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Partial-wave and helicity operators for the scattering of two hadrons in lattice QCD

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Partial-wave operators for lattice QCD are developed in order to facilitate the identification of the spins of two-hadron scattering states corresponding to zero total momentum. Taking the periodic boundary conditions for lattice states into account, orthogonal sets of partial-wave operators for orbital angular momentum are identified. When combined with the intrinsic spins of the hadrons, orthogonal sets of parent operators for total angular momentum J and projection M are obtained. The parent operators are subduced to irreducible representations of the octahedral group in order to obtain descendant operators for use in lattice calculations. The descendant operators retain orthogonality with respect to J . The spin of a state can be identified by the spin of parent operators that dominate creation of the state. For nonzero total momentum, operators are developed for a range of helicities and they are subduced to irreducible representations corresponding to the different directions of total momentum. Sets of operators that include a sufficient range of helicities allow identification of spin J when a state couples to operators with helicities less than or equal to J , but not to operators with higher helicities.

I. INTRODUCTION

Lattice operators subduced from irreducible representations (irreps) of group, $SU(2)$, to irreps of the octahedral group, O_h , have been used to determine the spins as well as the energies of single-hadron states in lattice QCD. Recent works used such operators at zero momentum to determine the excited-state spectroscopy of mesons, based on two-quark operators [1], and baryons, based on three-quark operators [2].

Subduction from $SU(2)$ associates each lattice operator with values of J and M , where J is the total angular momentum and M is its projection along the z-axis.

Using operators that are smeared as in Ref. [3], rotational invariance is realized approximately for bound states that fit within the lattice volume, i.e., there is an approximate orthogonality between operators subduced from different values of J and M . Using a different method to smear operators over many lattice sites, Ref. [4], finds that the leading rotational-symmetry violating contributions from the finite lattice spacing, a , are suppressed by $\alpha_s a^2$ as $a \rightarrow 0$, where $\alpha_s = g_s^2/(4\pi)$ and g_s is the strong coupling constant.

The analyses of Refs. [1, 2] obtain lattice correlation matrices that are approximately block-diagonal, with each block corresponding to a group of operators subduced from the same value of J . Lattice excited states are found to be created predominantly by operators subduced from a single value of J . That identifies the spins of excited states created by single-hadron operators.

However, multiparticle operators must be considered in view of the fact that excited states of hadrons show up as resonances in the scattering of two hadrons. For example, the Δ baryon, is a wide resonance in πN scattering for spin $J = \frac{3}{2}$ and isospin $I = \frac{3}{2}$ [5]. The quantum numbers

match those of a three-quark state in the quark model, or in lattice QCD.

In a well-known paper, Lüscher[6] has shown how phase shifts for the scattering of two hadrons can be extracted from lattice QCD. The Lüscher method has been extended to systems with nonzero total momentum, unequal masses, coupled channels and intrinsic spins [7–13]. It has been applied to coupled-channel scattering in Refs. [14–16].

In principle, the spins of scattering states can be identified by matching i), the pattern of approximately degenerate states found in lattice irreps with ii), the pattern of subductions of a given spin to the irreps of the lattice symmetry group. However, the combination of accidental degeneracies and statistical uncertainties can give ambiguous patterns of lattice states, e.g., the assignment of two or more values of J may be compatible with them.

In this work, sets of lattice operators based on partial waves are developed for the scattering of two hadrons with zero total momentum, and operators based on helicity are developed for nonzero total momentum. The operators are designed to facilitate the identification of the spin in calculations of phase shifts.

Periodic partial waves and their orthogonality properties are discussed in Section II. Operators based on partial waves are defined in Section III. Using the partial-wave operators, intrinsic spins are included to obtain operators that create lattice states at zero total momentum corresponding to total spin J in Sec. IV. These are called parent operators. They are subduced to irreps of O_h for use in lattice QCD. The subduced operators are called descendant operators. Sets of mutually orthogonal parent operators are identified that correspond to a range of different total spins.

Section IV C develops parent operators based on helicity for nonzero total momenta. These are subduced to lattice irrep operators, the descendant operators, that involve combinations of $\pm\lambda$. [17] Sets of mutually orthog-

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onal operators are identified that correspond to a range of different helicities. Section V provides a brief summary of the work.

II. PERIODIC PARTIAL WAVES

Periodic boundary conditions in spatial directions apply to quark propagators on a lattice. Thus, lattice states created by quark-field operators generally are periodic in spatial directions. In spectroscopy based on single-hadron operators, the effects of the boundary conditions are reduced if the operators create states that fit approximately within the lattice volume. Scattering states are affected strongly by periodic boundary conditions.

Generally, scattering calculations incorporate the periodic boundary conditions by using operators that involve combinations of plane-waves with momenta restricted to $\mathbf{k} = \frac{2\pi\mathbf{n}}{L}$, where L is dimension of the lattice in units of the lattice spacing and \mathbf{n} is a vector with integer components along the axes of the lattice.

Partial waves, $f_{\ell,m}(\mathbf{x}) = j_\ell(k|\mathbf{x}|)Y_{\ell,m}(\hat{x})$, involving momenta $k = \frac{2\pi|\mathbf{n}|}{L}$, no longer obey the same periodicity as the plane waves. However, partial-wave operators create lattice states that must obey the periodic boundary conditions. Such lattice states can be discussed in terms of periodic partial waves that are constructed from the formula,

$$[f_{\ell,m}(\mathbf{x})]^{(per)} = C \sum_{\mathbf{n}} f_{\ell,m}(\mathbf{x} + \mathbf{n}L). \quad (1)$$

The integer-valued components of \mathbf{n} are limited by $-N \leq n_i \leq N$ for $i = 1$ to 3 and the factor, $C = (2N+1)^{-3}$, provides a normalization. In the limit $N \rightarrow \infty$, the function $[f_{\ell,m}(\mathbf{x})]^{(per)}$ is periodic,

$$[f_{\ell,m}(\mathbf{x} + \mathbf{n}L)]^{(per)} = [f_{\ell,m}(\mathbf{x})]^{(per)}, \quad (2)$$

where \mathbf{n} is any vector with integer components.

Periodic partial waves for orbital angular momentum, ℓ , and projection along the z-direction, m , have restricted orthogonality. Consider the overlap matrix,

$$O_{\ell',m';\ell,m} = \int d^3x \quad [j_{\ell'}(k|\mathbf{x}|)Y_{\ell',m'}^\dagger(\hat{x})]^{(per)} \times [j_\ell(k|\mathbf{x}|)Y_{\ell,m}(\hat{x})]^{(per)}. \quad (3)$$

The integration symbol in Eq. (3) should be read as a sum over $(L+1)^3$ lattice points that are inside or on the boundaries of the L^3 lattice volume.

In order to make diagonal overlaps equal to unity, define normalization factors and construct the normalized matrix of overlaps as follows,

$$N_{\ell,m} = \sqrt{O_{\ell,m;\ell,m}}, \quad Z_{\ell',m';\ell,m} = \frac{1}{N_{\ell',m'}N_{\ell,m}} O_{\ell',m';\ell,m}. \quad (4)$$

TABLE I: Pattern of even-parity matrix elements $Z_{\ell',m';\ell,m}$: **1** for diagonal elements, blank for zero elements and **x** for large off-diagonal elements. The top row shows the ℓ, m indices and the left column shows the ℓ', m' indices.

