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Lattice QCD with a Dumbbell-Like Operator**

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# Towards high partial waves in lattice QCD with a dumbbell-like operator

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## Abstract

An extended two-hadron operator is developed to extract the spectra of irreducible representations (irreps) in the finite volume. The irreps of the group for the finite volume system are projected using a coordinate-space operator. The correlation function of this operator is computationally efficient to extract lattice spectra of the specific irrep. In particular, this new formulation only requires propagators to be computed from two distinct source locations, at fixed spatial separation. We perform a proof-of-principle study on a  $24^3 \times 48$  lattice volume with  $m_\pi \approx 900$  MeV by isolating various spectra of the  $\pi\pi$  system with isospin-2 including a range of total momenta and irreps. By applying the Lüscher formalism, the phase shifts of  $S$ -,  $D$ - and  $G$ -wave  $\pi\pi$  scattering with isospin-2 are extracted from the spectra.

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## I. INTRODUCTION

The numerical simulation of quark and gluon fields on a finite lattice enables a study of the hadron spectrum and strong interactions of QCD via first principles. Recently, there has been tremendous progress in lattice QCD calculations of the hadron spectrum and interactions (see Refs. [1–3] for recent reviews). From the energy levels of lattice QCD, there is a clear strategy for how to extract scattering information for two-body systems, such as the  $\pi\pi$  system [4–8]. In order to map out the energy-dependence of the scattering phase shifts various methods have been developed to access more finite-volume energy levels, such as the variational analysis for the excited energy eigenvalues [9–12], moving systems [4, 6], and twisted boundary conditions [13, 14]. An important requirement to isolate distinct partial waves is the need to distinguish the energy levels in different irreducible representations (irreps), such as done in Ref. [6].

With improved control of orbital motion, there is potential for lattice QCD to provide insight into the phenomenology of high-spin systems. For instance, the relatively narrow dibaryon resonance observed by WASA-at-COSY [15, 16] suggests significant coupling to the  $np$   $G$ -wave amplitude. There is also potential to shed light on the nuclear  $A(y)$  puzzle [17–19] or the dynamics underlying Regge trajectories [20–22]. While each of these objectives will (ultimately) also require advances in many-body systems on the lattice [23, 24], the physics of many-body channels can often be suppressed at large unphysical quark masses on the lattice—such as the recent high- $J$  study of Ref. [25].

The study of high angular momentum systems is an ongoing challenge in lattice QCD. On the cubic finite volume of a 4-dimensional lattice, the relevant symmetry group is a subgroup of the octahedral group ( $O_h$ )—or the relevant little group when considering systems at finite momenta. Importantly, the full  $SO(3)$  group of the infinite volume physical theory is broken, and consequently, numerical investigations are limited to the discrete symmetry of the lattice. The issue of partial-wave mixing, and influence on discrete spectra, has been investigated theoretically and numerically in previous work, e.g. Refs. [26–41].

In this paper, we introduce a novel operator construction, designed to provide an efficient method to isolate different lattice irreps in a two-hadron system. The method relies upon constructing an operator that corresponds to a “dumbbell” in coordinate space, where the two body operator is the product of two single particle operators separated by a fixed distance. The construction shares similarities with the “cube” source employed in Ref. [37]. In our case, as will be shown, we sum over the rotations of the dumbbell at the sink in order to project correlation functions onto the desired irrep. The two distinguishing features of this method are that only the total momentum of the two-hadron system is fixed and only two point-source Dirac matrix inversions are required. As an exploratory exercise, we study the isospin-2  $\pi\pi$  system, for which several alternative methods have already been explored [5–7]. We demonstrate that we are able to successfully determine energy levels of the various representations with different total momenta.

In Section II, the two-hadron operator and correlation functions for specific irreps are constructed. In Section III, a lattice-QCD calculation for isospin-2  $\pi^-\pi^-$  scattering is presented with lattice size  $24^3 \times 48$  and the energy levels for various irreps with different total momentum are extracted. These energy levels are then used to determine the phase shifts of  $\pi^-\pi^-$  scattering. Finally, results are summarised in Section IV.

