The hadron spectrum from lattice QCD

Mike Peardon

School of Mathematics, Trinity College Dublin, Ireland

Abstract. Lattice spectroscopy is becoming increasingly sophisticated. This review will introduce the methodology and describe progress made recently probing the spectrum of excitations of QCD. The focus will be on describing new developments that enable excited states, exotic quantum numbers and resonances to be explored.

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INTRODUCTION

Predicting the spectrum of hadrons directly from the QCD lagrangian has been a central research theme for lattice physicists since the birth of the subject [1]. Many technical challenges and unanswered puzzles remain, in spite of substantial progress in methods, numerical algorithms and the enormous rise in available computer power over the past decades. At this meeting we heard a great deal about the continuing experimental efforts to understand the dynamics of confined quarks and gluons. Lattice methods have an important role to play if a comprehensive link is to be made between the theory of QCD and this ever-emerging observed phenomenology.

The aim of lattice spectroscopy is to provide ab initio precision determinations of the spectrum of resonances. A goal for an ambitious current project should be to compute the energies of all resonances below about 2-3 GeV to a few percent and to start making determinations of the contributions to the widths of these resonances for two-body decay, aiming for a precision at about the ten- to twenty-percent level. Some information should be obtained regarding the constituent nature of these states whenever this is a plausible description that can be disentangled from the data (the “scalargators” described at this meeting [2] are an example where this may prove intractable). Whether all these ambitions can be achieved in full remains mostly speculation at this stage. The aim of this review is to present the best efforts the community is making to achieve these aims and to help non-experts form their own opinions on how well the lattice is doing and what the near future might reveal.

Representing QCD on the lattice provide theorists with a non-perturbative, gauge-invariant regulator of the path integral. Space-time is replaced with a four-dimensional mesh of points with neighbours connected via links. The quark fields are given support only on the sites of the grid while the gluon fields are represented as degrees of freedom living on the links. Typically in large, modern simulations, the lattice spacing $a \approx 0.1$ fm or less. For details, excellent reviews of the state-of-the-art and current challenges can be found in the most recent proceedings of the annual lattice symposium [3, 4, 5].

Monte Carlo simulations of lattice QCD are forced to use importance sampling of the vacuum to reduce the variance of estimators to manageable levels. This necessitates finding a useful positive-definite sampling measure on the gauge fields, which is only feasible for the theory defined on space-time with a Euclidean metric. This Wick rotation turns out to be first a blessing and then a curse for spectroscopy. It helps tremendously by giving a means of projecting onto the ground state (and lowest-lying excitations) reliably. The unfortunate consequence is that we lose direct contact with dynamical properties of the field theory, such as information about decay widths. These must be inferred in more indirect ways which are reviewed later.

THE QCD VACUUM

Once the lattice regularisation has been defined and a set of simulation parameters suitable for the accessible lattice volumes have been chosen, the task of computing observables by Monte Carlo can begin. The first step is to generate a sufficiently large ensemble of gauge-field configurations drawn from the importance sampling measure given by the chosen discretisation. Alternatively, many in the lattice community have recognised the value of open-source data sharing via grids, and the International Lattice Data Grid (ILDG) [6] provides open access to large ensembles.
Ensembles are generated by repeatedly applying a suitable Markov process with the importance sampling measure as its fixed-point. Doing this efficiently is a challenge [7], and the noughties have seen some substantial progress [8, 9, 10] in the techniques available for large-scale simulation. The computational challenge arises since the fermion fields cannot be manipulated directly in the computer, the quark path integral must be evaluated analytically before numerical work can begin. The analytic integration is a simple procedure in QCD, since the fermion action is a bilinear. On the lattice, this action is represented by first finding a matrix $M$ whose continuum limit is the Dirac operator. The action is then simply given by $S_q = \bar{\psi} M \psi$. After then integrating out the $N_f$ quark fields, the QCD lattice path integral is

$$Z = \int \mathcal{D}U \det M^{N_f} [U] e^{-S_q[U]}.$$  

A Markov process is designed to have sampling measure proportional to the integrand of Eqn. 1. There are many means of achieving this end and an introduction can be found in Ref. [11]. The process generates a sequence of states and a sample average measured on this ensemble has an expected value equal to the QCD path integral by the ergodic theorem.

