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Meson Spectroscopy from Lattice QCD

Abstract Some recent progress in using lattice QCD to perform first-principles calculations of the spectra of mesons is discussed. In particular, I highlight some new results on resonances, near-threshold states and related scattering phenomena—this is a theoretically and experimentally interesting area where we have made significant advances in the last few years.

1 Introduction

There has been a resurgence of interest in hadron spectroscopy in the last decade or so driven by the emergence of a wealth of high-quality experimental data. In particular, a number of unexpected states have been observed, e.g. various charmonium and bottomonium-like structures ("X, Y, Z's") and the charm-strange $D_{s0}(2317)$ [49,53], and there are also longer-standing puzzles such as the makeup of the light scalar mesons [55,57]. There has been a lot of theoretical work and speculation about their nature [6,50]—possibilities include tetraquarks (containing two quarks and two antiquarks), molecular states of hadrons, hadro-quarkonia and hybrid mesons (where the gluonic field is excited). States with exotic quantum numbers, i.e. those which cannot arise from solely a quark-antiquark pair, are particularly interesting because they are a smoking gun for physics beyond a model of a quark and an antiquark moving in a potential. For example, exotic spin (J), parity (P), charge-conjugation (C) combinations (e.g. $J^{PC} = 0^{--}, 0^{+-}, 1^{-+}, 2^{+-}$) or exotic flavour states (such as charged charmonium and bottomonium-like states).

Lattice Quantum Chromodynamics (Lattice QCD) is a method which enables first-principles computations of the spectra and properties of hadrons: four-dimensional space-time is discretised on a finite four-dimensional hypercubic lattice and the calculation of quantities in the path integral formulation then becomes an ordinary (but very large) integration problem. If a Euclidean (imaginary-time) space-time metric is used, the integrals can be evaluated effectively using importance-sampling Monte Carlo methods. The masses and other properties of hadrons then follow from analyzing correlation functions involving interpolating operators built from quark and gluon fields. Precise calculations of the spectrum of low-lying hadrons have long been benchmarks of lattice QCD (e.g. see Refs. [17,23]) but only relatively recently has there been significant progress in using lattice QCD to study excited hadrons.

Most hadrons are unstable with respect to the strong interaction and appear as resonances in the scattering of two or more lighter hadrons. In particular, many of the recently-observed puzzling states appear close to or above the threshold for strong decay—this must be taken into account in theoretical approaches and when analyzing experimental data. In recent years there have been significant advances in using lattice QCD to study resonances, near-threshold states and related scattering phenomena and I will discuss some highlights of this

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work in these proceedings. These calculations often use unphysically-heavy light quarks, corresponding to a pion mass, m_π, larger than the experiment pion mass and do not usually have a precise control over all the systematic uncertainties—details will not be given here and I refer to the references for further information.

After a brief description of some of the lattice QCD methodology in Sect. 2, in Sect. 3 I discuss calculations of the ρ resonance in $\pi\pi$ scattering. Some other channels relevant for light and strange mesons are discussed in Sect. 4 followed by heavy-light and charmonium-like resonances in Sect. 5. I conclude in Sect. 6 with an outlook.[1]

2 Excited Spectroscopy and Scattering in Lattice QCD

In lattice QCD the discrete spectrum of states in a finite volume follows from analyzing the dependence on the time separation, t, of two-point correlation functions,

$$C_{ij}(t) = \langle 0|\mathcal{O}_i(t)\mathcal{O}_j^\dagger(0)|0\rangle \,.$$

Here the interpolating operator $\mathcal{O}_j^\dagger(0)$ creates the states of interest at time 0 and $\mathcal{O}_i(t)$ annihilates them at time t—all states with the quantum numbers of the operators contribute to the correlation function. The variational method [5,43,44] enables excited states to be extracted reliably: a matrix of correlation functions involving a basis of N operators with the required quantum numbers is computed, $C_{ij}(t)$, where $i, j = 1, 2, \ldots, N$. A generalised eigenvalue problem,

