The Excited-state Spectrum of QCD through Lattice Gauge Theory Calculations

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Abstract. I describe the computation of the spectrum of Quantum Chromodynamics through first principles calculations using lattice gauge theory. I begin outlining briefly the formulation of QCD on a lattice, and then describe some of the challenges in computing the exciting state spectrum of the theory. I then present recent results for the spectrum for mesons containing both the light and heavier charm quarks, and for baryons containing the light quarks. A particular emphasis will be laid on the role played by gluons within the spectrum. I conclude by some of the challenges that remain, notably those due to strong decays, and the prospect for future calculations.

1. Introduction
A quantitative description of the spectrum of QCD goes to the core of our understanding of the theory, and is therefore the focus of intense experimental and theoretical effort. The experimental investigation of the spectrum has undergone a resurgence: the observation of new states in the Charmonium system at Belle, BaBar, CDF, D0 and CLEOc with future experiments at BESIII and PANDA, the search for the so-called missing baryon resonances of the quark model at CLAS at JLab@6GeV, and the flagship search for exotic mesons in the GlueX experiment at JLab@12GeV. These experimental initiatives are matched by increasingly vigorous theoretical efforts aimed at obtaining the QCD spectrum from first principles, where lattice QCD enables many quantities in QCD to be solved rather than modelled.

The potential of lattice QCD to enhance our understanding of hadronic and nuclear physics was recognized at Jefferson Laboratory when Nathan Isgur established a lattice initiative at the laboratory. Over the last decade, that initiative has become a core activity of the laboratory, comprising the three major components of a successful lattice effort. Firstly, the development of the computational and software infrastructure by both the Theory Center and the High-Performance Computing Group under the auspices of the Department of Energy’s SciDAC (Scientific Discovery through Advanced Computing) Initiative. Secondly, the development and operation of hardware, based on commodity clusters and latterly heterogeneous architectures, optimized for lattice QCD, and now serving as a national facility. Finally, a rigorous research effort dedicated to addressing the key scientific questions posed by the Jefferson Laboratory program. In this talk, I will focus on the scientific impact of the lattice program, and in particular on our understanding of the excited-state spectrum of both mesons and of baryons.
2. The Excited State Spectrum in Lattice QCD

Lattice gauge calculations solve QCD on a four-dimensional lattice, or grid, of points in Euclidean space. The quarks reside on the points of the grid, whilst the gluons are associated with the links joining those points. Lattice calculations proceed through a Monte Carlo method, in which ensembles of gauge configurations are generated with a probability distribution prescribed by the Euclidean QCD action.

The low-lying spectrum of QCD has long been an important benchmark for lattice QCD calculations, encapsulating both our ability to confront first-principles calculations with well-established observational results, and of our understanding of how QCD changes as the masses of the quarks are varied. A comprehensive picture of resonances requires that we go beyond a knowledge of the ground state mass in each channel, and obtain the masses of the lowest states of a given quantum number. This we can accomplish through the use of the variational method\cite{1, 2}. Rather than measuring a single correlator $C(t)$, we determine a matrix of correlators

$$C_{ij}(t) = \sum_{\vec{x}} \sum_{\vec{y}} \langle O_i(\vec{x}, t) O_j^\dagger(\vec{y}, 0) \rangle,$$

where $\{O_i; i = 1, \ldots, N\}$ are a basis of interpolating operators with given quantum numbers. We then solve the generalized eigenvalue equation

$$C(t) u = \lambda(t, t_0) C(t_0) u$$

to obtain a set of real (ordered) eigenvalues $\lambda_n(t, t_0)$, where $\lambda_0 \geq \lambda_1 \geq \cdots \geq \lambda_{N-1}$. At large Euclidean times, these eigenvalues then delineate between the different masses

$$\lambda_n(t, t_0) \rightarrow e^{-M_n(t-t_0)} + O(e^{-\Delta M_n(t-t_0)}).$$

where $\Delta M_n = \min\{| M_n - M_i | : i \neq n \}$. The eigenvectors $u$ are orthogonal with metric $C(t_0)$, and a knowledge of the eigenvectors can yield information about the partonic structure of the states.

The (hyper-) cubic lattice does not possess the full rotational symmetry of the continuum. Thus in a lattice calculation, states at rest are classified not according to the spin $(J, J_z)$, but rather according to the irreducible representations (irreps) of the symmetry group of the cube; for states of higher spin, the different continuum degrees of freedom are distributed across several lattice irreps. This reduced symmetry has proved a formidable barrier to the interpretation of lattice calculations by making the assignment of the continuum spins to the energy eigenstates problematic. In our work, the choice of interpolating operators is crucial to the assignment of spins both for mesons and for baryons. For the excited meson spectrum, our starting point is a set of interpolating operators

$$O = \sum_{\vec{x}} \bar{\psi}(\vec{x}) \Gamma_i \hat{D}_i \hat{D}_j \ldots \psi(\vec{x}) \quad (1)$$

