubly charmed baryons were studied (for a pion mass of 400 MeV) and spin identification up to 7/2 was performed. The baryon lattice operators were constructed by subduction of continuum operators to the lattice symmetry. Up to 11 excitation energy levels were presented; the observed multiplet structure matches the non-relativistic quark spinor model with symmetry $SU(6) \times O(3)$.

The bulk of results was extracted from correlation functions of single hadrons, i.e., either baryonic three-quark operators or mesonic quark-antiquark operators. Although we know that in quantum field theory all possible multi-quark intermediate states can contribute due to the dynamical vacuum with fermion loops, in practical lattice calculations using single hadron correlations these contributions are suppressed. This explains why one finds signals for resonances although they are not asymptotic states. The influence of coupled channels and associated thresholds is effectively neglected. It also means that an observed excited level do not necessarily give the position of the resonance peak. One has to allow for multi-hadron operators in the set of lattice interpolators.

Multi-Hadron Approach

This led to a changed point of view: One does not study the resonance correlators but the scattering process where resonances may appear. Due to the finite volume the energy spectrum of the scattering process is discrete. Lüscher derived a relation [44, 45] between the spectrum in finite volume to the phase shift in the continuum for elastic meson-meson scattering. This has been extended to moving frames and hadron-hadron scattering in general. In recent years there has been an explosion of contributions in that direction.

What are the challenges in that approach? First one needs to consider a larger set of operators - single hadron as well as hadron-hadron operators - and cross-correlations $C_{ij}(t)$ between them. In that correlation elements one has (for baryon-baryon scattering) up to six valence quark propagators. Secondly, there will be quark-antiquark annihilations
Zpotential related to the Nambu-Bethe-Salpeter equation is determined in a coupled channel formalism [72]. amplitude (in the elastic regime) may be parametrized by were identified, both in good agreement with experiment. \[ \psi \] interpolators for two pion masses (266 MeV and 157 MeV). Below threshold the cross-correlation matrix. All observed levels (covering the energy range up to 4.1 GeV) could be identified with \( 18 \) interpolators of meson-meson type with \( c \). Following several studies of elastic \( \pi \pi \) and \( \pi K \) scattering as well as coupled channels model calculations [56, 57] the last year has finally brought the first coupled channel simulation. Dudek et al. [58] investigated \( s \), \( p \), and \( d \)-waves of the coupled \( \pi K - \eta K \) system. Three lattice sizes with up to 70 identified energy levels and an interpolating model allows the determination of phase shifts and inelasticity up to 1600 MeV. Due to the large pion mass of 391 MeV the \( K^+ \) comes as a bound state but in particular in \( s \) and \( d \) wave the main features are successfully reproduced. This promising result was followed by a \( \pi \pi \), \( KK \) coupled channel study [59]. These results for a pion mass of 236 MeV have then been extrapolated to the physical point [60]. More details can be found in the contributions of J. Dudek, D. Wilson and D. Bolton to this conference.

A first application of \( \pi N \) scattering was presented already two years ago [61, 62] demonstrating the importance of scattering states. Earlier results for the \( \frac{1}{2}^- \) channel did show two energy levels tentatively attributed to the \( N(1535) \) and \( N(1650) \), but the splitting was too large. In the new study the lowest \( \pi N \) \( s \)-wave level was correctly identified close to threshold and the next two level had the right splitting and position of \( N(1535) \) and \( N(1650) \). Meanwhile further results with multi-hadron interpolators have appeared [63].

Nucleon-nucleon scattering needs six valence quark propagators but none of the quarks is backtracking. Such a study needs large spatial lattice size; results for \( s \), \( p \), \( d \), and \( f \) partial waves and spatial extent 4.6 fm was presented recently [64]. The pion mass there is quite high (800 MeV) but further studies closer to the physical values are to be expected.

**Heavy Quarks**

Recent reviews on lattice results in the heavy flavor sector are [65, 66, 67]. At present it is hopeless to perform a full coupled channel phase shift lattice calculation in the charmonium sector - there are too many coupled channels in the interesting energy regions. On the way towards that far-lying goal we can, however, learn something from the measured energy levels. An example for this “level hunting” is the search for a signal of the \( Z_c^+(3900) \) state. In [68] 18 interpolators of meson-meson type with \( c\bar{c}ud \) quark content as well as four tetraquark operators were included in the cross-correlation matrix. All observed levels (covering the energy range up to 4.1 GeV) could be identified with (expected) meson-meson states and no extra state (which then could be associated to the \( Z_c^*(3900) \)) was found in this \( I^G(J^{PC}) = 1^+(1^{-+}) \) channel. This agrees with other lattice studies [69, 70]. There is an ongoing discussion whether the \( Z_c(3900) \) might be a threshold effect. This has been also discussed in the so-called HALQCD approach [71]. There a potential related to the Nambu-Bethe-Salpeter equation is determined in a coupled channel formalism [72].