	0,0	2,2	2,1	2,0	2,-1	2,-2	4,4	4,3	4,2	4,1	4,0	4,-1	4,-2	4,-3	4,-4
0,0	1						x				x				x
2,2		1				x			x				x		
2,1			1							x					x
2,0				1			x				x				x
2,-1					1			x				x			
2,-2		x				1			x				x		
4,4	x			x			1				x				x
4,3					x			1				x			
4,2		x				x			1				x		
4,1			x							1				x	
4,0	x			x			x				1				x
4,-1					x			x				1			
4,-2		x				x			x				1		
4,-3			x							x				1	
4,-4	x			x			x				x				1

Numerical calculations for finite lattice spacings show that,

$$Z_{\ell',m';\ell,m} = 0, \quad \text{if } \ell' \neq \ell \pmod{2} \text{ and } m' \neq m \pmod{4}, \quad (5)$$

holds to high precision. The pattern of zero elements in Eq. (5) is the same as for Lüscher's matrix, $\mathcal{M}_{\ell',m';\ell,m}$, that is central to the method for determining phase shifts. As shown in Ref. [6], the zeroes are exact because of cubic symmetry for a finite box with no discretization. For a discrete lattice spacing, the orthogonality is found in Appendix A not to depend on the momentum in the spherical Bessel functions, or on the difference between scattering wave functions and spherical Bessel functions. In a lattice QCD calculation, the orthogonality should be realized approximately after averaging over gauge configurations.

There is one exception to the $\text{mod } 2$ in Eq. (5): overlaps of periodic partial waves involving $\ell', \ell = 0, 2$, or $2, 0$, are zero. Thus, the $\ell = 0, 1$ and 2 periodic partial waves are orthogonal to one another, except for the $m = \pm 2$ values that are affected by the $\text{mod } 4$ rule, i.e., the $\langle \ell', m' | \ell, m \rangle = \langle 2, 2 | 2, -2 \rangle$ and $\langle 2, -2 | 2, 2 \rangle$ overlaps are of order 1.

Periodic partial waves of opposite parities are orthogonal. Tables I and II show the patterns of orthogonality of $Z_{\ell',m';\ell,m}$ for partial waves of the same parity, using a blank to indicate a matrix element that is zero, **1** to indicate a diagonal element and *x* to indicate a large off-diagonal element.

Periodic operators with $\ell = 0, 1$ and 2 unavoidably couple to states of higher ℓ because of the cubic symmetry. For example, a periodic operator for angular momentum $\ell = 1$ couples with $\ell = 3, 5, \dots$ states. Thus, assuming

TABLE II: Pattern of odd-parity matrix elements $Z_{\ell', m'; \ell, m}$. Symbols are the same as in Table I. The top row shows the ℓ, m indices and the left column shows the ℓ', m' indices.

	1,1	1,0	1,-1	3,3	3,2	3,1	3,0	3,-1	3,-2	3,-3
1,1	1					x				x
1,0		1					x			
1,-1			1	x				x		
3,3			x	1				x		
3,2					1				x	
3,1	x					1				x
3,0		x					1			
3,-1			x	x				1		
3,-2					x				1	
3,-3	x					x				1

that $\ell \geq 5$ can be neglected, there is a need to distinguish which states are $\ell = 1$ versus $\ell = 3$. The blank elements in Tables I and II show that it is possible to construct periodic operators for $\ell = 3$ that are orthogonal to those for $\ell = 1$. For example, $\ell, m = 3, 2$ is orthogonal to $\ell, m = 1, 1, 1, 0$ and $1, -1$. Thus, including a tracer operator that couples to states with $\ell \geq 3$ but does not couple to $\ell = 1$ states, provides a means to distinguish lattice states involving $\ell = 3$ from those involving $\ell = 1$. Similarly, states involving $\ell = 4$ can be distinguished from ones involving $\ell = 2$ by use of suitable tracer operators. That provides the motivation for the use of partial-wave operators corresponding to distinct values of ℓ and m .

III. PLANE-WAVE, LATTICE IRREP AND PARTIAL-WAVE OPERATORS

A. Plane-wave operators

Consider two point-like fields for distinct, scalar mesons that are labeled by indices 1 and 2.

The field operator for a single scalar meson at $t=0$, keeping only the creation part, is

$$m_1^\dagger(\mathbf{x}, 0) = \frac{1}{(2\pi)^{3/2}} \int d^3p \frac{1}{(2E_p)^{1/2}} a_{\mathbf{p}}^\dagger e^{-i\mathbf{p} \cdot \mathbf{x}}. \quad (6)$$

Fourier transformation of the field gives the creation operator for a plane-wave state,

$$\begin{aligned} m_1^\dagger(\mathbf{k}, 0) &= \frac{1}{(2\pi)^{3/2}} \int d^3x e^{i\mathbf{k} \cdot \mathbf{x}} m_1^\dagger(\mathbf{x}, 0), \\ &= a_{\mathbf{k}}^\dagger \frac{1}{(2E_{\mathbf{k}})^{1/2}}. \end{aligned} \quad (7)$$

For total momentum and time both equal to 0, a two-meson operator is,

$$m_1^\dagger(\mathbf{k}, 0) m_2^\dagger(-\mathbf{k}, 0) = a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger \frac{1}{2E_{\mathbf{k}}}. \quad (8)$$

Acting on the vacuum, this operator creates a two-meson state with equal and opposite momenta,

$$m_1^\dagger(\mathbf{k}, 0) m_2^\dagger(-\mathbf{k}, 0) |0\rangle = |\mathbf{k}, -\mathbf{k}\rangle \frac{1}{2E_{\mathbf{k}}}. \quad (9)$$

In a cubical volume of dimension L , the state is periodic when the momentum is $\mathbf{k} = \frac{2\pi\mathbf{n}}{L}$, where \mathbf{n} is a vector whose components are integers.

In the sink operator for two scalar mesons, destruction operators, $a_{\mathbf{k}'}$, are kept and in general the momentum of the sink operator, \mathbf{k}' , has a different direction but the same magnitude as \mathbf{k} ,

$$m_1(\mathbf{k}', 0) m_2(-\mathbf{k}', 0) = a_{\mathbf{k}'} a_{-\mathbf{k}'} \frac{1}{2E_{\mathbf{k}}}. \quad (10)$$

Correlation functions involve the operators at $t = 0$ and the Euclidean-time propagator, which is written as a sum over a complete set of eigenstates, $|n\rangle$, of the lattice Hamiltonian, as follows,

$$\begin{aligned} C(t) &= \sum_n \langle 0 | m_1(\mathbf{k}', 0) m_2(-\mathbf{k}', 0) | n \rangle e^{-E_n t} \\ &\quad \times \langle n | m_1^\dagger(\mathbf{k}, 0) m_2^\dagger(-\mathbf{k}, 0) | 0 \rangle, \end{aligned}$$

yielding a correlation function for plane-wave states of two mesons,

$$C(t) = \sum_n \langle \mathbf{k}', -\mathbf{k}' | n \rangle e^{-E_n t} \langle n | \mathbf{k}, -\mathbf{k} \rangle \frac{1}{4E_{\mathbf{k}}^2}. \quad (11)$$

B. Lattice irrep operators

Lattice irrep operators involve sums of plane-wave operators over sets of momenta that are related to one another by rotations that leave the lattice invariant. In general, the use of lattice irrep operators leads to mixings of various partial waves.

