Multi-hadron states in Lattice QCD spectroscopy

J. Foley*, J. Bulava†, K.J. Juge**, C. Morningstar*, M. Peardon‡ and C.H. Wong*

*Dept. of Physics, Carnegie Mellon University, Pittsburgh, PA 15213, USA
†NIC, DESY, Platanenallee 6, 15738 Zeuthen, Germany
**Dept. of Physics, University of the Pacific, Stockton, CA 95211, USA
‡School of Mathematics, Trinity College, Dublin 2, Ireland

Abstract. The ability to reliably measure the energy of an excited hadron in Lattice QCD simulations hinges on the accurate determination of all lower-lying energies in the same symmetry channel. These include not only single-particle energies, but also the energies of multi-hadron states. This talk deals with the determination of multi-hadron energies in Lattice QCD. The group-theoretical derivation of lattice interpolating operators that couple optimally to multi-hadron states is described. We briefly discuss recent algorithmic developments which allow for the efficient implementation of these operators in software, and present numerical results from the Hadron Spectrum Collaboration.

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A stated aim of the Hadron Spectrum Collaboration is the determination of the low-lying hadron spectra across all flavor sectors for pion masses approaching the physical value. The ability to reliably extract a hadronic energy level from a lattice QCD simulation hinges on the accurate determination of all lower-lying energies in the same symmetry channel. Thus, a critical component of a spectroscopy calculation is the identification of a large and diverse set of interpolating operators that couple to all low-lying states. The stationary-state energies accessible to Monte Carlo studies receive contributions not only from single-particle states, but also from multi-hadron excitations. Considerable effort has already gone into the identification of an optimal set of single-particle interpolators [1, 2], and initial scans of the baryon, isovector meson, and kaon sectors have been promising [3]. However, a complete analysis of the spectrum must include interpolating operators specifically designed to couple to multi-hadrons. The Wick contraction of multi-hadron operators can produce diagrams which contain quark lines that begin and end on a single time slice. In studies which use only single-particle operators, such diagrams are confined to the flavor-singlet meson channels. Until recently, precision measurements of the contributions from these diagrams to lattice correlation functions were prohibitively expensive. Fortunately, due to recent advances in lattice algorithms [3, 4], it is now feasible to accurately compute the contributions from these diagrams, even on larger lattice volumes, and a comprehensive study of the spectrum including the light isosinglet meson sectors and multi-particle states appears within reach.

Group-theoretical construction of multi-hadron operators

The multi-hadron operators in question are formed by combining single-particle operators (e.g. fermion bilinears in the meson sector) to form composite interpolators, which are expected to couple well to multi-particle states. To facilitate the extraction and identification of energies, interpolating operators are constructed to transform irreducibly under the lattice symmetry group. As in the continuum, operators project onto definite flavor sectors and meson interpolators have definite G-parity.

The lattice space group is the semi-direct product of the group of spatial lattice translations and the cubic point group $O_h$. Irreducible representations (irreps) of the space group are conventionally labeled by a momentum vector $\mathbf{k}$ and a second label denoting irreps of the little group of $\mathbf{k}$. In our numerical studies, we enforce periodic boundary conditions in the spatial directions. Hence, the components of the momentum vector $\mathbf{k}$ are quantized in units of $2\pi/L_s$, where $L_s$ is the spatial extent of the lattice.

Hadron rest energies can be classified according to the $\mathbf{k} = 0$ space-group irreps. The corresponding little group is $O_h$, which has ten single-valued irreps. Following Mulliken convention, these are labeled $A_{1g}/u$, $A_{2g}/u$, $E_{g}/u$, $T_{1g}/u$, $T_{2g}/u$, $A_{1u}/g$, $A_{2u}/g$, $E_{u}/g$, $T_{1u}/g$, $T_{2u}/g$. Our simulations use a Wilson-type quark action and are performed in the isospin limit: $m_u = m_d$. 