$$C_{ij}(t)v_j^{(n)} = \lambda^{(n)}(t)C_{ij}(t_0)v_j^{(n)} \,,$$

is then solved for an appropriate reference time t_0. The time dependence of an eigenvalue, $\lambda^{(n)}(t)$, is related to the energy of the n'th state. The eigenvectors, $v_i^{(n)}$, are related to the operator-state overlaps, $Z_i^{(n)} \equiv \langle 0|\mathcal{O}_i|n\rangle$, which can be used to probe the structure of states and also give the optimal (in a variational sense) linear combination of operators to create the n'th state. To accurately determine the spectrum, the basis of operators must have a sufficiently wide range of structures to disentangle the various states that appear.

Although it is not possible to compute scattering properties directly in the Euclidean formulation of lattice QCD, the Lüscher method [40–42] and its extensions [7,8,16,25,27,32,38,39,62] allow indirect access to *infinite-volume* scattering amplitudes from *finite-volume* spectra, at least in the case of any number of two-hadron coupled channels. For elastic scattering, there is a one-to-one correspondence[2] between an energy level with centre-of-mass energy E_{cm} and the scattering phase shift δ at E_{cm} or equivalently the scattering t-matrix, $t(E_{\text{cm}})$. For coupled-channel two-hadron scattering, extracting an energy level E_{cm} constrains the scattering t-matrix at E_{cm} but this is in general an under-constrained problem. For example, with two coupled channels there are three energy-dependent parameters but only one constraint at each E_{cm}. One solution is to parameterize the E_{cm}-dependence of the t-matrix with a relatively small number of parameters—the spectrum resulting from this t-matrix is fit to the computed spectrum by varying these parameters. With the t-matrix in hand, its singularity structure can be investigated to determine the bound state and resonant content. The former corresponds to a pole below threshold on the real axis of the physical Riemann sheet, whereas the latter corresponds to poles away from the real axis on unphysical sheets.

3 The ρ Resonance in $\pi\pi$ Scattering

One of the simplest resonances, and the one that has attracted the most initial attention from lattice QCD [1, 2,24,33,56], is the $\rho(770)$ which appears in $\pi\pi$ scattering in $L = 1$ (P-wave) with $J^{PC} = 1^{--}$ and isospin $I = 1$; empirically the ρ decays almost entirely to $\pi\pi$ [53]. The results of a recent lattice QCD calculation [65] of the elastic $I = 1$ $\pi\pi$ scattering phase shift by the Hadron Spectrum Collaboration (HSC) are shown in Fig. 1. The computations have dynamical strange and degenerate up and down quarks, "$N_f = 2 + 1$", corresponding to $m_\pi \approx 240$ MeV, and used 469 gauge field configurations; the spatial (temporal) lattice extent is $L \sim 4$ fm ($T \sim 9$ fm). The plot also shows results from an earlier calculation with $m_\pi \approx 390$ MeV. A combination of

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[1] This talk was based on a similar talk I gave at the Confinement XII conference and this write-up is similar to Ref. [63].

[2] Ignoring complications arising from the mixing of partial waves due to the reduced symmetry of a finite box which we will not discuss here.
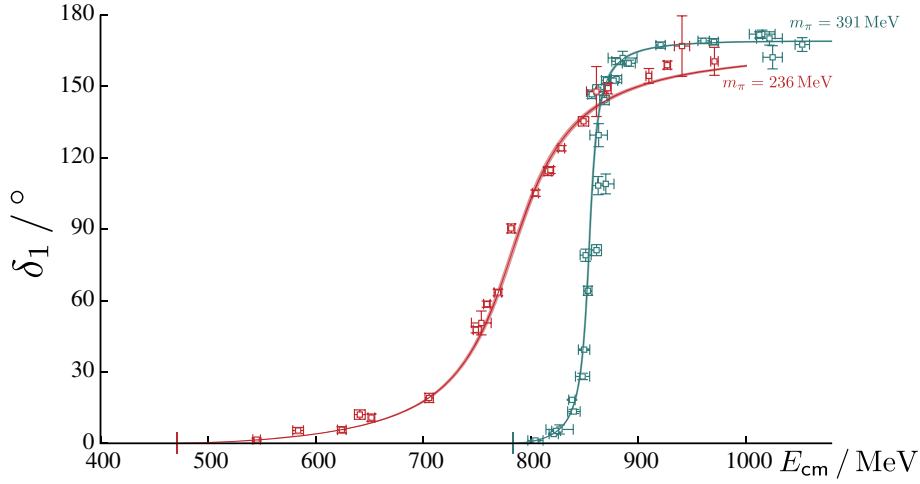
Fig. 1 From Ref. [65]. The P-wave $I = 1$ $\pi\pi$ elastic scattering phase shift plotted from $\pi\pi$ threshold to the inelastic $K\bar{K}$ threshold, from dynamical lattice QCD calculations with $m_\pi \approx 240$ MeV [65] and $m_\pi \approx 390$ MeV [20]. Points are from an energy-level by energy-level analysis and the curves are from a relativistic Breit Wigner parameterization as described in [65]