An illustrative case is row 2 of the T_1 lattice irrep, for which the source operator is a sum of two terms,

$$\frac{1}{2} m_1^\dagger(\mathbf{k}, 0) m_2^\dagger(-\mathbf{k}, 0) - \frac{1}{2} m_1^\dagger(-\mathbf{k}, 0) m_2^\dagger(\mathbf{k}, 0), \quad (12)$$

where \mathbf{k} is along the z direction. The sink operator has a similar form except with annihilation operators. The correlator can be written as,

$$\begin{aligned} C_{T_1, 2}(t) &= \frac{1}{4E_{\mathbf{k}}^2} \sum_n \frac{1}{2} \left(\langle \mathbf{k}', -\mathbf{k}' | - \langle -\mathbf{k}', \mathbf{k}' | \right) | n \rangle \\ &\quad \times e^{-E_n t} \langle n | \frac{1}{2} \left(|\mathbf{k}, -\mathbf{k}\rangle - |-\mathbf{k}, \mathbf{k}\rangle \right). \end{aligned} \quad (13)$$

Inserting complete sets of states, $|\mathbf{x}_1, \mathbf{x}_2\rangle$, and using $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$, $\mathbf{X} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2)$ (similarly for \mathbf{x}' and \mathbf{X}'), leads

to

$$C_{T_1,2}(t) = \frac{1}{4E_k^2} \sum_n e^{-E_n t} \times \int d^3 x'_1 d^3 x'_2 \frac{1}{2} \left(e^{i\mathbf{k}' \cdot \mathbf{x}'} - e^{-i\mathbf{k}' \cdot \mathbf{x}'} \right)^\dagger \Psi_n(\mathbf{x}', \mathbf{X}') \times \int d^3 x_1 d^3 x_2 \Psi_n^\dagger(\mathbf{x}, \mathbf{X}) \frac{1}{2} \left(e^{i\mathbf{k} \cdot \mathbf{x}} - e^{-i\mathbf{k} \cdot \mathbf{x}} \right), \quad (14)$$

where $\Psi_n(\mathbf{x}, \mathbf{X}) = \langle \mathbf{x}_1, \mathbf{x}_2 | n \rangle$ is the wave function of state $|n\rangle$. For this example, partial-wave expansion of the factors involving plane-waves contain odd ℓ values,

$$\frac{1}{2} \left(e^{i\mathbf{k} \cdot \mathbf{x}} - e^{-i\mathbf{k} \cdot \mathbf{x}} \right) = \sum_{\text{odd } \ell} 4\pi i^\ell j_\ell(k|\mathbf{x}|) Y_{\ell,0}^\dagger(\hat{k}) Y_{\ell,0}(\hat{x}). \quad (15)$$

Thus, the correlator becomes,

$$C_{T_1,2}(t) = \sum_n e^{-E_n t} \frac{1}{4E_k^2} \left(\sum_{\text{odd } \ell'} 4\pi i^{\ell'} Y_{\ell',0}(\hat{k}') \Phi_{n,\ell',0}(k) \right) \times \left(\sum_{\text{odd } \ell} 4\pi i^\ell \Phi_{n,\ell,0}^\dagger(k) Y_{\ell,0}^\dagger(\hat{k}) \right), \quad (16)$$

where

$$\Phi_{n,\ell,m}(k) = \int d^3 x j_\ell(k|\mathbf{x}|) Y_{\ell,m}^\dagger(\hat{x}) \Phi_n(\mathbf{x}), \quad (17)$$

and

$$\Phi_n(\mathbf{x}) = \int d^3 X \Psi_n(\mathbf{x}, \mathbf{X}). \quad (18)$$

The matrix elements, $\Phi_{n,\ell,m}(k)$, show that the coupling of operators to lattice states involves the $j_\ell(k|\mathbf{x}|) Y_{\ell,m}^\dagger(\hat{x})$ part of the operator.

When the mesons do not interact, the wave function, $\Phi_n(\mathbf{x})$, corresponds to two mesons with the same momenta as in the operator that creates the state. The wave function can be expanded in partial waves as follows,

$$\Phi_n(\mathbf{x}) = \sum_{\mathcal{L}, \mathcal{M}} a_{\mathcal{L}, \mathcal{M}} j_{\mathcal{L}}(k|\mathbf{x}|) Y_{\mathcal{L}, \mathcal{M}}(\hat{x}). \quad (19)$$

Substituting this expansion into Eq. (17) and taking into account the periodic boundary conditions leads to sums over the the overlaps of Eq. (3).

When the two mesons interact, the scattering wave function generally differs from $j_{\mathcal{L}}(k|\mathbf{x}|)$. Appendix A describes numerical tests that show that the interactions do not have a significant effect on the orthogonality.

C. Lattice partial-wave operators

In the analysis above, the two-meson operator at $t = 0$ contains the plane-wave factor, $e^{i\mathbf{k} \cdot \mathbf{x}}$, and can be written as,

$$m^\dagger(\mathbf{k}, 0) m^\dagger(-\mathbf{k}, 0) = \frac{1}{(2\pi)^3} \int d^3 x_1 \int d^3 x_2 e^{i\mathbf{k} \cdot \mathbf{x}} m^\dagger(\mathbf{x}_1, 0) m^\dagger(\mathbf{x}_2, 0). \quad (20)$$

This is a form that is useful for lattice QCD. In order to restrict the source or sink operator to a single partial wave, the plane-wave factor is replaced by a partial-wave factor, defined as follows,

$$\left[e^{i\mathbf{k} \cdot \mathbf{x}} \right]_{\ell, m} \equiv j_\ell(k|\mathbf{x}|) Y_{\ell, m}(\hat{x}), \quad (21)$$

where a factor $4\pi i^\ell Y_{\ell, m}(\hat{k})$ is omitted. The partial-wave operator is based on the factors that occur in the matrix elements between operators and lattice states, as in Eq. (17). The result is equivalent to projecting the plane-wave factor $e^{i\mathbf{k} \cdot \mathbf{x}}$ in Eq. (20) to a partial wave using $Y_{\ell, m}(\hat{k})$.

The partial-wave operator is defined by,

$$\left[m^\dagger(\mathbf{k}, 0) m^\dagger(-\mathbf{k}, 0) \right]_{\ell, m} = \frac{1}{(2\pi)^3} \int d^3 x_1 \int d^3 x_2 \left[e^{i\mathbf{k} \cdot \mathbf{x}} \right]_{\ell, m} m^\dagger(\mathbf{x}_1) m^\dagger(\mathbf{x}_2). \quad (22)$$

When used in a lattice QCD calculation, a partial-wave operator creates periodic states.

The quantization of momentum for noninteracting plane-waves that obey periodic boundary conditions implies that $q = \frac{kL}{2\pi} = |\mathbf{n}|$, where \mathbf{n} is a vector with integer components. Interactions modify the wave functions but they should remain close to the noninteracting waves with momenta corresponding to $\mathbf{n}^2 = 1, 2, 3, 4 \dots$. While there is no restriction that limits the momentum values, the noninteracting momenta provide a reasonable choice for the momenta in the partial-wave operators. The $j_\ell(k|\mathbf{x}|)$ factor can also be viewed as simply providing a spatial smearing with a smearing parameter, k , that may be chosen to maximize the coupling of the operator to states of interest.

A matrix of correlation functions could be obtained by using partial-wave operators with orbital angular momentum indices ℓ' and m' at the sink point together with indices ℓ and m at the source point, which gives,

$$C_{\ell', m'; \ell, m}(t) = \sum_n e^{-E_n t} \Phi_{n, \ell', m'}(k) \Phi_{n, \ell, m}^\dagger(k), \quad (23)$$

where $\Phi_{n, \ell, m}(k)$ is defined by Eq. (17). In this case, one can select operators corresponding to an orthogonal set of states, including tracer operators to indicate the presence of higher spins, in order to facilitate the identification of spins. However, the partial-wave operators are not used directly. They serve as parent operators that are subduced to lattice irreps before use in lattice calculations.