**Quark-field dynamics**

Most large-scale computational groups currently perform dynamical simulations. Computing the effects of the quark field through the fermion determinant is the most expensive part of these calculations and its cost (using current methods) diverges as the quark mass goes to zero and the pion correlation length becomes infinite. As a result, most simulations are done at up- and down-quark masses above their physical values. There is a substantial interest then in understanding and controlling the extrapolation of observables to the chiral limit and a substantial literature exists covering that topic (see Refs. [12, 13] for an introduction).

In many modern simulations, the dynamics of both up, down and strange quarks are included in the sampling measure and the physical point is getting close enough for extrapolations to be manageable. An example of the precision coming from a recent large-scale simulation [14] of the low-lying states is presented in Fig. 1.

The first simulations at the physical strange and light quark masses have been reported recently by the PACS-CS collaboration [15]. To get to the physical point, a technical trick allowing reweighting of the ensembles was used but this was well controlled and did not substantially increase statistical uncertainty. The difficulties with light quark simulations are not all resolved however and there is some uncertainty about how reliably the Markov chains of configurations used are sampling the QCD vacuum sectors with distinct topological charge. More experience will resolve the extent of these effects and their impact on physics outputs.

![FIGURE 1. The spectrum of low-lying hadrons in QCD with dynamical up, down and strange quarks, extrapolated to their physical values and to the continuum limit, computed by the Budapest-Marseille-Wupperlal collaboration [14].](image-url)
Testing universality

There are infinitely many ways of representing QCD on a lattice. All these representations should agree on the spectrum for a particular set of quark mass inputs. The different ways of representing the fields of QCD have their own merits and drawbacks; as an unfortunate rule of thumb, if a scheme does a better job of preserving a symmetry of QCD in the continuum, it is more expensive to implement numerically. For example, the Neuberger overlap [16] maintains an unbroken symmetry that closely resembles chiral symmetry but is very computationally expensive.

This diversity can be turned into a strength and the use of different discretisations for the quark and gluon actions by different collaborations means universality of the continuum limit of QCD can be checked. To date, no dramatic upsets have been reported. For a review, see Ref. [3]. For calculations of energies of highly excited states, anisotropic discretisations [17] have proved very useful. Here, the lattice has distinct grid spacings $a_s$ and $a_t$ for the spatial and temporal directions, with $a_t < a_s$. Since spectroscopy requires precise determination of temporal correlations, using a fine spacing in that domain improves resolution without the extreme rise in cost associated with making all four grid directions finer.

VACUUM PROBES

With a suitable ensemble of gauge field configurations available, physics measurements can begin. Quantum mechanical expectation values are determined by sampling a given observable on the ensemble. To investigate spectroscopy, appropriate vacuum probes must be defined to extract energies of eigenstates of the QCD Hamiltonian.

Spectroscopic techniques

The Euclidean metric turns out to be very helpful when it comes to studying the spectroscopy of stable states and narrow resonances. If the correlation function between two identical creation and annihilation operators with the quantum numbers of interest is measured, a simple analysis shows

$$C(t) = \langle \Phi(t + t')|\Phi(t') \rangle = \langle \Phi|e^{-\mathcal{H}t}|\Phi \rangle = \sum_\alpha |\langle \Phi|\alpha \rangle|^2 e^{-E_{\alpha}t},$$

(2)

and as the separation between the source operators is extended, we find

$$\lim_{t \to \infty} C(t) \propto e^{-E_{\alpha}t}.$$  

(3)

The correlation function falls exponentially where $E_0$ is the energy of the lowest-lying state with the quantum numbers of the creation operator. In principle then, the Euclidean metric gives a simple means of extracting the ground-state energy of QCD states with particular quantum numbers; if the fall-off of the correlation function can be measured in a region where the first term in the tower of exponentials dominates and a statistical analysis can be performed to extract $E_0$ from a fit, then an ab initio mass determination from the QCD lagrangian has been made.