techniques were used to calculate extensive finite-volume spectra with high statistical precision: the distillation approach [54] was used to compute correlation matrices involving large bases of carefully-constructed fermion-bilinear [18,64] and multi-hadron interpolating operators [19,20] (between 10 and 37 operators in each of 12 different irreducible representations of the relevant symmetry group). The correlation matrices were analysed using the variational method and the resulting spectra, with 22 energy levels in the elastic region, enabled the energy dependence of the scattering phase shift to be mapped out in detail via the the Lüscher method.

The figure shows convincingly the rapid rise in the phase shift from 0° through 90° to 180° that is expected in the presence of a single isolated resonance. The resonance mass ($M_R = 790 \pm 2$ MeV) is not too different from experiment (775.49 ± 0.3 MeV) but the width is significantly smaller ($\Gamma = 87 \pm 2$ MeV compared to 149.1 ± 0.8 MeV experimentally). This is simply because the pion mass in this study is larger than the physical value and so the phase space for decay is reduced. The coupling, g, with the phase space factor divided out, defined by $\Gamma = \frac{g^2}{6\pi} \frac{p_{cm}^3}{M_R^2}$, where p_{cm} is the cm-frame scattering momentum, shows little dependence on m_π and is in reasonable agreement with experiment.

Ref. [65] also extends the analysis to the coupled-channel $\pi\pi$, $K\bar{K}$ energy region using 34 energy levels. Negligible coupling between the channels is found in the energy range explored.

The RQCD Collaboration have recently studied the ρ resonance with $m_\pi \approx 150$ MeV, close to the physical value [3]. However, in these "$N_f = 2$" computations only the light up and down quarks were dynamical whereas the strange quarks were quenched (not present in the sea). As can be seen from the comparison of different lattice QCD results in Ref. [3], the resonance mass is sensitive to whether or not the strange quarks are quenched (unlike g which appears to be insensitive to this and to m_π). The same effect was observed in recent $N_f = 2$ computations by Guo et. al. [26] with $m_\pi = 226$ and 315 MeV, as is discussed in Ref. [31].

Going beyond the resonance mass and width, recently the form factor of an unstable hadron has been calculated for the first time in lattice QCD [10,12]. From computations of the $\pi\pi \to \pi\gamma^*$ transition amplitude, the resonant $\rho \to \pi\gamma^*$ transition form factor and the radiative decay width were extracted.