IV. OPERATORS FOR TWO HADRONS WITH INTRINSIC SPINS 0 OR $\frac{1}{2}$

It is interesting to consider operators for hadrons with the simplest intrinsic spins, namely, $s = 0$ and $s = \frac{1}{2}$. The total intrinsic spin of the two-hadron system can be

$S = 0$ (for example, $\pi\pi$ or NN), $S = \frac{1}{2}$ (πN) or $S = 1$ (NN).

The representations of the intrinsic spins of hadrons with $s \leq \frac{3}{2}$ are orthogonal, like the spin states in quantum mechanics,

$$\langle s, m_s | s', m'_s \rangle = \delta_{s,s'} \delta_{m_s, m'_s}, \quad (24)$$

where s is the spin and m_s is its projection along the z -axis. This orthogonality follows on the lattice because each irreducible representation of the double-cover octahedral group, $[\Lambda, r]$, is equivalent to a set of quantum states, $|s, m_s\rangle$, for a single value of s . Spin $s = 0$ is equivalent to $\Lambda = A_1$, $s = \frac{1}{2}$ to G_1 , $s = 1$ to T_1 and $s = \frac{3}{2}$ to H . With the convention used, the spin projection, m_s , is equivalent to a unique row index, r , of the irrep.

Parent operators for the scattering of two hadrons with zero total momentum are constructed in Sec. IV A by coupling the intrinsic spin angular momenta with a partial wave of orbital angular momentum to make total spin J and projection M . The final step, outlined in Sec. IV B is to produce descendant operators by subducing the parent operators from J and M to lattice irreps of O_h .

When total momentum is nonzero, operators are constructed based on total helicity in Sec. IV C. Lattice irrep operators are constructed in Sec. IV E.

A. Parent operators for total momentum $\mathbf{P} = 0$

Consider zero total momentum: $\mathbf{P} = \mathbf{k}_1 + \mathbf{k}_2 = 0$. The relative momentum is $\mathbf{k} = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ and it follows that $\mathbf{k}_1 = \mathbf{k}$ and $\mathbf{k}_2 = -\mathbf{k}$. The masses of the hadrons are m_1 and m_2 , and the energies are $E_1 = \sqrt{\mathbf{k}^2 + m_1^2}$ and $E_2 = \sqrt{\mathbf{k}^2 + m_2^2}$. For fixed energies of the hadrons, relative momentum, \mathbf{k} , is a vector of fixed magnitude, k .

Two equivalent ways of writing the lattice coordinates of the operators are,

$$\mathbf{x}_1 = \mathbf{X} + \frac{1}{2}\mathbf{x}, \quad \mathbf{x}_2 = \mathbf{X} - \frac{1}{2}\mathbf{x}, \quad (25)$$

and

$$\mathbf{X} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2), \quad \mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2. \quad (26)$$

We switch between them without further comment.

Consider a product of hadron operator, $A_{s_1, m_{s_1}}(\mathbf{x}_1, t)$, and hadron operator, $B_{s_2, m_{s_2}}(\mathbf{x}_2, t)$, where s_1 and s_2 are intrinsic-spin labels, and m_{s_1} and m_{s_2} are labels for the z -components of intrinsic spins. The desired parent operator involves coupling intrinsic spins and relative orbital angular momentum to total angular momentum, J , and projection, M , as follows,

$$\begin{aligned} (AB)_{JPM}(\mathbf{P} = 0, k, t) &= \int d^3x_1 \int d^3x_2 \sum_{\substack{s_1, s_2 \\ m_{s_1}, m_{s_2} \\ \ell, m}} \mathcal{C}_{JM} \\ &\times \left[e^{i\mathbf{k} \cdot \mathbf{x}} \right]_{\ell, m} A_{s_1, m_{s_1}}(\mathbf{x}_1, t) B_{s_2, m_{s_2}}(\mathbf{x}_2, t), \end{aligned} \quad (27)$$

where \mathcal{C}_{JM} denotes the following product of the usual Clebsch-Gordan coefficients for coupling the spins and orbital angular momenta,

$$\mathcal{C}_{JM} = \langle s_1 m_{s_1} s_2 m_{s_2} | S m_S \rangle \langle S m_S \ell m | J M \rangle, \quad (28)$$

and the partial wave of relative momentum is given by Eq. (21).

A matrix of correlation functions for the hadron-hadron system based on parent operators is,

$$\begin{aligned} C_{J'M':JM}(\mathbf{P} = 0, k, t) &= \langle 0 | (AB)_{J', M'}(\mathbf{P} = 0, k, t) \\ &\times \overline{(AB)}_{JM}(\mathbf{P} = 0, k, 0) | 0 \rangle. \end{aligned} \quad (29)$$

Sets of mutually-orthogonal parent operators for two-hadron scattering states are given in Table III for total intrinsic spin $S = 0$, in Table IV for $S = \frac{1}{2}$ and Table V for $S = 1$. The tables provide the quantum numbers corresponding to nonzero Clebsch-Gordan coefficients for the coupling of intrinsic spins with orbital angular momenta $\ell = 0, 1, 2, 3$ and 4. Some of the listed operators are orthogonal to others because their couplings involve pairs of ℓ, m values that are orthogonal, or pairs of m_s values that are orthogonal. Other operators, for example $\frac{3}{2}^+, \frac{3}{2}$ and $\frac{5}{2}^+, \frac{3}{2}$, involve combinations of Clebsch-Gordan coefficients that give orthogonality. Note that each ℓ, m component involved must be normalized to the same value in order to realize the orthogonality due to the Clebsch-Gordan coefficients.^[1]

It is straightforward to add operators for other momenta in order to build a variational basis of operators with respect to energy within each set of J, M values. For each additional momentum included, all operators of Table III (or Table IV or Table V) can be used. Orthogonality is then between subsets of operators that have different J, M values.

Isospin and the Pauli Principle provide limits on the partial wave operators that should be used. For example, the $\pi\pi$ system can occur in states of isospin 0, 1 or 2 and the system must be symmetric with regard to the exchange of the pions. Similarly, the NN system can occur in states of isospin 0 or 1 and the system must be antisymmetric with regard to exchange of the two nucleons. Operators that do not obey the correct symmetry should be omitted.

B. Descendant operators in lattice irreps for $\mathbf{P} = 0$

When the total momentum of a two-hadron operator is zero, the lattice is invariant with respect to the elements of the octahedral group. The parent operators given

[1] It is straightforward to use the orthogonality properties of C-G coefficients to project out the ℓ, m components corresponding to a given m_s .

TABLE III: Mutually-orthogonal parent operators for the scattering of two hadrons with total intrinsic spin $S = 0$, for example, $\pi\pi$ or NN . The final column provides conventional labels of the form $^{2S+1}L_J$ for the NN system with $S = 0$.

Operator	J^P, M	ℓ, m	$^{2S+1}L_J$
1	$0^+, 0$	$0, 0$	1S_0
2	$1^-, 1$	$1, 1$	1P_1
3	$1^-, 0$	$1, 0$	1P_1
4	$2^+, 2$	$2, 2$	1D_2
5	$2^+, 1$	$2, 1$	1D_2
6	$2^+, 0$	$2, 0$	1D_2
7	$3^-, 3$	$3, 3$	1F_3
8	$3^-, 2$	$3, 2$	1F_3
9	$4^-, 3$	$4, 3$	1G_4

TABLE IV: Mutually-orthogonal parent operators for the scattering of two hadrons with total intrinsic spin $S = \frac{1}{2}$, for example, πN . Each row of the table gives the combinations of ℓ, m and m_s quantum numbers that occur in the Clebsch-Gordan expansion to form J^P and M .