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amongst themselves under the action of the little group (or, in the case of baryon operators, the corresponding double group) generates a representation of the little group, is defined to be a zero-displacement operator: \( \tilde{\chi} \), and

\[
T^i_\varphi \rightarrow A_1 \oplus B_1
\]

where the subscripts \( g \) and \( u \) denote even- (gerade) and odd- (ungerade) representations respectively. Baryons at rest are classified according to the fermionic, or double-valued, irreps of \( O_h \). These are obtained from the single-valued irreps of the double cubic group \( O^D_4 \). The double group has sixteen single-valued irreps. Of these, ten are identical to the single-valued irreps of \( O_h \), while the remaining six representations, \( G_{13g/u}, G_{2g/u}, H_{g/u} \), form double-valued irreps of \( O_h \). The simplest accessible multi-hadrons are made up of two single-particle states at rest. However, on large spatial lattice volumes, most of the low-lying multi-hadron states are expected to consist of hadrons with non-zero relative momenta. To date, we have analyzed the finite-momentum space-group irreps needed to construct operators for the lowest-lying multi-hadron states. These include space-group irreps that correspond to momenta directed along lattice axes, such as \( \mathbf{k} = (0, 0, k) \), as well as momenta in planar-diagonal and cubic directions, for example, \( \mathbf{k} = (0, k, k) \) and \( \mathbf{k} = (k, k, k) \). The corresponding little groups are the point groups \( C_{4v}, C_{2v}, \) and \( C_{3v} \), respectively. \( C_{4v} \) has five single-valued irreducible representations and two fermionic irreps, \( C_{3v} \) has three single-valued irreps and three fermionic irreps, and \( C_{2v} \) has four single-valued irreducible representations and just one fermionic irrep. Table 1 contains the decomposition of the single-valued irreps of \( O_h \) subduced onto \( C_{4v} \) into irreps of \( C_{4v} \). \( A_1, A_2, B_1 \) and \( B_2 \) are one-dimensional irreps, and \( E \) is two-dimensional. The decompositions of the subduced representations show, for example, that the finite-momentum operators which transform according to the \( A_2 \) representation of \( C_{4v} \) project onto states with rest energies in the \( A_1, E \) and \( T^i_\varphi \) irreps of \( O_h \). Space-group irreps for the lattice momentum vector \( \mathbf{k} \) can be induced from the unitary irreps of the little group of \( \mathbf{k} \). The dimensions of these space-group representations are equal to the dimension of the star of \( \mathbf{k} \) (the set of distinct momentum vectors obtained by applying \( O_h \) to \( \mathbf{k} \)) times the dimensions of the little group irreps. Hence, the space-group irrep with momentum \((0, 0, k)\) induced from the \( A_2 \) irrep of \( C_{4v} \) is six-dimensional. A comprehensive discussion of the group theory for finite-momentum and multi-particle states can be found in Refs. [5, 6], whose results for the irreps which arise in this study we have independently verified.

To obtain a complete set of basis operators for the space-group irrep characterized by the lattice momentum \( \mathbf{k} \) and the little group irrep \( \Lambda \), we first identify a set of operators with definite momentum \( \mathbf{k} \) that transform amongst themselves according to the irrep \( \Lambda \) under the little group of \( \mathbf{k} \). These form a subset of operators in the basis of the space-group irrep. The other basis operators are obtained by applying rotations to this initial operator set. To identify irreducible single-particle operators for the lattice little groups, we have adapted the operator construction algorithm described in Ref. [1]. Irreducible operators are formed from linear superpositions of more basic gauge-invariant operators, termed elemental operators. The general expression for the single-particle elemental operators from which irreducible meson annihilation operators are constructed is

\[
\phi_{\alpha\beta,i,j,k}(t,\mathbf{k}) = \sum_x e^{-i\mathbf{k}\cdot\mathbf{x}} \left( \tilde{\chi}_\alpha \tilde{D}_i^{(p)\dagger}(x,t) \left( \tilde{D}_j^{(p)}(x) \tilde{\psi}_\beta \right)(x,t) \right),
\]