4 Other Scattering Channels Relevant for Light and Strange Mesons

Moving to other scattering channels relevant for light and strange mesons, using a similar setup to that described above with $m_\pi \approx 390$ MeV and three lattice volumes, the HSC investigated coupled-channel $K\pi$, $K\eta$ scattering with $I = 1/2$ [21,66], the first study of coupled-channel scattering on the lattice. In total 73 energy levels were extracted and these enabled the energy dependence of the scattering matrix to be mapped out. A number of interesting features emerged including a broad $J^P = 0^+$ scalar resonance in S-wave [c.f. the $K_0^*(1430)$], a P-wave 1^- vector bound state [c.f. the $K^*(892)$], a narrow 2^+ tensor resonance in D-wave [c.f. the $K_2^*(1430)$] and a suggestion that the κ, a scalar resonance with physical-mass light quarks, corresponds to a virtual bound
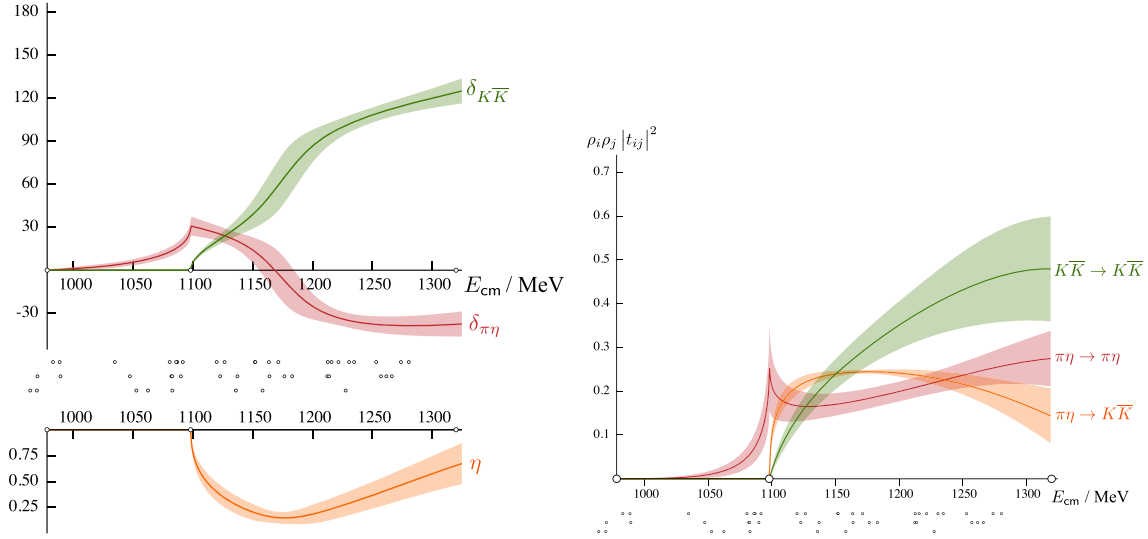
Fig. 2 From Ref. [22]. The *S*-wave $I = 1\,\pi\eta$, $K\bar{K}$ coupled-channel scattering amplitudes ($J^{PC} = 0^{++}$) from a lattice calculation with $m_\pi \approx 390\,\text{MeV}$. *Left panel* shows phase shifts, δ_i, and inelasticity, η, and the *right panel* shows quantities proportional to cross sections. *Open circles* on the *horizontal axis* indicate $\pi\eta$, $K\bar{K}$ and $\pi\eta'$ thresholds. The *dots* below the figures show energy levels used to constrain the amplitudes

state[3] when $m_\pi \approx 390\,\text{MeV}$. The latter observation is consistent with how the κ behaves in unitarised chiral perturbation theory as the π mass is varied [48]. The exotic-flavour $I = 3/2\,K\pi$ channel was also studied.

The RQCD Collaboration have studied *P*-wave elastic $K\pi$ scattering in a $N_f = 2$ calculation with light quarks corresponding to $m_\pi \approx 150\,\text{MeV}$ [3]. They find a vector resonance, consistent with the expectation that the bound state found by the HSC with $m_\pi \approx 390\,\text{MeV}$ becomes a resonance as the light-quark masses are reduced.