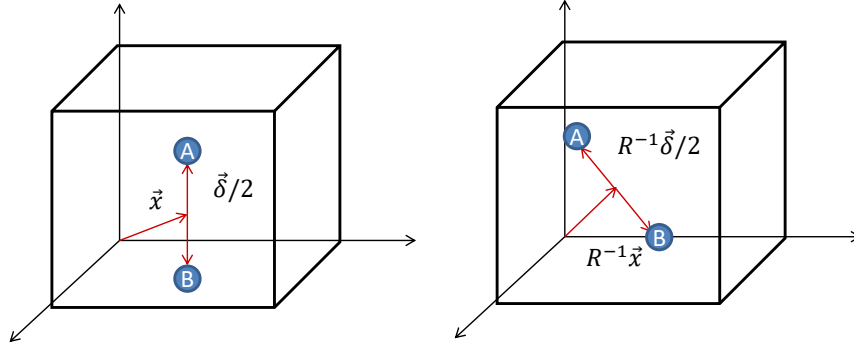


FIG. 1. Illustration of the 2-hadron “dumbbell” interpolating operator. A fixed source location is indicated in the left image, and the sink on the right indicates that the separation of the pointwise interpolating fields are summed over all lattice rotations,  $R$ .

## II. FORMALISM

### A. Operators in coordinate space

Our goal is to construct extended interpolating operators which project onto states of both definite momenta and irreps of the lattice rotation group. To minimise the numerical cost associated with inversion of Dirac matrices, we seek a construction which allows our correlation functions to be constructed from just two conventional local sources. The projection onto definite Fourier momenta and rotational irreps are to be performed at the sink, as depicted in Fig. 1. To construct the appropriate projections we start from a composite operator of two hadrons with a separation  $\boldsymbol{\delta}$  between them:

$$\Phi(\mathbf{x}, \boldsymbol{\delta}) \equiv \phi(\mathbf{x} + \boldsymbol{\delta}/2)\phi'(\mathbf{x} - \boldsymbol{\delta}/2), \quad (1)$$

where time-dependence has been suppressed and the operator  $\phi$  (or  $\phi'$ ) denotes a conventional, local single-hadron operator. For example, in the following calculation, we consider the standard  $\pi^-$  operator given by

$$\phi(\mathbf{x}) = \phi'(\mathbf{x}) \equiv \sum_a \bar{u}^a(\mathbf{x})\gamma_5 d^a(\mathbf{x}), \quad (2)$$

with a sum over the color index  $a$ .

We consider the set of operators,  $\{\Phi_{\hat{R}}\}$ , which are related by a lattice rotation,  $\hat{R} \in O_h$ . Under such a rotation, the transformed operators take the form:

$$\begin{aligned} \Phi_{\hat{R}}(\mathbf{x}, \boldsymbol{\delta}) &\equiv \hat{P}_{\hat{R}} \Phi(\mathbf{x}, \boldsymbol{\delta}) \hat{P}_{\hat{R}^{-1}} = \Phi(\hat{R}^{-1}\mathbf{x}, \hat{R}^{-1}\boldsymbol{\delta}) \\ &= \phi(\hat{R}^{-1}(\mathbf{x} + \boldsymbol{\delta}/2))\phi'(\hat{R}^{-1}(\mathbf{x} - \boldsymbol{\delta}/2)), \end{aligned} \quad (3)$$

as being represented in the right panel of Fig. 1. To maximally span the space of lattice irreps, we choose to work with separation vectors satisfying  $0 < \delta_x < \delta_y < \delta_z$  such that  $\hat{R}\boldsymbol{\delta} \neq \boldsymbol{\delta}$  (for  $\hat{R} \neq I$ ). We then have 24 different operators that are related by a lattice rotation — in the case of non-identical particles, there are 48 operators. While the single-hadron operators must lie on lattice sites, the center of the composite operator,  $\mathbf{x}$ , need

not be on a lattice site. In the numerical results presented here, we work with the choice  $\boldsymbol{\delta} = (1, 3, 5)$  and  $\mathbf{x} = (1/2, 1/2, 1/2)$ . We note that choosing all even values for  $\boldsymbol{\delta}$  would place the origin of the extended operator on a lattice site and maintain the same discrete rotational symmetries. In principle, combinations of even and odd displacements by  $\boldsymbol{\delta}$  would be possible, but it would lead to a (short distance) modification of the rotational symmetries discussed here.