where $\hat{D}$ is a discretized covariant derivative, and $\psi(\bar{\psi})$ a quark (antiquark) field. From this set, we can construct a basis of interpolating operators $O^{J,M}$ that in the continuum have definite spin,

$$\langle 0 | O^{JM} | J', M' \rangle = Z^J \delta_{J,J'} \delta_{M,M'}.$$

It is these operators that are now subduced to the lattice irreducible representations:

$$O^{[J]}_{\Lambda, \Lambda} = \sum_M S^{JM}_{\Lambda, \Lambda} O^{JM},$$

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where Λ, λ denote the lattice irrep and its row respectively, and $S^{J,M}_{Λ,λ}$ are calculable coefficients. Whilst the resulting operators $O^{[J]}_{Λ,λ}$ interpolate to any state whose spin is subduced to the irrep Λ, we find that in practice the operator interpolates strongly to states of spin $J$, and that the resulting overlaps $Z^J$ are common across the different subductions; the method is described in detail in ref. [3]. Thus the operators $O^{[J]}_{Λ,λ}$ retain a strong memory of their continuum antecedents, and this property enables us to identify the spins of the states for the effectively single-hadron states we have observed in the following calculation.

Our ability to calculate correlation functions efficiently for the large basis of operators that this methodology entails has been greatly advanced through the development of a new method, “distillation” [4], that enables all the elements of the correlation matrix to be computed, with time-sliced sums at both source and sink.

The final ingredient in the spectroscopy effort has been the generation of so-called anisotropic lattices, with finer temporal than spatial discretisation, enabling the fall-off of the principle correlators introduced above to be discerned at short temporal separations. This has been accomplished through the generation of lattices with two flavors of fully dynamical light and a dynamical strange quark, using the clover fermion action. An important milestone was the tuning of the parameters of the action, beginning with the three-flavor theory [5], and the development of a means of specifying the values of the quark masses, in particular those for the light $u/d$ and $s$ quarks, in a way that enables lattice calculations to be extrapolated to the physical values of these masses [6].

3. Excited Meson Spectrum

The new Hall D of the JLab 12GeV upgrade centers on the study of meson states produced in photoproduction reactions in the GlueX experiment. Photoproduction has been proposed, within QCD-motivated models, as a favorable method for the production of exotic mesons, that is those mesons having $J^{PC}$ outside the set allowed to a fermion-antifermion pair. The “hybrid” hypothesis is that these quantum numbers arise from an excited gluonic field, in addition to a quark-antiquark pair.

The availability of the large ensembles of $N_f = 2 + 1$ anisotropic clover lattices, together with the efficient operator-construction admitted by “distillation”, has enabled us to compute the isovector meson spectrum for states composed of the light and strange quarks [7, 3], at pion masses down to around 400 MeV. Masses of highly excited states have been calculated, with the quantum numbers reliably delineated, including for the first time in a lattice calculation states of spin 4. Figure 1 summarizes the results on exotic states and compares those results with previous lattice QCD results from Refs. [8, 9, 10, 11, 12, 13]. Further, we see evidence for “hybrid” states, that is those in which the gluons play a vital structural role but with non-exotic quantum numbers, as we show below.

3.1. Isoscalar meson spectrum

The calculation of the isoscalar meson spectrum, and the study of the hidden-flavor composition of states, is a challenging undertaking, since it requires the computationally demanding task of including quark-annihilation contributions to hadronic correlation functions. The “distillation” method provides a computationally highly efficient way of including these contributions, by enabling the most demanding part of the calculation, that of the so-called perambulators (the parallel transporters of the method) to be computed with using GPUs, with the remaining parts of the calculation performed on CPUs. This feature was exploited to perform a high-precision calculation of the isoscalar spectrum [14], revealing not only the masses but also the hidden flavor-mixing angles for the states.
Figure 1. Summary of extracted isovector exotic states at two volumes, and at four quark masses. For comparison $1^{-+}$ results from Refs. [8, 9, 10, 11, 12, 13] are also plotted.

We employ as our basis of operators

$$O^l_A(t) = \frac{1}{\sqrt{2}} (\bar{u}\Gamma^A_l u + \bar{d}\Gamma^A_l d)$$

$$O^s_A(t) = \bar{s}\Gamma^A_l s,$$

where $u$, $d$, and $s$ are the up, down and strange quark fields, and the $\Gamma^A_l$ are operators, of the form of eqn. (1), acting in color, Dirac spin, and also in space [4], at a time slice, $t$; in the following we have $SU(2)$ flavor symmetry and therefore use $l$ to denote the light ($u, d$) quarks. The results for the isoscalar spectrum, together with the isovector results presented above, are summarized in Figure 2. For each value of $J^{PC}$, we find that the isoscalar energy eigenvalues occur in pairs. For a particular combination of creation and annihilation operators, we are able to diagonalize the resulting two-by-two correlation matrix in flavor space, thereby revealing the hidden flavor-mixing angles, shown as the fraction of black ($l$) and green ($s$) in the bars of the figure. For “conventional” mesons, we found near ideal mixing other than in the pseudoscalar and axial states. We also computed, for the first time in a lattice calculation, isoscalar “exotic” states; these appear at a mass scale comparable to their isovector cousins. Though these calculations are as yet incomplete, their implication for the Jefferson Laboratory program is profound; they suggest the presence of numerous states of exotic quantum numbers in the energy range accessible to the GlueX experiment.