The HSC have also studied coupled $\pi\eta$, $K\bar{K}$, $\pi\eta'$ scattering in $I = 1$ with $m_\pi \approx 390\,\text{MeV}$ on three lattice volumes: $L \approx 1.9$, 2.4 and 2.9 fm using respectively 479, 603 and 553 configurations [22]. The *S*-wave coupled-channel $\pi\eta$, $K\bar{K}$ scattering amplitudes constrained by 47 energy levels are shown in Fig. 2. Here the phase shifts, δ_i, and inelasticity, η, are defined in terms of elements of the *t*-matrix,[4]

$$t_{ij} = \begin{cases} \frac{\eta\, e^{2i\delta_i} - 1}{2i\,\rho_i} & (i = j) \\ \frac{\sqrt{1-\eta^2}\, e^{i(\delta_i + \delta_j)}}{2\sqrt{\rho_i\,\rho_j}} & (i \neq j) \end{cases} \tag{1}$$

where i, j label scattering channels and $\rho_i = 2\,p_{\text{cm},i}/E_{\text{cm}}$ is the phase space factor for channel i. The amplitudes show a cusp-like enhancement in $\pi\eta \to \pi\eta$ near $K\bar{K}$ threshold and a rapid turn on of amplitudes to $K\bar{K}$. This behaviour originates from an $a_0(980)$-like resonance which is strongly coupled to both $\pi\eta$ and $K\bar{K}$—the first strongly-coupled meson-meson scattering system extracted in a lattice QCD calculation. The corresponding pole appears on a single unphysical Riemann sheet, unlike a canonical two-channel resonance where poles would be expected on two unphysical sheets, and this may be a sign that the state binds through the long-range interaction between a pair of mesons. Ref. [22] also presents results with the $\pi\eta'$ channel included and considers *D*-wave scattering where a narrow tensor resonance is found.

Using a similar setup again, the HSC have recently determined the elastic $\pi\pi$ *S*-wave $I = 0$ scattering phase shift for the first time in a lattice QCD computation [11]. Two different light quark masses were used corresponding to $m_\pi \approx 240\,\text{MeV}$ and 390 MeV. For the lighter mass the scattering amplitude has a pole on the unphysical Riemann sheet with a large imaginary part, corresponding to a broad resonance, in qualitative agreement with experiment. At the heavier mass a pole is found below threshold on the real axis of the physical sheet, corresponding to a bound state. Work is ongoing to extend this calculation into the coupled-channel region above $K\bar{K}$ threshold where a $f_0(980)$-like resonance is expected, the final component of a study of the scalar meson nonet using lattice QCD.

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[3] A pole below threshold on the real axis of an unphysical Riemann sheet.

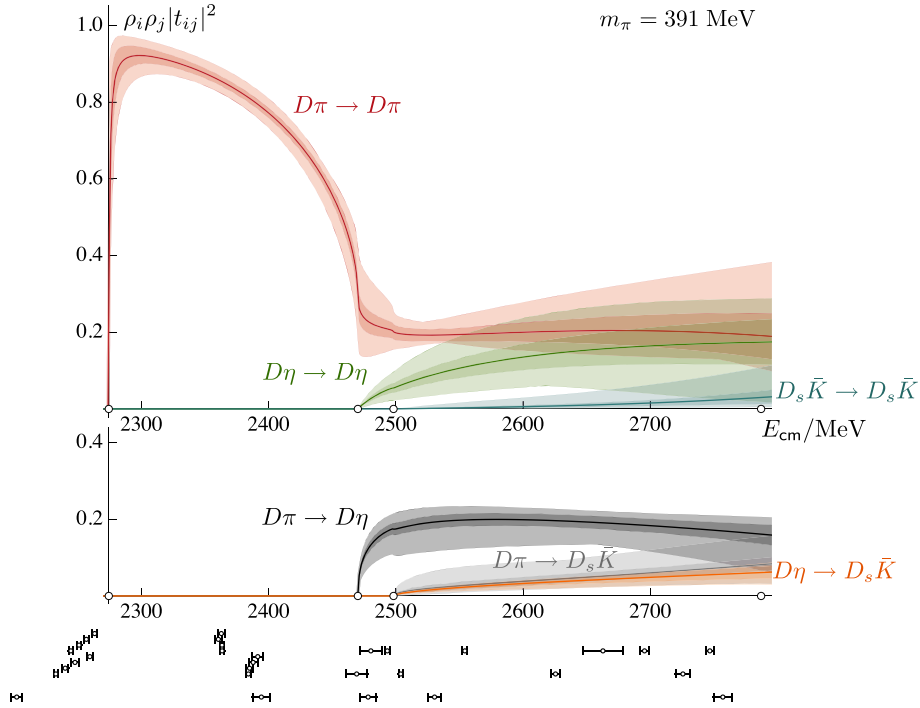[4] Note that $\eta = 1$ would indicate no coupling between channels.