A Fourier transform with respect to the coordinate  $\mathbf{x}$  project onto states of definite momenta:

$$\langle \Phi(\mathbf{P}, \boldsymbol{\delta}) | = \langle \Omega | \sum_{\mathbf{x}} e^{-i\mathbf{P}\cdot\mathbf{x}} \Phi(\mathbf{x}, \boldsymbol{\delta}). \quad (4)$$

In just the same way that the Fourier transform projects onto states of definite momenta, particular linear combinations of operators related by lattice rotations, Eq. (3), will project onto particular irreducible representations. In particular, for  $(|\mathbf{p}|L/2\pi)^2 = 0, 1, 2,$  and  $3,$  operators are constructed to project onto the irreps of the groups commonly denoted  $O_h,$   $C_{4\nu},$   $C_{2\nu}$  and  $C_{3\nu},$  respectively (see for instance, Ref. [42]). The projection onto these irreps has been discussed in a number of previous works [4, 31, 33, 34, 43]. For completeness and to set our notation, we briefly summarise the relevant features here.

The states  $|\Phi_{\hat{R}}(t; \mathbf{x}, \boldsymbol{\delta})\rangle$  where  $\hat{R}$  belong to the corresponding group will transform as vectors of the regular representation as follows:

$$\hat{P}_{\hat{R}} |\Phi_{\hat{R}'}(\mathbf{x}, \boldsymbol{\delta})\rangle = \sum_{\hat{R}'' \in G^{\mathbf{p}}} |\Phi_{\hat{R}''}(\mathbf{x}, \boldsymbol{\delta})\rangle \left( \bar{B}(\hat{R}) \right)_{\hat{R}'', \hat{R}'}, \quad (5)$$

where  $\left( \bar{B}(\hat{R}) \right)_{\hat{R}'', \hat{R}'} = \delta_{\hat{R}\hat{R}'', \hat{R}'},$  and  $G^{\mathbf{p}}$  denotes the rotation group for specific total momentum  $\mathbf{p}$  (see Table VI).

The regular representation of any non-trivial group is reducible. Thus,  $\bar{B}$  can be made block diagonal according to the irreps of the symmetry group via a unitary transformation matrix  $\bar{S}$ . For example, in the  $O_h$  group,

$$\bar{S}^{-1} \bar{B}(\hat{R}) \bar{S} = 1\bar{A}_1^{\pm}(\hat{R}) \oplus 1\bar{A}_2^{\pm}(\hat{R}) \oplus 2\bar{E}^{\pm}(\hat{R}) \oplus 3\bar{T}_1^{\pm}(\hat{R}) \oplus 3\bar{T}_2^{\pm}(\hat{R}) \equiv \bar{A}(\hat{R}), \quad (6)$$

where  $\bar{\Gamma}(\hat{R})$  denotes the representation matrix of  $\hat{R}$  in the irrep  $\Gamma,$  and the number before  $\bar{\Gamma}$  indicates the number of occurrences of  $\Gamma$  in the regular representation. Using  $(i, \Gamma, n)$  to label the  $n$ -th vector of the  $i$ -th occurrence of an irrep  $\Gamma,$  the matrix  $\bar{A}$  takes the block diagonal form:

$$\bar{A}_{i\Gamma n, i'\Gamma' n'}(\hat{R}) = \delta_{i'i} \delta_{\Gamma'\Gamma} \bar{\Gamma}_{n, n'}(\hat{R}). \quad (7)$$

With the unitary transformation matrix  $\bar{S},$  one can construct the states  $|\Psi_{i, \Gamma, n}^{\dagger}\rangle$  as

$$|\Phi_{i, \Gamma, n}^{\dagger}\rangle = \sum_{\hat{R}} |\Phi_{\hat{R}}^{\dagger}\rangle \bar{S}_{R, i\Gamma n}, \quad (8)$$

which will satisfy

$$\hat{P}_R |\Phi_{i, \Gamma, n}^{\dagger}\rangle = \sum_{i', \Gamma', n'} |\Phi_{i', \Gamma', n'}^{\dagger}\rangle \left( \bar{A}(\hat{R}) \right)_{i'\Gamma' n', i\Gamma n}. \quad (9)$$