Operator	J^P, M	ℓ, m, m_s	ℓ, m, m_s
1	$\frac{1}{2}^+, \frac{1}{2}$	$0, 0, \frac{1}{2}$	
2	$\frac{1}{2}^-, \frac{1}{2}$	$1, 0, \frac{1}{2}$	$1, 1, -\frac{1}{2}$
3	$\frac{1}{2}^-, -\frac{1}{2}$	$1, -1, \frac{1}{2}$	$1, 0, -\frac{1}{2}$
4	$\frac{3}{2}^-, \frac{3}{2}$	$1, 1, \frac{1}{2}$	
5	$\frac{3}{2}^-, \frac{1}{2}$	$1, 0, \frac{1}{2}$	$1, 1, -\frac{1}{2}$
6	$\frac{3}{2}^+, \frac{3}{2}$	$2, 1, \frac{1}{2}$	$2, 2, -\frac{1}{2}$
7	$\frac{3}{2}^+, \frac{1}{2}$	$2, 0, \frac{1}{2}$	$2, 1, -\frac{1}{2}$
8	$\frac{5}{2}^+, \frac{5}{2}$	$2, 2, \frac{1}{2}$	
9	$\frac{5}{2}^+, \frac{3}{2}$	$2, 1, \frac{1}{2}$	$2, 2, -\frac{1}{2}$
10	$\frac{5}{2}^+, \frac{1}{2}$	$2, 0, \frac{1}{2}$	$2, 1, -\frac{1}{2}$
11	$\frac{5}{2}^-, \frac{5}{2}$	$3, 2, \frac{1}{2}$	$3, 3, -\frac{1}{2}$
12	$\frac{7}{2}^-, \frac{5}{2}$	$3, 2, \frac{1}{2}$	$3, 3, -\frac{1}{2}$
13	$\frac{7}{2}^+, \frac{7}{2}$	$4, 3, \frac{1}{2}$	$4, 4, -\frac{1}{2}$

above are subduced to irreps of the octahedral group, which produces descendant operators that can be used in lattice calculations.

The subduction coefficients, $S_{\Lambda, r}^{J, M}$, are given in Ref. [1] for integer spins and in Ref. [2] for half-integer spins. They should be applied as follows to the operators of Eq. (27) that are labeled by J, M to obtain operators that are labeled by the octahedral group irrep Λ and row r ,

$$(AB)_{\Lambda, r}(\mathbf{k}_1, \mathbf{k}_2, t) = \sum_M S_{\Lambda, r}^{J, M} (AB)_{JM}(\mathbf{k}_1, \mathbf{k}_2, t). \quad (30)$$

As shown in appendix B of Ref. [2], the subduction coefficients are real and they obey,

$$\sum_M S_{\Lambda', r'}^{J, M} S_{\Lambda, r}^{J, M} = \delta_{\Lambda', \Lambda} \delta_{r', r}. \quad (31)$$

TABLE V: Mutually-orthogonal parent operators for the scattering of two hadrons with total intrinsic spin $S = 1$, for example, NN . Each row of the table gives the combinations of ℓ, m and m_s quantum numbers that have nonzero coefficients in the Clebsch-Gordan expansion to form J and M . The final column provides conventional labels of the form $^{2S+1}L_J$ for the NN system with $S = 1$.

Operator	J, M	ℓ, m, m_s	ℓ, m, m_s	ℓ, m, m_s	$^{2S+1}L_J$
1	$0, 1$	$0, 0, 1$			3S_1
2	$0, 0$	$0, 0, 0$			3S_1
3	$0, -1$	$0, 0, -1$			3S_1
4	$0, 0$	$1, 1, -1$	$1, 0, 0$	$1, -1, 1$	3P_0
5	$1, 1$	$1, 1, 0$	$1, 0, 1$		3P_1
6	$1, 0$	$1, 1, -1$	$1, -1, 1$		3P_1
7	$2, 2$	$1, 1, 1$			3P_2
8	$2, 1$	$1, 1, 0$	$1, 0, 1$		3P_2
9	$2, 0$	$1, 1, -1$	$1, 0, 0$	$1, -1, 1$	3P_2
10	$1, 1$	$2, 2, -1$	$2, 1, 0$	$2, 0, 1$	3D_1
11	$1, 0$	$2, 1, -1$	$2, -1, 1$		3D_1
12	$2, 2$	$2, 2, 0$	$2, 1, 1$		3D_2
13	$2, 1$	$2, 2, -1$	$2, 1, 0$	$2, 0, 1$	3D_2
14	$2, 0$	$2, 1, -1$	$2, -1, 1$		3D_2
15	$3, 3$	$2, 2, 1$			3D_3
16	$3, 2$	$2, 2, 0$	$2, 1, 1$		3D_3
17	$3, 1$	$2, 2, -1$	$2, 0, 1$	$2, 0, 1$	3D_3

This property causes descendant states to be orthogonal with respect to J when they are obtained by subducing a set of mutually orthogonal parent states. This is shown for quantum states of angular momentum, $|J, M\rangle$, and their descendant states, labelled by lattice irreps, that are subduced from a single value of J , i.e., $|\Lambda[J], r\rangle = \sum_M S_{\Lambda, r}^{J, M} |J, M\rangle$, as follows,

$$\begin{aligned} \langle \Lambda'[J'], r' | \Lambda[J], r \rangle &= \sum_{M, M'} S_{\Lambda', r'}^{J', M'} S_{\Lambda, r}^{J, M} \langle J', M' | J, M \rangle, \\ &= \sum_{M, M'} S_{\Lambda', r'}^{J', M'} S_{\Lambda, r}^{J, M} \delta_{J', J} \delta_{M', M} \\ &= \delta_{\Lambda', \Lambda} \delta_{r', r} \delta_{J', J}. \end{aligned} \quad (32)$$

Spin identification is based on an orthogonal set of parent operators. A matrix of correlation functions is calculated based on the descendant, irreducible operators. Because of the orthogonality of Eq. (32), the matrices are approximately block-diagonal with respect to the values of the parent spin, J , from which the irreducible operators are subduced. Use of the variational method[18, 19] to extract the energies of states, and operator overlaps [1, 2], $Z_{nm} = \langle n | O_m | 0 \rangle$, to identify the couplings of operators to the states, then identifies which parent spins, J , are predominant in the creation of a lattice state. Generally, when a spin- J operator couples to a state, that identifies J as a lower bound of the spin. If two or more operators couple to a state, the highest

value of J identifies the lower bound of the spin.

The phase shift can be calculated using the Luscher method, which is based on the deviation of the energy of a scattering state from the energy when there is zero interaction. The latter energy may be calculated from the masses of the hadrons and the quantized momenta that obey periodic boundary conditions.

C. Two-hadron operators with total momentum $\mathbf{P} \neq 0$

Nonzero total momentum is of considerable interest because it provides a way to increase the number of c.m. energies that can be obtained using a given lattice.

The helicity, λ , is the eigenvalue of J_z in the c.m. frame. Invariance with respect to boosts along the direction of the total momentum shows that helicity takes the same value in the c.m. frame and the lattice frame, where it can be determined.