Charmonium levels in the single hadron approximation are in good agreement with experiment only below the \( D\bar{D} \) threshold. In [73] charmonium \( \psi(3770) \) was studied in a system of 15 operators of \( c\bar{c} \) type as well as two \( D\bar{D} \) interpolators for two pion masses (266 MeV and 157 MeV). Below threshold \( \psi(2S) \) and above threshold \( \psi(3770) \) were identified, both in good agreement with experiment.

Of particular interest are resonances or bound states close to thresholds. The reciprocal partial wave scattering amplitude (in the elastic regime) may be parametrized by

\[
\text{Re}[f^{-1}_G(s)] = \rho(s) \cot \delta_1(s) - i \rho(s) \equiv k^{-1}(s) - i \rho(s) \quad \text{with the phase space factor} \quad \rho(s) = 2\rho_e s^{1/2} / \sqrt{s} \quad (5)
\]

and in the Lüscher-type analysis each energy level gives a value of \( \text{Re}(f^{-1}) = c \sum_\omega \left( \frac{m^2}{m^2} \right)^2 \) (cf. Fig. 3). Above threshold each point gives a value of the phase shift. Interpolation and continuation below threshold allows to retrieve threshold parameters as well bound state energies or resonance position and coupling.
FIGURE 3. Left: Schematic description of the Lüscher analysis: Red curves are the theoretically possible values, the measured energy values then lead to the values of $k^{-1}(s)$ lying on that curves. Right: Example for this scenario for $B_s(0^+)$ $BK$ scattering (Fig. from [74]); note that below threshold the analytic continuation of the phase space factor contributes to the real part leading to the bound state position.

FIGURE 4. Left: Fig. from [75] for the $I=0$ channel with $c\bar{c}$ and $c\bar{c}(u\bar{u}+d\bar{d})$ interpolators. The tetraquark operators appear to have little effect on the spectrum. The red squares are dominated by $c\bar{c}$ operators and are attributed to $X_{c1}$ and $X(3872)$. Right: Fig. from [76]; results for $D_s$ states derived for a gauge field ensemble “Ens.2” with pion mass of 157 MeV [77].

In the $0^+(1^{++})$ channel lies the $X(3872)$; this state was postdicted in a lattice study (for the first time) [78]. This was confirmed in [69]. A recent study [75] extended the set of coupled channel operators significantly (22 interpolators including $DD^*$, $J/\psi\omega$, $\eta_c\sigma$, $X_{c1}\sigma$, as well as four tetraquark operators). The $X(3872)$ closely below $DD^*$ threshold was reconfirmed with a strong $c\bar{c}$ Fock component. It is not seen, if the $c\bar{c}$ interpolators are not included.

Phenomenological models as well as lattice calculations gave controversial results for the $D_s$ in $0^{++}$ and $1^{++}$. In both cases there is a nearby threshold: $KD$ and $KD^*$, respectively, and it was suggested that these channels may be important components of the states [79]. Indeed a lattice study [80, 76] including these channels reproduced the pattern from experiment and identified bound states $D_{s0}(2315)$ and $D_{s1}(2460)$ and, above the $KD^*$ threshold $D_{s1}(2536)$ (Fig. 4). The levels were consistently higher than experiment due to larger than physical pion mass of 157 MeV and quark mass tuning effects but the splitting and distance to threshold agreed with experiment.

Motivated by these results a similar study was then done for $B_s$ in $0^+$, $1^+$ and $2^+$ with $BK$ and $B^*K$ contributions [74]. In $0^+$ a bound state $B_{s0}$ with a mass of 5.711(13)(19) GeV and in $1^+$ a bound state $B_{s1}$ with a mass of 5.750(17)(19) GeV was predicted. Close to threshold a weakly coupled $B_{s1}^0$ at a mass of 5.831(9)(6) GeV was identified close to the experimental state at 5.8288(4) GeV.

Summary

The lattice formulation of QCD is mathematically well defined and provides a controlled continuum limit. With increasing compute power and algorithmic improvements we have come close to that ambition. Lattice structure results approach the quality needed for an input to experiment analysis, although they are not yet precise enough and one still has to understand the origin of deviations. Efficient methods for disconnected graph contributions are needed. Our understanding of lattice scattering has improved considerably and hadron spectroscopy has entered a new era. Processes involving several coupled channels are still a challenge.
ACKNOWLEDGMENTS

Many thanks go to my collaborators of recent years Sasa Prelovsek, Daniel Mohler, Luka Leskovec and Padmanath Madanagopalan. I thank Sara Collins and Martha Constantinou for their help with the data collection and Constantia Alexandrou, Raul Briceño, Christine Davies, Michael Engelhardt, Gian-Carlo Rossi and André Walker-Loud for information. Support by the Austrian Science Fund FWF: I1313-N27 is gratefully acknowledged.

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