Correspondingly, a new type of two-hadron operator can be defined as in Eq.(A6) as

$$\Phi_{i, \Gamma, n}^{\dagger} = \sum_{\hat{R}} \Phi_{\hat{R}}^{\dagger} \bar{S}_{R, i\Gamma n}. \quad (10)$$

## B. Correlation function

The elementary two-point correlation function is constructed from  $\Phi_{\hat{R}}(t; \mathbf{x}, \boldsymbol{\delta})$  at the source and sink as follows:

$$G_{\hat{R}, \hat{R}'}(t; \mathbf{p}; \mathbf{x}, \boldsymbol{\delta}) = \sum_{(\mathbf{y}-\mathbf{x}) \in \mathbb{Z}^3} e^{-i\mathbf{p} \cdot (\mathbf{y}-\mathbf{x})} \left\langle \text{T} \left( \Phi_{\hat{R}}(t; \mathbf{y}, \boldsymbol{\delta}), \Phi_{\hat{R}'}^\dagger(0; \mathbf{x}, \boldsymbol{\delta}) \right) \right\rangle$$

where the angle brackets denote the ensemble average across gauge ensembles and T the time-ordered product of field operators. While this generally involves the full set of rotations at source and sink, we can exploit the translational and rotational symmetry of this correlator to obtain:

$$G_{\hat{R}, \hat{R}'}(t; \mathbf{p}; \mathbf{x}, \boldsymbol{\delta}) = G_{\hat{R}\hat{R}^{-1}, \hat{I}}(t; \mathbf{p}; \mathbf{x}, \boldsymbol{\delta}) \quad \forall \hat{R}, \hat{R}' \in G^{\mathbf{p}}. \quad (11)$$

The projection of the correlation function onto definite irreps of the lattice rotation group is then given by

$$\tilde{G}_\Gamma(t; \mathbf{p}; \mathbf{x}, \boldsymbol{\delta}) = \sum_{(\mathbf{y}-\mathbf{x}) \in \mathbb{Z}^3} e^{-i\mathbf{p} \cdot (\mathbf{y}-\mathbf{x})} \left\langle \text{T} \left( \Phi_{i, \Gamma, n}(t; \mathbf{y}, \boldsymbol{\delta}), \Phi_{i, \Gamma, n}^\dagger(0; \mathbf{x}, \boldsymbol{\delta}) \right) \right\rangle \quad (12)$$

$$= \frac{1}{l_\Gamma} \sum_{\hat{R}} \chi_{\hat{R}}^\Gamma G_{\hat{R}, \hat{I}}(t; \mathbf{p}; \mathbf{x}, \boldsymbol{\delta}), \quad (13)$$

where  $\chi_{\hat{R}}^\Gamma$  is the character number of element  $\hat{R}$  of the group in the irrep  $\Gamma$ , and  $l_\Gamma$  is the dimension of the irrep  $\Gamma$ . See Appendix A for an in depth discussion.

A demonstration of the technique introduced here is performed in the  $\pi^- \pi^-$  system. The individual contributions,  $G_{\hat{R}^{-1}, \hat{I}}$ , to the target correlation functions are given in terms of the Wick contractions shown in Fig. 2, given explicitly by:

$$\begin{aligned} G_{\hat{R}^{-1}, \hat{I}}(t; \mathbf{p}; \mathbf{x}, \boldsymbol{\delta}) &= \sum_{(\mathbf{y}-\mathbf{x}) \in \mathbb{Z}^3} e^{i\mathbf{p} \cdot (\mathbf{y}-\mathbf{x})} \\ &\times \left\langle \left\{ \text{Tr} [S_d(\mathbf{y}_R^-, t; \mathbf{x}^-) S_u^\dagger(\mathbf{y}_R^-, t; \mathbf{x}^-, 0)] \text{Tr} [S_d(\mathbf{y}_R^+, t; \mathbf{x}^+, 0) S_u^\dagger(\mathbf{y}_R^+, t; \mathbf{x}^+, 0)] \right. \right. \\ &\quad + \text{Tr} [S_d(\mathbf{y}_R^+, t; \mathbf{x}^-, 0) S_u^\dagger(\mathbf{y}_R^+, t; \mathbf{x}^-, 0)] \text{Tr} [S_d(\mathbf{y}_R^-, t; \mathbf{x}^+, 0) S_u^\dagger(\mathbf{y}_R^-, t; \mathbf{x}^+, 0)] \\ &\quad - \text{Tr} [S_d(\mathbf{y}_R^-, t; \mathbf{x}^-, 0) S_u^\dagger(\mathbf{y}_R^+, t; \mathbf{x}^-, 0) S_d(\mathbf{y}_R^+, t; \mathbf{x}^+, 0) S_u^\dagger(\mathbf{y}_R^-, t; \mathbf{x}^+, 0)] \\ &\quad \left. \left. - \text{Tr} [S_d(\mathbf{y}_R^+, t; \mathbf{x}^-, 0) S_u^\dagger(\mathbf{y}_R^-, t; \mathbf{x}^-, 0) S_d(\mathbf{y}_R^-, t; \mathbf{x}^+, 0) S_u^\dagger(\mathbf{y}_R^+, t; \mathbf{x}^+, 0)] \right\} \right\rangle. \quad (14) \end{aligned}$$

Here we have made use of the notation

$$\mathbf{x}^\pm = \frac{2\mathbf{x} \pm \boldsymbol{\delta}}{2}, \quad \mathbf{y}_R^\pm = \frac{2\mathbf{y} \pm \hat{R}\boldsymbol{\delta}}{2}, \quad (15)$$

and  $S_q(\mathbf{y}, t; \mathbf{x}, 0)$  denotes a conventional point-to-all propagator. The quark flavours,  $q = u$  or  $d$ , are shown explicitly, however in the following numerical calculation we assume isospin symmetry,  $S_u = S_d$ .

Given the form of the correlator construction, we note that the correlation function can be efficiently calculated by only performing Dirac matrix inversions from two distinct sites  $\mathbf{x}^\pm$ . Furthermore, in the moving frame, the same spectra are extracted from the set of

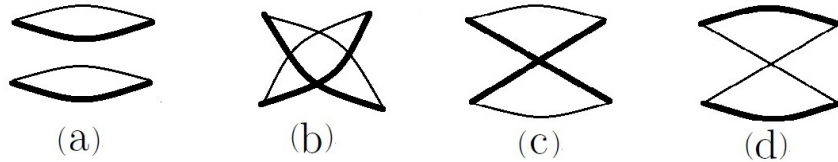


FIG. 2. Diagrams for Wick contractions. Thick and thin lines are to distinguish  $d$  and  $u$  propagators, respectively.

$\tilde{G}_\Gamma(t; \mathbf{p}; \mathbf{x}, \boldsymbol{\delta})$  with the same  $|\mathbf{p}|$ . One can therefore sum over each direction to reduce the statistical variance, *i.e.*,

$$\tilde{G}_\Gamma(t; P; \mathbf{x}, \boldsymbol{\delta}) = \sum_{\mathbf{p}, |\mathbf{p}|=P} \sum_{\hat{R} \in G^{\mathbf{p}}} \chi_{\hat{R}}^\Gamma G_{\hat{R}, \hat{I}}(t; \mathbf{p}; \mathbf{x}, \boldsymbol{\delta}), \quad (16)$$

where, as above,  $G^{\mathbf{p}}$  denotes the rotation group for specific total momentum  $\mathbf{p}$ .

In the following Section we present numerical results for the determination of the ground states in each of the considered irreps up to  $P^2 = 3P_0^2$ , where  $P_0$  defines the basic momentum unit in the box  $P_0 \equiv 2\pi/L$ .