Because $J \geq |\lambda|$, the use of operators for a range of helicity values provides the following signature. A state with spin J couples to the operators with $\lambda \leq J$, and not to the operators for higher helicity.

It is useful to decompose coordinates and momenta into parts that are perpendicular and parallel to \mathbf{P} , which are denoted by subscripts, \perp and \parallel , respectively. Rotations that keep \mathbf{P} invariant also leave the parallel components of other vectors invariant, e.g., $k_{1\parallel}$, $k_{2\parallel}$ and $k_{\parallel} = \frac{1}{2}(k_{1\parallel} - k_{2\parallel})$. Vectors that are perpendicular to the total momentum, e.g., $\mathbf{k}_{1\perp} = -\mathbf{k}_{2\perp} = \mathbf{k}_{\perp}$, are invariant with respect to boosts along the direction of the total momentum. Energies are $E_1 = \sqrt{m_1^2 + k_{\perp}^2 + k_{1\parallel}^2}$ and $E_2 = \sqrt{m_2^2 + k_{\perp}^2 + k_{2\parallel}^2}$, where $k_{\perp} = |\mathbf{k}_{\perp}|$ is invariant with respect to rotations that keep \mathbf{P} invariant.

D. Parent helicity operators for $\mathbf{P} \neq 0$

Two-hadron operators are labelled by the total helicity when $\mathbf{P} \neq 0$. For two spin-zero hadrons, the helicity values are constructed in the lattice frame using a cylindrical function in place of the spherical harmonic that appears in Eq. (21), as follows,

$$\left[e^{i\mathbf{k}_{\perp} \cdot \mathbf{x}_{\perp}} \right]_m = J_m(k_{\perp} x_{\perp}) e^{im\phi_x}, \quad (33)$$

where ϕ_x is the azimuthal angle of \mathbf{x}_{\perp} and J_m is a Bessel function. An overall factor $i^m e^{-im\phi_k}$ is omitted, where ϕ_k is the azimuthal angle of \mathbf{k}_{\perp} , because it plays no role in the final analysis.

A two-hadron parent operator incorporates intrinsic

spins of the hadrons as follows,

$$(AB)_{\lambda}(\mathbf{P}, k_{\parallel}, k_{\perp}, t) = \int d^3x_1 \int d^3x_2 e^{i\mathbf{P} \cdot \mathbf{X}} e^{ik_{\parallel} x_{\parallel}} \sum_{\substack{s_1, s_2 \\ m_{s_1}, m_{s_2}, m}} \mathcal{C}_{\lambda} \left[e^{i\mathbf{k}_{\perp} \cdot \mathbf{x}_{\perp}} \right]_m A_{s_1, m_{s_1}}(\mathbf{x}_1, t) B_{s_2, m_{s_2}}(\mathbf{x}_2, t), \quad (34)$$

where \mathcal{C}_{λ} denotes the following product of a Clebsch-Gordan coefficient for spin and a delta function,

$$\mathcal{C}_{\lambda} = \langle s_1 m_{s_1} s_2 m_{s_2} | S m_S \rangle \delta_{m_S + m, \lambda}. \quad (35)$$

This operator is constructed to create a state with helicity, λ , that is the sum of the orbital helicity, m , and spin helicity, m_S .

The matrix of correlation functions for the two-hadron system based on parent operators is,

$$C_{\lambda'; \lambda}(\mathbf{P}, k_{\parallel}, k_{\perp}, t) = \langle 0 | (AB)_{\lambda'}(\mathbf{P}, k_{\parallel}, k_{\perp}, t) \times \overline{(AB)_{\lambda}(\mathbf{P}, k_{\parallel}, k_{\perp}, 0)} | 0 \rangle. \quad (36)$$

E. Descendant operators in lattice irreps for $\mathbf{P} \neq 0$

When the total momentum of the two-hadron system is nonzero, the lattice symmetry group is C_{nv} (alternatively known as Dic_n for the double group), for $n=4, 3$, or 2 . For C_{4v} , the total momentum is directed along one of the axes of the cube; for C_{3v} , it is along a body diagonal; for C_{2v} it is parallel to a face diagonal. For each of these cases, we label the direction of total momentum as the z-axis. Altmann and Herzig [20] have developed the subductions from $SU(2)$ to irreps of the point groups C_{nv} ; their notation is followed in this work. Equivalent results are given in Refs. [17, 21, 22].

The C_{nv} group applies for integer spins and the C_{nv} double group applies for half-integer spins. The group elements are n rotations about the z direction, $R_z(\theta)$, with equally spaced θ values in the range $0 \leq \theta < 2\pi$ (or $2n$ rotations in the range $0 \leq \theta < 4\pi$ for the double group). In addition, there is an equal number of reflections, $R_z(\theta)\Pi_{yz}$, that involve the same rotations and a reference reflection, which is chosen to be Π_{yz} , the reflection in the yz -plane. The group elements transform helicity states as follows,

$$R_z(\theta)|\lambda\rangle = e^{-i\lambda\theta}|\lambda\rangle, \quad \Pi_{yz}|\lambda\rangle = \eta|-\lambda\rangle, \quad (37)$$

where $\eta = (-1)^J P$ and P is the parity. The phase factor, η , is equal to $\tilde{\eta}$ in the analysis of Ref. [17], where it is shown to follow from the choice of Π_{yz} as the reference reflection,

Representations of C_{nv} involve a linear combination of helicity states, $|\lambda\rangle$ and $|-\lambda\rangle$. In this work, they are chosen to diagonalize the reference reflection and are labeled by the positive helicity, $\lambda > 0$, and a sign, \pm ,

which serves as the row index of the representation, as follows,

$$|\lambda, \pm\rangle \equiv \sqrt{\frac{1}{2}} \left(|\lambda\rangle \pm \eta |-\lambda\rangle \right). \quad (38)$$

The action of group elements is to transform the $|\lambda, \pm\rangle$ representations into linear combinations of one another,

$$\begin{aligned} R_z(\theta)|\lambda, +\rangle &= \cos(\lambda\theta)|\lambda, +\rangle - i\sin(\lambda\theta)|\lambda, -\rangle, \\ R_z(\theta)|\lambda, -\rangle &= -i\sin(\lambda\theta)|\lambda, +\rangle + \cos(\lambda\theta)|\lambda, -\rangle, \\ \Pi_{yz}|\lambda, \pm\rangle &= \pm(-1)^J|\lambda, \pm\rangle, \end{aligned} \quad (39)$$

where the eigenvalue of the reference reflection is seen to be $\pm(-1)^J$. Note that a two-dimensional representation is reducible to two one-dimensional irreps when $\sin(\lambda\theta)$ vanishes for each group rotation angle, θ . Otherwise $|\lambda, +\rangle$ and $|\lambda, -\rangle$ provide the rows of a two-dimensional irrep.