Excited states

The lattice method does not just enable computations of ground-state energies, however. Any excited state is accessible in principle. A range of methods for approaching this problem have been developed, but the most robust uses information from correlations between more than one source. To compute a higher-lying state in the spectrum, a matrix of correlation functions between $n$ creation and annihilation operators rather than just one [18, 19] can be used.

With such a basis, $\{\Phi_i\}, i = 1 \ldots n$ the correlation matrix is

$$C_{ij}(t) = \langle \Phi_i(t + t')|\Phi_j(t') \rangle.$$  

(4)

Now if the generalised eigenvalue problem of the form

$$C_{ij}(t_1)v_j = \lambda C_{ik}(t_0)v_k,$$

(5)

is solved for suitably chosen $t_1$ and $t_0$ then the $p$-th eigenvalue $\lambda(p)$ is related to the $p$-th excited energy level. More detail can be found in Ref. [20].
Smearing

The correlation function falls rapidly as the source and sink operator are moved further apart. At the same time, for most symmetry channels, the statistical variance in the Monte Carlo estimator remains constant and so there is a limited range of time separations over which the fall-off can be observed reliably. It is crucial then that the asymptotic form of equation 3 is reached as rapidly as possible. This issue has been understood for as long as spectroscopy calculations on the lattice have been performed and methods have been devised to build creation operators whose overlap onto low-lying states is large while contributions from very high-lying states are minimised. These techniques are usually termed “smearing”. Many variants exist. The most useful ones preserve the gauge-covariant structure of quark fields.

A new smearing method has recently been proposed and tested by the Hadron Spectrum Collaboration [21]. The technique, termed “distillation”, uses a low-rank projection operator to define a small space of gauge-covariant “smooth” fields and creation operators for hadrons are constructed exclusively in that space. A simple analogy is with image compression; most digital images use a projection algorithm to extract the most important features and discard others and this greatly reduces the amount of information needed to store and reproduce the picture. Similarly distillation attempts to extract only the salient long-range features of the quark vacuum. The main benefit of this is the resulting system is rather small in practice and so all elements of the quark propagator from any basis vector in the distillation spaces on two different time-slices can be computed affordably for modest lattice volumes (about 2fm).

The most substantial problem with the method is the cost growth. This meeting heard first results [22] from the attempts by the collaboration to ameliorate this expense using new stochastic estimator methods. The new technique is in its infancy but is showing clear promise.

Spin

As we have seen, once operators with a particular quantum number are constructed, ground states and excitation energies can be measured. The issue of constructing operators with the right quantum numbers is complicated by the reduced symmetry of the lattice. When the fields are regulated on the lattice, they take values only on the sites or links and so the relevant symmetry operations are those of the cubic point group $O_h$ rather than the Lie group of rotations $SO(3)$. So states on the lattice, rather than being classified by a spin quantum number that labels which irreducible representation of $SO(3)$ they transform according to, they have a “quantum letter” labelling an irreducible representation of $O_h$. To understand the link between these two sets of labels, the irreducible representations of $SO(3)$ must be subduced in $O_h$. The link between $J = 0$ and 1 is simple; they transform according to the $A_1$ and $T_1$ irreps. At $J = 2$ the first complication appears; the largest irreps of $O_h$ have dimension three so the subduced $J = 2$ irrep of $SO(3)$ must be reducible. The $J = 2$ irrep appears both in the $E$ and $T_2$ of $O_h$. Whether parity is a good quantum number depends on the details of the regularisation of the quark fields; the formulations most widely used for spectroscopy do preserve parity although there are exceptions.