### III. NUMERICAL RESULTS

#### A. Lattice setup

Following the prescription given by Eqs. (14) and (16) and Tables V and VI, the correlation functions of the  $\pi^-\pi^-$  system are analysed for various total momenta and irreps of the lattice rotation group. The present calculation is performed on an ensemble with 2 flavours of dynamical  $\mathcal{O}(a)$ -improved Wilson fermions with  $\beta = 5.29$ ,  $\kappa = 0.13550$  on a  $24^3 \times 48$  volume, corresponding to  $a = 0.71$  fm and  $m_\pi \simeq 900$  MeV, from the QCDSF Collaboration [44].

Results are collected from 376 configurations using 16 different randomised source locations, totalling  $\mathcal{O}(6,000)$  measurements. With two distinct propagators required for each source, the comparative computational cost of the present calculation is  $\mathcal{O}(12,000)$  measurements. For comparison, other calculations of the isospin-2  $\pi\pi$  system in lattice QCD have used various amounts of computation, depending the complexity of the observable:  $\mathcal{O}(4,500)$  by NPLQCD to extract the  $S$ -wave scattering length [45];  $\mathcal{O}(290,000)$  by NPLQCD [46] for the energy-dependent  $S$ -wave phase shifts [7]; and  $\mathcal{O}(270,000)$  by Dudek et al. to isolate  $S$ - and  $D$ -wave phase shifts [6].

#### B. Spectra

In this study, we consider correlation functions with total momentum up to three lattice units  $|\mathbf{p}| \leq \sqrt{3}P_0$ . The correlation functions for each irrep are fit with a parameterisation taking the form:

$$G(t) = A (e^{-Et} + e^{-E(T-t)}) + B (e^{-\Delta Et} + e^{-\Delta E(T-t)}), \quad (17)$$



where the fit parameters  $A$  and  $E$  correspond to the amplitude and 2-point energy of interest. The term involving  $B$  is provided to isolate the leading contribution arising from thermal states, as is familiar in studies of multi-hadron correlators [6, 47–52]. For the present study, this corresponds to one pion propagating forwards and the other backwards in Euclidean time. The value of the exponent in the thermal contribution is held fixed to  $\Delta E = E_\pi(\mathbf{p} - \mathbf{k}) - E_\pi(\mathbf{k})$ , for single-pion energies  $E_\pi$ , and  $\mathbf{k}$  chosen to correspond to the lightest single pion state contributing to the given correlator. At large temporal extent, the coefficient  $B$  should scale according to  $e^{-E_\pi(\mathbf{k})T}$ . While we don't have numerical results at different  $T$ , we see that the fitted values of  $B$  are always suppressed by this order of magnitude compared to  $A$ .

After subtracting the contributions from thermal states, Figure 3 displays the effective mass for different total momenta and irreducible representation. We see a clear separation of the energy levels in distinct irreps. As expected, the low-lying  $A_1$  irreps are generally cleaner statistically, whereas the signal quality degrades for the irreps corresponding to the resolution of higher-spin partial waves.