where \( \tilde{\chi}(x,t) \) and \( \tilde{\psi}(x,t) \) represent smeared lattice quark fields with flavor indices \( \alpha \) and \( \beta \). \( \tilde{D}_i^{(p)} \) is a \( p \)-link quark-field displacement operator: \( \tilde{D}_i^{(p)} \rho(x,t) = \tilde{U}_i(x,t) \ldots \tilde{U}_i(x+(p-1)i,t) \rho(x+pi,t) \), for \( i = \pm 1, \pm 2, \pm 3 \), where \( \tilde{U} \) are stout-smeared link variables. Our labeling convention also permits \( i = 0 \), where \( \tilde{D}_0^{(p)} \) is defined to be a zero-displacement operator: \( \tilde{D}_0^{(p)} \rho(x,t) = \rho(x,t). \) A set of elemental operators which transform amongst themselves under the action of the little group \( W \), which is in general reducible. Given the unitary irrep matrices \( \Gamma^\lambda \), one can define a projection matrix

\[
P^{\lambda\bar{\lambda}} = \frac{d_A}{N_D} \sum_{gd} \Gamma^\lambda_{gd}(gd) W(gd),
\]
the order of the double group. Applied to the elementals, this projection matrix returns a set of operators that transform according to the row symmetry channel, a slight horizontal offset distinguishes energies with different relative momenta. The figure suggests that, even where \( \Delta \) is approximately true for small lattice momenta. While the results of this qualitative analysis must be treated with caution, it does provide a ball-park estimate for multi-hadron thresholds and a first approximation for the density of multi-hadron states in each symmetry channel.

Having performed a first scan of the spectrum using single-particle operators, we get a rough estimate for the number and types of multi-hadron operators required in each symmetry channel from the spectrum of states consisting of multiple non-interacting hadrons. Figure 1 shows results for systems of two non-interacting isovector mesons on a lattice volume of approximately \((1.9 \text{ fm})^3\). The energies of the moving single-particle states were calculated assuming zero total momentum. The meson rest masses were obtained from low-statistics measurements with a 380 MeV pion on a target of multiple non-interacting hadrons. Figure 1 shows results for systems of two non-interacting isovector mesons with \( \Lambda^4 \) representations of \( O_h \). In analogy to Eq. 2, we form projection matrices to get the required irreducible multi-hadron interpolating operators.

By varying the displacement combinations in Eq. 1, a large number of operator bases can be generated. However, these bases may include operators that have little overlap onto the states of interest, as well as sets of operators that all couple strongly to the same state. Hence, a rigorous pruning procedure has been applied to the zero-momentum single-particle operators to identify a manageable subset of operators that couple to different low-lying states. We expect that the best multi-hadron operators are formed by combining single-particle operators that couple well to the constitutent hadrons. Therefore, we apply the same rigorous selection process to the finite-momentum single-particle operators. Operator pruning is implemented as follows: first, we compute Euclidean-time correlation functions for a sample operator in each basis set in low-statistics Monte Carlo runs. The interpolating operators that produce the largest statistical errors are identified and discarded. From the remaining operator set, smaller subsets are used to compute the normalized correlation matrices \( \tilde{C}_{ij}(t) = C_{ij}(t)/\sqrt{C_{ii}(t)C_{jj}(t)} \), with \( C_{ij}(t) = \langle O_i(t)\bar{O}_j(0) \rangle \). The subscripts \( i \) and \( j \) distinguish different operators transforming according to a single row of a particular lattice irrep. We then select a set of operators that has a well-conditioned correlator matrix at small values of \( t \). A condition number close to unity indicates that the operators are almost orthogonal and therefore couple to different states.