**TABLE 1.** The art of subduction. The subduced representations of $SO(3)$ up to spin-4 in $O_h$, which indicate where continuum spin states appear in the five allowed lattice channels

<table>
<thead>
<tr>
<th>Spin</th>
<th>$O_h$ irrep</th>
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<tbody>
<tr>
<td>$J=0$</td>
<td>1</td>
</tr>
<tr>
<td>$J=1$</td>
<td>1</td>
</tr>
<tr>
<td>$J=2$</td>
<td>1 1 1</td>
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<tr>
<td>$J=3$</td>
<td>1 1</td>
</tr>
<tr>
<td>$J=4$</td>
<td>1 1</td>
</tr>
</tbody>
</table>

General frameworks for constructing basic operators on quark fields that transform irreducibly under $O_h$ have been established and exploited in large calculations [23, 24, 25]. More recently, [26, 27] a construction has been developed that subduces representations made from continuum operators built from products of gauge-covariant derivatives and replaces them with their lattice equivalents. This provides extra tagging information that allows states in distinct lattice irreps to be identified as coming from continuum irreps with some confidence. The extra information has enabled a much clearer identification of hybrid states and high-spin states, with three spin-four mesons being identified.
Hadron spectroscopy

Consider now the computational steps that must be performed to compute the mass of hadrons and their excitations. These Monte Carlo calculations proceed in multiple steps; first the observable is defined as a function on the fields in the lagrangian and a path integral representation is written. The quark field integral is done analytically at this stage, yielding a path integral representation over the gluons alone, with the memory of valence quark fields appearing in the quark propagators given by the allowed Wick contractions and the memory of sea quarks in the determinant weight. The expression involving valence propagators is thus measured on the appropriate importance sampling ensemble.

Details and recent results can be found in [23, 24, 25, 35]. Consider applying this procedure to the measurement of a correlation function between operators that create an isovector or flavoured meson. After the Wick contraction integration over the up- and down-quark fields, we arrive at

\[ C_{I=1}(t_2 - t_1) = \sum_{\Delta t} \langle \text{Tr} \left( M^{-1}[x_1, t_1; s_2, t_2] \Gamma M^{-1}[x_2, t_2; x_1, t_1] \Gamma \right) \rangle. \] (7)

The operator \( \Gamma \) can depend on the gluon fields too, enabling hybrid mesons to be created [34]. These measurements have been developed extensively over the past five years yielding much better precision and reliability [28, 29, 30, 31, 32, 33] Heavy quarks can be dealt with similarly, although extra care must be taken to account for the practical problem that the heavy quark mass-scale is close to or exceeds the lattice cut-off. Recent progress [36] in determining the spectrum of mesons built from a static colour source and a light quark shows precision is possible and the effects of the finite heavy quark mass can be accounted for.

Similarly for a baryon, following the rules of Wick contraction yields expressions for the correlation function in terms of the quark propagation matrix. If a creation operator for a \( \Lambda \) baryon (to pick an example) was written \( \chi(x, t) = \epsilon_{ijk} \Gamma u_{i}(x, t)d_{j}(x, t)\bar{s}_{k}(x, t) \) with \( \Gamma \) an appropriate operator on the spin indices, then the object to be measured would read

\[ C_{\Lambda}(t_2 - t_1) = \sum_{\Delta t} \epsilon_{ijk} \epsilon_{\mu\nu} \Gamma \bar{\Gamma} M^{-1}[x_1, t_1; x_2, t_2] \bar{u}_{\mu} M^{-1}[x_1, t_1; x_2, t_2] \bar{u}_{\mu} M^{-1}[x_1, t_1; x_2, t_2] \bar{s}_{\nu}. \] (8)

Details and recent results can be found in [23, 24, 25, 35].