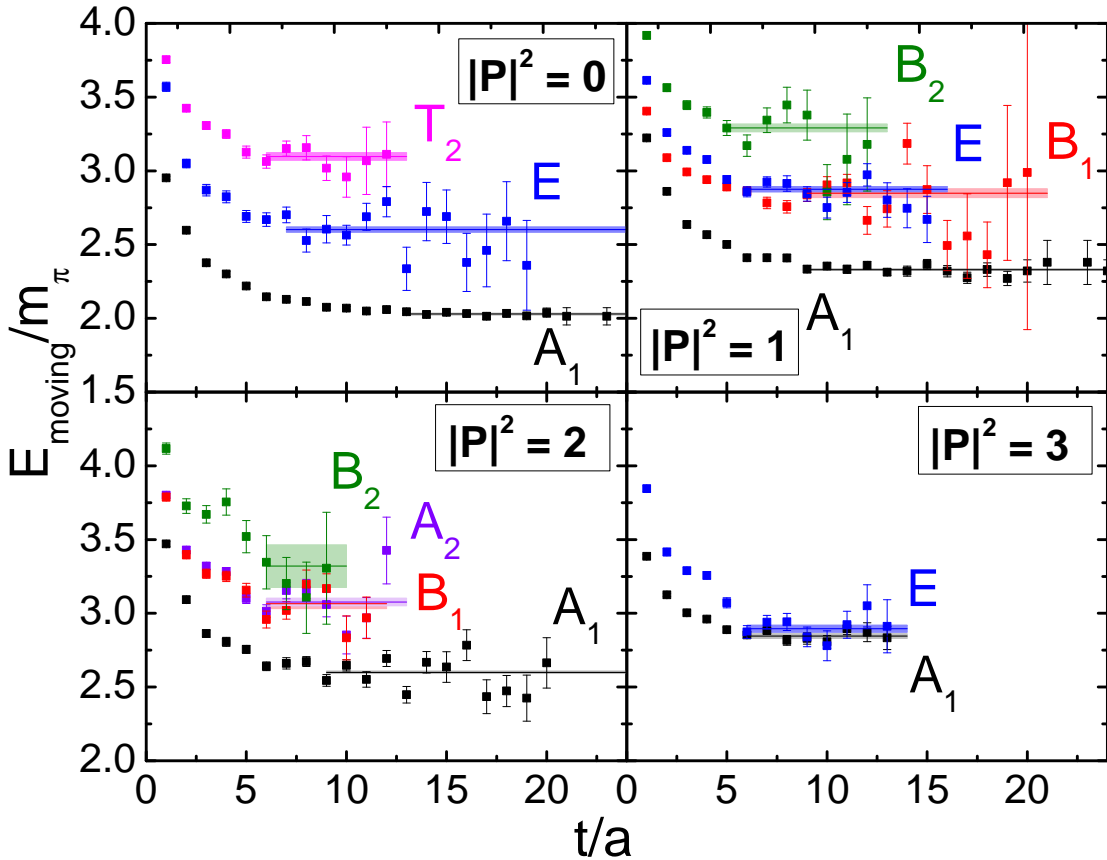


FIG. 3. The effective energies for different total momenta  $P$  (in multiples of  $2\pi/L$ ), and different irreps. The bands display the two-pion energies fitted to Eq. (17). The horizontal width of the bands indicates the corresponding fit window.

The results for the extracted energy levels are shown by the black circles in Fig. 4. For comparison, the low-lying non-interacting energy levels in each system are displayed by the grey lines. Each of the energy levels isolated are consistent with some degree of

weak repulsion, as expected for the  $I = 2$  state. For most of the states considered, the first excited state is expected to be clearly separated, and hence the ground-state isolation should be reliable (to within the statistical uncertainties of this work). However, there are three particular channels where multiple low-lying states are anticipated, arising from the clustering of non-interacting two-particle energy levels. These include  $A_1$  at  $P^2 = 2P_0^2, 3P_0^2$  and  $B_2$  at  $P^2 = 2P_0^2$ . In these cases, we do not expect that our correlation functions are dominated by a single ground-state energy and hence the fitted parameters are not representative of eigenenergies of the system.