In order to access the most important multi-hadron states on our target lattice volumes, we estimate that we require moving single-particle operators corresponding to the lowest two to four energy levels in most irreps. Our studies
FIGURE 2. Effective masses for the three lowest-lying states in a channel containing moving $\pi$ and $a$ mesons. The meson momentum is $L_s k/(2\pi) = (0, 0, 1)$, and the figure shows results for the $A_2$ irrep of the little group $C_{4v}$. The resulting energy values are consistent with measurements of the ground-state rest masses in the $A_{1u}$, $E_u$ and $T_{1g}$ irreps of $O_h$. These measurements were performed on 93 configurations using a set of six single-site and singly-displaced interpolating operators which had been selected using the pruning procedure outlined in the text. For clarity, a fourth level, which also exhibits a reasonable plateau, has been omitted. The operators employed here will feature in the set of single-particle operators used in the construction of composite, multi-hadron operators.

suggest that all the required operators can be formed from linear superpositions of local, or single-site, elementals and elemental operators containing a straight-line displacement in a single direction. Figure 2 shows effective masses for single-particle isovector, negative G-parity meson operators with the momentum $L_s k/(2\pi) = (0, 0, 1)$. These are results for the $A_2$ irrep of $C_{4v}$, which includes the energy of a pion in flight. The effective masses were extracted from a variational analysis of a $6 \times 6$ correlator matrix on 93 configurations. There is a discernible plateau in each of the three lowest-lying effective masses, although due to low statistics the third level is somewhat noisy, and we have verified that the fitted energies are consistent with ground-state rest-mass measurements in the $A_{1u}$, $E_u$ and $T_{1g}$ irreps. The fourth level, which is not included in the figure, also exhibits an acceptable plateau. However, it overlaps the third level within errors, and has been omitted for the sake of clarity.

Computing multi-hadron correlators

Finally, we turn to the recent algorithmic advances which facilitate the accurate evaluation of the required multi-hadron correlators on our target lattice volumes. We present only a brief outline of progress in this area and refer the reader to Refs. [3, 4] for more detailed descriptions.

The first major development was the realization that one does not need to compute the quark-propagator components directly in order to evaluate hadron correlation functions; instead, only the matrix elements of the propagator between eigenvectors of the quark-field smearing operator are required. Since the smearing operator acts to suppress excited-state contamination, only a subset of smearing eigenvectors that preserves the important long-distance physics needs to be included in the calculation. These ideas form the basis for a technique for computing correlation functions, known as distillation. A simple but effective implementation of this method involves defining the quark-field smearing operator to be a gauge-covariant laplacian with a hard cutoff imposed on high-momentum modes. This defines the Laplacian-Heaviside, or Laph, smearing scheme.

The distillation algorithm makes it feasible to compute the correlation functions of interest on smaller lattice volumes. However, the number of smearing eigenvectors needed to capture the essential low-energy physics increases linearly with the spatial volume, reducing the efficacy of this method on larger lattices. More recently, a new method for evaluating correlation functions, which combines distillation with a stochastic estimator, has been developed. The new algorithm utilizes noise dilution [7] to reduce the variance in correlation functions, and exact distillation is recovered in the maximal dilution limit. In test studies, this method has consistently produced correlators with variances that are very close to the gauge-noise limit, but at considerably lower computational cost than exact distillation. An example of
FIGURE 3. The left-hand side shows a quark-line diagram that arises in the evaluation of a two-pion correlation function. The plot on the right is the contribution of this diagram to a correlator obtained using the stochastic Laph method described in the text. This test measurement was performed on 99 gauge-field configurations generated at the three-flavor point on a $12^3 \times 96$ lattice, and the correlator was averaged over four source times. The operator used was designed to project onto two pions at rest. The dilution schemes for the quark lines connecting the source and sink time slices and for the quark lines restricted to a single time slice, which are given in parentheses, are explained in Ref. [3].

results obtained for the box-diagram contribution to a two-pion correlation function using the stochastic Laph scheme is shown in figure 3.

Conclusions

Recent progress in lattice algorithms, combined with advances in computer infrastructure, has made it possible to incorporate explicit multi-hadron operators into our spectroscopy calculations. Our current focus is the construction of sets of multi-hadron operators for each lattice symmetry channel. To that end, we have put considerable effort into identifying good single-particle operators for hadrons with non-zero momenta. Pruning of the finite-momentum isovector meson operators is complete, and operator pruning in other meson and baryon sectors is underway. We plan to begin measurements using the resulting operator set in the coming months.

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