Descendant operators for $\mathbf{P} \neq 0$ transform as irreps of C_{nv} . They involve the positive helicity, $\lambda > 0$, and the row index, \pm , and have a composition similar to Eq. (38),

$$\begin{aligned} (AB)_{\lambda, \pm}(\mathbf{P}, k_{\parallel}, k_{\perp}, t) &= \sqrt{\frac{1}{2}} \left((AB)_{\lambda}(\mathbf{P}, k_{\parallel}, k_{\perp}, t) \right. \\ &\quad \left. \pm \eta (AB)_{-\lambda}(\mathbf{P}, k_{\parallel}, k_{\perp}, t) \right). \end{aligned} \quad (40)$$

The rows of a two-dimensional irrep are orthogonal and they produce the same correlation function as the average over rows, which is the same as the average over \pm signs. Using the descendant operators of Eq. (40), the average over rows is,

$$\overline{C}_{\lambda} = \frac{1}{2} (C_{\lambda, +; \lambda, +} + C_{\lambda, -; \lambda, -}). \quad (41)$$

A little algebra shows that this is equal to the average over the helicities, λ and $-\lambda$, that appear when the expression above is expanded in terms of the correlation functions $C_{\lambda', \lambda}$ of Eq. (36). Using $\eta^* \eta = 1$, the row average is evaluated as follows,

$$\begin{aligned} \overline{C}_{\lambda} &= \frac{1}{4} (C_{\lambda, \lambda} + \eta^* C_{-\lambda, \lambda} + \eta C_{\lambda, -\lambda} + \eta^* \eta C_{-\lambda, -\lambda}) \\ &\quad + \frac{1}{4} (C_{\lambda, \lambda} - \eta^* C_{-\lambda, \lambda} - \eta C_{\lambda, -\lambda} + \eta^* \eta C_{-\lambda, -\lambda}), \\ &= \frac{1}{2} (C_{\lambda, \lambda} + C_{-\lambda, -\lambda}). \end{aligned} \quad (42)$$

The parity-dependent phase factor, η , cancels out of the average over rows.

Each one-dimensional irrep also involves both λ and $-\lambda$, as in Eq. (38). For most purposes, it is adequate to average the two one-dimensional irreps for a given helicity, λ , in the same manner as the rows of a two-dimensional irrep. When this is done, the result is the same as in Eq. (42), i.e., the parity-dependent phase factor, η , cancels out. Thus, correlation functions can be

TABLE VI: Pattern of matrix elements $Z_{m'm}$ for group C_{4v} . For group C_{3v} , the x's shift to horizontal positions that are a multiple of three units away from the diagonal and for group C_{2v} the x's move to positions that are a multiple of 2 units away from the diagonal. Symbols have the same meaning as in Table I. The top row shows the m indices and the left column shows the m' indices.

	-4	-3	-2	-1	0	1	2	3	4
-4	1				x				x
-3		1				x			
-2			1				x		
-1				1				x	
0	x				1				x
1		x				1			
2			x				1		
3				x				1	
4	x				x				1

calculated directly from parent operators, as in Eq. (36), and then averaged over the $\pm\lambda$ values in order to obtain the same result as would be obtained from averaging over the rows of correlation functions based on the irrep operators of Eq. (40).

Although the average over helicities provides a simple and straightforward analysis, the irrep operators are given in Appendix B for completeness.

The orthogonality of periodic orbital-helicity functions involves the following matrix of overlaps,

$$\begin{aligned} Z_{m'm} &= \int d^3x [J_m(k_{\perp}x_{\perp})e^{im\phi_x}]^{(per)\dagger} \times \\ &\quad [J_{m'}(k_{\perp}x_{\perp})e^{im'\phi_x}]^{(per)}. \end{aligned} \quad (43)$$

This matrix is normalized as in Eq. (4) in order to make diagonal elements equal to one. Then the zero elements depend on index n of group C_{nv} as follows,

$$Z_{m',m} = 0 \text{ if } m' \neq m \pmod{n}. \quad (44)$$

Table VI shows the pattern of matrix elements based on Eq. (43).

The best case for spin identification is group C_{4v} because it has the largest range of orbital helicities that can be included in an orthogonal set. The orbital-helicity states that are orthogonal are limited to $m = 0$ and ± 1 for both C_{3v} and C_{2v} . For each of these groups, the resulting sets of mutually-orthogonal operators for two-hadron scattering states are given in Table VII for total intrinsic spin $S = 0$, in Table VIII for $S = \frac{1}{2}$ and Table IX for $S = 1$. As each irrep operator includes helicity values, λ and $-\lambda$, quantum numbers m and $-m$ are included for the cylindrical harmonics. Orthogonality for $S = 0$ is limited because each m -component must be orthogonal to all the other m -components in the table. For example, $m = \pm 3$ cannot be included because $m = \pm 1$ is included.

When intrinsic spin states are included, orthogonality depends on each m, m_s pair being orthogonal to each

TABLE VII: Mutually orthogonal helicity operators for group C_{4v} and total intrinsic spin $S = 0$. Each row lists the irrep label, λ , and the m values included in the operator. For groups C_{3v} and C_{2v} , only rows 1 and 2 involving $m = 0$ and ± 1 are orthogonal.

No.	λ	m	$-m$
1	0	0	0
2	1	1	-1
3	2	2	-2

TABLE VIII: Mutually orthogonal helicity operators for group C_{4v} and total intrinsic spin $S = \frac{1}{2}$. Each row lists the irrep label, λ , and the m, m_s values included in the operator. For groups C_{3v} and C_{2v} , only the rows involving $m = 0$ and ± 1 are orthogonal.

No.	λ	m, m_s	$-m, -m_s$
1	$\frac{1}{2}$	$0, \frac{1}{2}$	$0, -\frac{1}{2}$
2	$\frac{1}{2}$	$1, -\frac{1}{2}$	$-1, \frac{1}{2}$
3	$\frac{3}{2}$	$1, \frac{1}{2}$	$-1, -\frac{1}{2}$
4	$\frac{5}{2}$	$2, \frac{1}{2}$	$-2, -\frac{1}{2}$

other pair. The orthogonality of spins allows more operators to be included.

V. SUMMARY

Operators are developed to facilitate the identification of spins in lattice QCD calculations of the scattering of two hadrons. In the case that the total momentum of the hadrons is $\mathbf{P} = 0$, partial-wave operators are used to create periodic partial waves of orbital angular momentum, ℓ , and projection, m . The operators are based on momenta of magnitude $k = \frac{2\pi|\mathbf{n}|}{L}$, where \mathbf{n} is a vector with integer components. These are the momenta for noninteracting plane waves on the cubic lattice, however, other values of k could be used to provide a different radial smearing of the operators. Phase shifts may

TABLE IX: Mutually orthogonal helicity operators for group C_{4v} and total intrinsic $S = 1$. Each row lists the irrep label, λ , and the m, m_s values included in the operator. For groups C_{3v} and C_{2v} , only the rows involving $m = 0$ and ± 1 are orthogonal.

No.	λ	m, m_s	$-m, -m_s$
1	0	0,0	0,0
2	0	1,-1	-1,1
3	1	0,1	0,-1
4	1	1,0	-1,0
5	1	2,-1	-2,1
6	2	1,1	-1,-1
7	2	2,0	-2,0

be obtained using the Lüscher method and its extensions. The periodic partial waves are orthogonal with respect to ℓ and m , subject to restrictions imposed by the cubical lattice. The partial waves provide an advantage relative to the use of combinations of plane waves in that there is freedom to select sets of orthogonal operators based on specific ℓ and m values.

The essential point of this work is to differentiate between lattice irreps that are subduced from different continuum spins. For example, the use of mutually orthogonal $\ell = 1$ and $\ell = 3$ parent operators based on partial waves provides orthogonal descendant operators after subduction to the T_1 lattice irrep. Strong coupling of a lattice state to one of these operators but not the other provides a signal for the spin of the state. While contributions of $\ell \geq 5$ can occur in the subduced operators, the short range of hadronic interactions and the centrifugal barrier at high ℓ suggest that the role of higher spins is suppressed.