3.2. Charmonium Spectroscopy

The emergence of new experimental states in the charmonium system has been an important driver for spectroscopy, and is an especially attractive area for lattice studies where calculations of the spectrum can be performed with high statistical precision. It is thus a particularly fruitful area in which to explore the phenomenology of the spectrum. Figure 3 shows the charmonium spectrum for channels, both exotic and non-exotic, in which we are able to identify “hybrid”
Figure 2. The left-hand panel shows the isoscalar meson spectrum labeled by $J^{PC}$, where the box height denotes the statistical uncertainty. The light-strange content of each state ($\cos^2\alpha, \sin^2\alpha$) is given by the fraction of (black, green) and the mixing angle is also shown. Grey boxes indicate the positions of isovector meson states extracted on the same lattice (taken from [3]). Pink boxes indicate the position of quenched glueballs [15]. The right-hand panel shows the GlueX experiment, together with an indication of the expected energy reach.

Figure 3. The charmonium spectrum for those channels in which “hybrid” mesons are identified, obtained on a $24^3$ spatial volume for a pion mass around 400 MeV. The red and blue boxes are suggested as the members of the lowest-lying and first-excited hybrid multiplets, respectively. The black lines are experimental values, whilst the dashed lines are the lowest non-interacting $D\bar{D}$ and $D_s\bar{D}_s$ levels, obtained on a $16^3$ ensemble (short green dashes), and using the experimental masses (long grey dashes).

states [16]. Notably, a lightest and a first-excited hybrid supermultiplet [17] in which the quark-antiquark pairs are coupled to a chromomagnetic gluonic excitation, are identified, indicated by the red and blue bars respectively.
4. Excited Baryon Spectrum

The recipe employed to determine the excited meson spectrum can be applied to determine the spectrum of baryons. A basis of continuum interpolating operators is constructed, including up to two derivatives, and which respect classical symmetries, which is then subduced to the appropriate lattice irreps. The overlaps of the interpolating operators with the extracted states is once again key to determining the spin of the states, exploiting the remarkable degree of rotational symmetry observed at the hadronic scale [18]. The nucleon and Δ excited-nucleon spectrum at the lightest of our pion masses is shown in Figure 4, and exhibits a counting of levels consistent with the non-relativistic $qqq$ constituent quark model.

In contrast to mesons, there are no “exotic” quantum numbers for baryons that demand a richer structure than that of three quarks with relative orbital angular momentum. As noted in reference [18], the operators associated with an excited gluon field, and which would vanish for a trivial gauge configuration, were not included in the basis. These operators were included in a subsequent reanalysis, shown in Figure 5, for the positive-parity N and Δ spectrum [19], and revealed the presence of “hybrid” baryons dominated by operators with an excited gluon field. Remarkably, the mechanism giving rise to such gluonic excitations appears common to both mesons and baryons, as shown in the right-hand panel of Figure 5, where the excitation energy of both “hybrid” mesons and “hybrid” baryons is shown.

5. Summary

The amalgam of theoretical, algorithmic and computational advances has enabled increasingly sophisticated studies of the spectrum of QCD. These are already having a notable impact, suggesting the important role played by gluonic degrees of freedom in describing the spectrum, the anticipated reach of GlueX to see states of exotic quantum numbers, and the rich spectrum of baryon resonances. The calculations outlined above are incomplete: all but the lightest states are resonances whose study requires the calculation of the momentum-dependent phase shifts. Lattice QCD provides a powerful means of relating infinite-momentum elastic phase information to energy shifts at finite volume [20], and the algorithmic advances discussed here have already been exploited to yield precise calculations of the momentum-dependent phase shifts in non-resonant $I = 2\pi\pi$ scattering [21, 22]. Thus most of the ingredients are in place for calculations of the spectrum that can not only confront but also predict the outcomes of future experiment.
Figure 5. The upper panel shows $N$ and $\Delta$ spectrum at $m_\pi = 396$ MeV with the “hybrid” operators included in the basis; blue boxes denote states dominated by such operators and thereby identified as “hybrids”. The lower panel shows the excitation spectrum of hybrid mesons and baryons at three values of the light-quark mass; for mesons we show $m - m_\rho$, while for baryons we show $m - m_N$.

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