The isovector mesons of QCD are more widely studied on the lattice compared to the isoscalar states. The reason for this is a practical one. As we have seen, quark fields are not manipulated directly on the computer and instead an analytic calculation integrates out the quark fields in the relevant observables needed. The Wick contraction rules for isovector and isoscalar mesons yield distinct propagator terms. The isoscalar meson includes an extra term, the “disconnected diagram”. Consider for example the correlation function of an operator exciting the strange quark field alone:

\[ C_{I=0}(t_2 - t_1) = \langle \langle \bar{s}(x_1, t_1) \Gamma \bar{s}(x_1, t_1) - \bar{s}(x_2, t_2) \Gamma \bar{s}(x_2, t_2) \rangle \rangle \] (9)

now the Wick contraction generates two diagrams;

\[ C_{I=0}(t_2 - t_1) = \langle \text{Tr} \left( M^{-1}[x_1, t_1; x_2, t_2] \Gamma M^{-1}[x_2, t_2; x_1, t_1] \Gamma \right) \rangle - \langle \text{Tr} \left( M^{-1}[x_1, t_1; x_2, t_2] \Gamma \right) \text{Tr} \left( M^{-1}[x_1, t_1; x_2, t_2] \Gamma \right) \rangle. \] (10)

As before, the single angle bracket indicates integration over the gluon fields alone. The second term comprises the product of two traces, each with an independent sum over the space-time indices. In the case of isovector mesons, \( \bar{\psi}_s \)-hermiticity was used to rewrite the first diagram in terms of propagators from a single source point. This trick will not work here, since there are two independent summation points in the two traces. All elements of the quark propagator are needed.

This limitation has substantially slowed progress in lattice simulations of the isoscalar sector, certainly in comparison to the isovector states. There have been significant inroads however [37, 38]. The first observation that enabled...
these calculations was the use of stochastic estimation to compute the disconnected terms [39] and these techniques have developed further [40, 41]. At their core, all these techniques start from a simple recipe. If a random field $\eta(x, t)$ is introduced which satisfies a simple property:

$$E[\eta(x_1, t_1)\eta^*(x_2, t_2)] = \delta_{x_1, x_2}\delta_{t_1, t_2},$$

and subsequently the linear system

$$M(x_1, t_1; x_2, t_2)\psi(x_2, t_2) = \eta(x_1, t_1),$$

is solved for $\psi$, then the outer product between $\psi$ and $\eta$ directly yields an unbiased estimator for any element of the quark propagator,

$$E[\psi(x_1, t_1)\eta^*(x_2, t_2)] = M^{-1}(x_1, t_1; x_2, t_2).$$

This simple observation now enables isoscalar meson computations on the computer. Unfortunately, the estimator can have a substantial variance and this results in poor statistical precision. Methods have been developed to improve on this simplest expression and reduce the noise. Distillation technology offers a new framework for these calculations and results presented at this meeting suggest it will be an efficient way of getting access to the isoscalar and other previously difficult measurements. Creation operators to make glueballs can also be studied. These calculations are well-established for the $SU(3)$ Yang-Mills theory [42, 43].

**New results**

This conference saw new results from the Hadron Spectrum collaboration [22, 54]. Highlights taken from determinations of the isovector meson [27] and $\Lambda$ baryon sectors are presented in Fig. 2. Note in the right-hand figure, the states are labelled by the irreps of $O_h$ with double cover; the lattice equivalents of spin $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$ states. The spectrum of excited baryons was presented. The distillation method has proved useful here but its cost still restricts the scope. Colin Morningstar described a new stochastic estimator that should substantially reduce the cost and extend the usefulness of the method. Robert Edwards showed results on baryon excitations using a modified basis to help spin identification.

A lot of new data on the meson spectrum has been published recently. Precision continues to improve, as does the framework for making measurements. The Hadron Spectrum collaboration recently presented new results on the spectrum of isovector mesons. This investigation found states in three exotic $J^{PC}$ channels ($0^+, 1^+$ and $2^+$) that are good hybrid meson candidates. Use of distillation technology has enabled unprecedented resolution to be reached and the statistical uncertainty in the mass determinations is now at the percent-level.