Parent operators for total spin, $J \leq 4$, and projection, M , are obtained by coupling the intrinsic spins of the hadrons and the partial waves of orbital angular momentum. Sets of mutually-orthogonal parent operators corresponding to different values of J and M are given for total intrinsic spin $S = 0, \frac{1}{2}$ and 1 based on omitting operators that are not orthogonal because of the cubic symmetry. When these parent operators are subduced to lattice irreps, their descendants retain orthogonality and lead to matrices of correlation functions that are block diagonal with respect to the different values of J . That allows the spin of a scattering state to be identified as the spin of the parent operators that dominate the creation of the state.

In the case that the total momentum is $\mathbf{P} \neq 0$, parent operators are designed to create states of total helicity by combining spin helicities and orbital helicity based on cylindrical harmonics. Mutually-orthogonal sets of parent operators for a sufficient range of total helicity values can be used to facilitate the identification of the spin, J , of a state. The signature is that a state of spin J couples to operators for all total helicity values $\lambda \leq J$, and not to operators for $\lambda > J$. However, there is a limitation owing to cubic symmetry. Total momenta that are parallel to an axis of the cubical lattice (symmetry group C_{4v}) allow the widest range of helicity values and, thus, provide the best case for spin identification based on helicity.

For either the partial-wave operators or the helicity operators, a variational basis can be constructed by using additional copies of the sets of mutually-orthogonal operators based on different momentum values.

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Appendix A: Lattice orthogonality of periodic partial waves.

A generalization of Eqs. (3) and (4) is considered in which the lattice state is assumed to be a scattering state described by the Lüscher formalism for various values of the phase shift,

$$Z_{\ell', m'; \ell, m} = \frac{1}{N_{\ell', m'} N_{\ell, m}} \times \int d^3 x [j_{\ell'}(k|\mathbf{x}) Y_{\ell', m'}^\dagger(\hat{x})]^{(per)} [\Psi_\ell(|\mathbf{x}|) Y_{\ell, m}(\hat{x})]^{(per)}, \quad (\text{A1})$$

where $\Psi_\ell(|\mathbf{x}|)$ is the radial wave function of the scattering state. When the phase shift, δ_ℓ is zero, $\Psi_\ell(|\mathbf{x}|)$ reduces to a spherical Bessel function, $j_\ell(k|\mathbf{x}|)$.

According to the Lüscher formalism, a scattering state for angular momentum ℓ and phase shift δ_ℓ involves a momentum value, k_{ext} , in the exterior region, $r > R$, where R is the range of interaction. Momentum k_{ext} is related to the energy of the scattering state through $W = \sqrt{m_1^2 + k_{ext}^2} + \sqrt{m_2^2 + k_{ext}^2}$, as shown by Lüscher [6]. The value of k_{ext} also is related to the phase shift as follows,

$$\delta_\ell = j\pi - \phi(q), \quad q = \frac{k_{ext}L}{2\pi}, \quad (\text{A2})$$

where the function $\phi(q)$ is obtained from

$$\cot(\phi) = -\frac{\mathcal{Z}_{00}(1; q^2)}{\pi^{3/2}q} = -\frac{1}{2\pi^2q} \sum_{\mathbf{n} \in \mathbb{Z}^3} \frac{1}{(\mathbf{n}^2 - q^2)}. \quad (\text{A3})$$

The integer j is chosen so that $\phi(q)$ is a continuous function of q and obeys the boundary condition $\phi(0) = 0$. These formulas neglect contributions from $\ell = 4$ or higher partial waves.

Since the interaction is not known, it is necessary to use a model to approximate the scattering wave function in the interior region, $0 < r < R$. A square-well potential gives a momentum, k_{int} , in the interior region and the scattering wave function is,

$$\begin{aligned} \Psi_\ell(r) &= j_\ell(k_{int}r), & 0 < r < R, \\ \Psi_\ell(r) &= A[\cos\delta_\ell j_\ell(k_{ext}r) - \sin\delta_\ell n_\ell(k_{ext}r)], & R < r < L/2, \end{aligned} \quad (\text{A4})$$

where j_ℓ and n_ℓ are spherical Bessel functions.

The scattering wave function is then obtained by choosing a phase shift, finding k_{ext} from Eq. (A2) and matching the interior and exterior wave functions in Eq. (A4), and their derivatives, at $r = R$ to obtain momentum k_{int} and coefficient A .

Calculations have used $R = L/4$ as the range of the interaction and $\delta_\ell/\pi = [0.0, 0.1, 0.25, 0.5, 0.75, 0.9]$. The lowest values of k_{ext} are used. The cubical volumes considered are 16^3 and 32^3 . The construction of periodic partial waves was done using $N = 5, 7, 9$ and 11 for the sum in Eq.(1). For all cases, the results confirm that matrix elements shown by blank entries in Tables I and II have numerical values less than 10^{-15} in magnitude for each considered value of the phase shift.

Appendix B: Irreducible representations for helicity states

As noted in the text, the two-dimensional representation of Eq. (38) is reducible when $\sin(\lambda\theta)$ vanishes for all group rotations. Then, the $|\lambda, \pm\rangle$ states are not mixed by the group rotations, as may be seen from Eq. (39).

The reduction occurs when $\lambda = 0, n/2, n, \dots$, where n is the index of group C_{nv} . Following the Mulliken convention[23] for labelling irreps, the helicity states $|\lambda, \pm\rangle$ provide irreps as listed in Table X. For $\lambda = 0$ or n , the $|\lambda, +\rangle$ state transforms as the A_1 irrep and the $|\lambda, -\rangle$ state transforms as the A_2 irrep. For $\lambda = n/2$ or $3n/2$, $|\lambda, +\rangle$ transforms as the B_1 irrep and $|\lambda, -\rangle$ transforms as the B_2 irrep.

For $\lambda = 1$, the $|\lambda, \pm\rangle$ are mixed by the action of group rotations for groups C_{4v} and C_{3v} , but not for C_{2v} . For $\lambda = 3$, the rotations mix the $|\lambda, \pm\rangle$ for group C_{4v} , providing two rows of the E_2 two-dimensional irrep. For groups C_{3v} and C_{2v} , there is no mixing and the $|\lambda, \pm\rangle$ provide one-dimensional irreps A_1 and A_2 for C_{3v} and B_1 and B_2 for C_{2v} .

For half-integer spins and helicities, the irreps are two-dimensional and are given labels $E_{\frac{1}{2}}$, $E_{\frac{3}{2}}$ and E , as shown in Table X. An equivalent table may be found in Ref. [22].

TABLE X: Helicity irreps for C_{nv} groups. $\Pi = \pm(-1)^J$ is the eigenvalue of the reference reflection and $\Pi/(-1)^J$ is the row index, namely, \pm .

λ	$\Pi/(-1)^J$	C_{4v}	C_{3v}	C_{2v}
0	+	A_1	A_1	A_1
0	-	A_2	A_2	A_2
$\frac{1}{2}$	\pm	$E_{\frac{1}{2}}$	$E_{\frac{1}{2}}$	E
1	+	E_2	E_2	B_1
1	-	E_2	E_2	B_2
$\frac{3}{2}$	\pm	$E_{\frac{3}{2}}$	$B_1 \oplus B_2$	E
2	+	B_1	E_2	A_1
2	-	B_2	E_2	A_2
$\frac{5}{2}$	\pm	$E_{\frac{5}{2}}$	$A_1 \oplus B_1$	E
3	+	E_2	A_1	B_1
3	-	E_2	A_2	B_2
$\frac{7}{2}$	\pm	$E_{\frac{7}{2}}$	$E_{\frac{1}{2}}$	E
4	+	A_1	E_2	A_1
4	-	A_2	E_2	A_2

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