Fig. 3 From Ref. [47]. The S-wave $I = 1/2$ $D\pi$, $D\eta$, $D_s\bar{K}$ coupled-channel scattering amplitudes from a lattice calculation with $m_\pi \approx 390$ MeV. Quantities proportional to the diagonal (off-diagonal) cross sections are plotted in the *top* (*bottom*) panel. *Open circles* on the *horizontal axes* indicate $D\pi$, $D\eta$, $D_s\bar{K}$ and $D^*\pi\pi$ thresholds. The *black points* below the plot show energy levels used to constrain the amplitudes

5 Heavy-Light and Charmonium-Like Resonances

Turning to channels relevant for heavy-light and quarkonium mesons, we begin with the charm-light (D) and charm-strange (D_s) sectors. The $D^*_{s0}(2317)$ and $D_{s1}(2460)$ present a long standing-puzzle: they were expected to be broad resonances, like the analogous $D^*_0(2400)$ and $D_1(2430)$ mesons, but were observed to be narrow states below the respective DK and D^*K thresholds [53]. Some early lattice calculations of elastic $D^*\pi$ and D^*K scattering can be found in Refs. [34,45,46].

The HSC have recently investigated $I = 1/2$ coupled-channel $D\pi$, $D\eta$, $D_s\bar{K}$ scattering with light-quark masses corresponding to $m_\pi \approx 390$ MeV on three lattice volumes: $L \approx 1.9$, 2.4 and 2.9 fm using respectively 479, 603 and 553 configurations [47]. Figure 3 shows the S-wave scattering amplitudes constrained by 47 energy levels—the broad feature in the $D\pi \rightarrow D\pi$ amplitude is associated with a $J^P = 0^+$ bound state very close to $D\pi$ threshold. Although, by contrast, the associated experimental state, $D^*_0(2400)$, is a resonance, they are similar in that they influence a broad energy range and couple predominantly to $D\pi$. The pole position lies between what is observed experimentally for the $D^*_{s0}(2317)$ and the $D^*_0(2400)$. In P-wave ($J^P = 1^-$), a deeply bound state was found and can be compared to the experimentally observed narrow resonance, $D^*(2007)$. A narrow 2^+ resonance was found in D-wave. The $I = 3/2$ elastic $D\pi$ channel was also investigated and a weakly repulsive interaction found in S-wave.

In the charmonium sector there have been a number of lattice QCD investigations [13–15,35,51,52,59–61] and there have been a couple in the bottom sector [36,37]. However, the calculations are somewhat less advanced than in the other sectors and studies have generally been exploratory, inconclusive or have not determined the phenomena in detail or robustly, and I will not discuss these here. More robust and detailed computations are required—one challenge is the number of channels to which a resonance can potentially couple and all these channels need to be considered in the calculations.

6 Conclusions

I have highlighted some recent lattice QCD studies of resonances and related scattering phenomena, an area which has seen significant advances in the last few years and where prospects for further progress are very

good. Although it may be seen as a disadvantage that many of the computations used unphysically-heavy light quarks, corresponding to m_π larger than the experimental value, and so cannot be compared quantitatively to experiment, it turns out that studying how states evolve as m_π varies is a useful tool in discerning their nature. As we go further up in the spectrum and undertake calculations with m_π closer to the physical value, in general calculations become more difficult because additional channels become relevant and, in particular, channels involving more than two hadrons open up. Work on the formalism for such situations is ongoing [4,9,28–30,58].

To stringently probe the structure of states we must go beyond solely computing masses and consider other properties of hadrons such as form factors and related quantities. There are also good prospects here with the recent appearance of the first lattice QCD calculation of a transition form factor involving a resonance [10,12].

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