The tetraquark states remain an active topic of investigation [44]. A full understanding of whether these exotic states play an important role in the low-energy spectrum of QCD is still a way off, since many theoretical questions remain and technical obstacles must be overcome.
High-precision glueball studies for the SU(3) Yang-Mills theory have been performed, but the expense of making very large ensembles of dynamical quark fields, combined with the much more intricate theoretical details of understanding mixing means measurements of glueball properties in QCD are in their infancy. Pioneering work has been done [45, 46, 47] and is reviewed in Ref. [48]. The next few years should bring a lot of new results.

COMPUTING RESONANCE WIDTHS

Lattice simulations of QCD are by necessity carried out in a space-time with a Euclidean metric. We have seen the benefits of this sleight-of-hand for computing the energies of low-lying states but the disadvantage arises when we turn our attention to resonances. Information on the dynamics of hadron-hadron scattering can not be directly computed; the notion of asymptotic “in” and “out” states is lost. The matrix elements that would be used to compute scattering cross-sections in Minkowski space do not contain the same information in their asymptotics.

A theoretical means of circumventing this apparent limitation exists, however [49, 19]. In a finite spatial box with periodic boundary conditions, QCD exhibits a discrete spectrum of states. These include the resonances and states more closely resembling two (and more) hadrons. A state comprising two mesons with momenta $p$ and $-p$ (so the total momentum of the state is zero) and where each constituent has mass $m$ has an energy approximately given by $E = 2\sqrt{m^2 + p^2}$. Since the boundary conditions quantise the allowed momentum, the energy spectrum has discrete, well separated levels. If one of these levels approaches the energy of a resonance as the box size is varied, the mixing between these states that is responsible in the continuum for the decay causes the two near degenerate states to repel. The width of the resonance can be inferred from this data. To date, pioneering tests of this technique in QCD have focused on studying the $\rho$-meson [50, 51, 52]. These studies measure the coupling $g_{\rho\pi\pi}$ that appears in a phenomenological model of rho decay and find a result consistent with a value extracted from experimental determination of the $\rho$ width. The Monte Carlo calculations yield about 20% statistical precision on the width.

Even with a clean determination of the spectrum, extracting resonance parameters is far from straightforward. Narrow low-lying resonances can be handled using Breit-Wigner fits and Lüscher’s method but broad structures above inelastic thresholds will be as difficult to interpret for the lattice as they are for experiments. New methods have been proposed [53] to identify resonances as peaks in histograms where the number of levels in an energy range are counted as the volume is varied. These studies will require large numbers of independent simulations on different lattice volumes to be performed, which will be accompanied by a correspondingly large bill for computer time requirements. The appropriate time-scale to watch the lattice literature for these results to emerge is probably about five years. First tests by the Hadron Spectrum Collaboration were presented at this meeting [54, 55].

SUMMARY

Lattice spectroscopy continues to develop at a significant pace, with new ideas and results giving increasingly high precision. The quenched approximation was a substantial hurdle to reliable QCD spectroscopy, since it destroyed the unitarity of the quark sector, rendering interpretation of resonances impossible. Developments in both computer technology and Markov Chain Monte Carlo algorithms have meant lattice practitioners can now carry out realistic simulations with the full quark dynamics included and run these simulations close to (or even at) the physical quark masses. The lattice spacings in most modern calculations are small enough so that discretisation errors do not dominate.

What will the next five years bring? I think new techniques and datasets will enable the isoscalar mesons and light baryons to be studied with much better precision. Better parallel computers will ensure lattice simulations will get very close to the physical quark masses although there are questions about whether our current sophisticated Markov Chain Monte Carlo algorithms are in fact sophisticated enough. The sudden rise of scientific computing on GPUs [56, 57] will open access to an unexplored seam of measurements of new hadronic vacuum probes and the inclusion of multi-hadron operators will become increasingly widespread, enabling much richer investigations of resonance physics to be performed. The recent excitement in charmonium spectroscopy will continue to inspire lattice physicists. The use of lattice techniques to study hadrons in nuclei and at high temperatures will continue to blossom. As the next generation of hadron experiments switch on, the lattice will deliver new predictions for the physics these machines will explore.

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