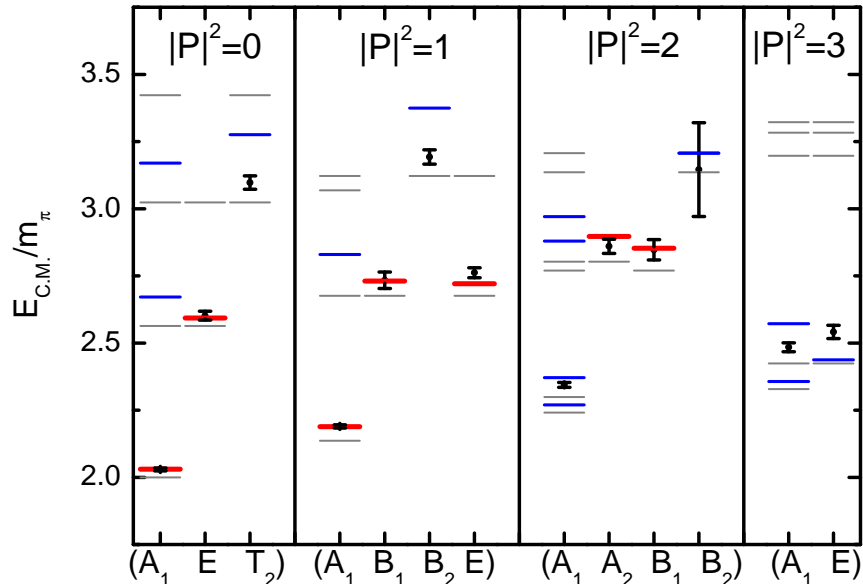


FIG. 4. The energy levels of the various systems with different total momenta and irreps. The black points show the extracted centre-of-momentum (CM) energies. The grey lines display the locations of the corresponding non-interacting energies. The red lines show the fitted energies according to fit (iii), as described in Table II, and the blue lines display further predicted eigenvalues based upon this fit.

Within the operator construction presented, only the total momentum is specified, whereas the momentum of each pion is not. In contrast to Refs. [7, 37], which involve momentum-projected hadrons at the sink, we use the same operators at both the source and sink. While staying within the paradigm of local sources, this method then lends itself to a variational analysis [11, 53, 54], where the operator basis can be extended by varying  $|\delta\rangle$ .

### C. Phase shifts

We use the following Lüscher formula [5, 26, 31], assuming that exponentially-suppressed corrections can be neglected, to extract phase shifts from finite-volume spectra:

$$\det[M_{\ell n, \ell' n'}^{\Gamma, \mathbf{p}}(q(\Gamma)) - \delta_{\ell, \ell'} \delta_{n, n'} \cot \delta_{\ell}(q(\Gamma))] = 0. \quad (18)$$

The matrix  $M_{\ell n, \ell' n'}^{\Gamma, \mathbf{P}}$  has been discussed extensively in the literature, see e.g. [28, 31, 34]. For completeness, we provide detail relevant to the present investigation in Appendix B.

As encoded by Eq. (18), each energy level determined on the lattice is constrained by multiple partial waves — see Table I. This necessitates the use of a parameterisation of the energy dependence of the phase shifts in order to isolate the individual partial waves. For the purpose of this investigation, we consider the parameterisation of the  $\ell$ -wave phase shifts by the effective range expansion:

$$q^{2\ell+1} \cot \delta_\ell = \frac{1}{a_\ell} + \frac{1}{2} r_\ell q^2, \quad (19)$$

for parameters  $a_\ell$  and  $r_\ell$  — for  $\ell = 0$  these are familiarly recognised as the scattering length and effective range, respectively. Such a parameterisation should be reasonable for the weakly-repulsive interactions anticipated in  $I = 2$  scattering.

TABLE I. The relationship between angular momentum and irrep in the various momentum. The total angular momentum quantum number for exact spherical symmetry are only quoted up to  $\ell = 4$ .

Group	$ \mathbf{p}L/2\pi ^2$	$\Gamma$	$\ell$
$O_h$	0	$A_1^+$	0, 4
		$A_2^+$	>4
		$E^+$	2, 4
		$T_1^+$	4
		$T_2^+$	2, 4
		$C_{4v}$	1
$C_{4v}$	1	$A_2$	>4
		$B_1$	2, 4
		$B_2$	2, 4
		$E$	2, 4
		$C_{2v}$	2
$C_{2v}$	2	$A_2$	2, 4
		$B_1$	2, 4
		$B_2$	2, 4
		$C_{3v}$	3
$C_{3v}$	3	$A_2$	> 4
		$E$	2, 4

As described above, we do not expect that our extracted energy levels in  $A_1$  at  $P^2 = 2P_0^2, 3P_0^2$  or  $B_2$  at  $P^2 = 2P_0^2$  are meaningful representations of an energy eigenstate, and hence these are excluded from any fits. This leaves up to 10 data points for constraining the phase shift parameterisation. We summarise a selection of fit prescriptions in Table II. In fit (i), we attempt to describe all 10 data points with just a leading order  $a_\ell$  in each partial wave. We find that the  $E$  representation at  $P^2 = 3P_0^2$  is incompatible with the fit form, as shown in Table III, and hence we drop this point also from subsequent fits. Just dropping this one point improves the reduced  $\chi^2$  ( $\chi_r^2$ ) significantly in fit (ii), yet still suggests some tension with the data. As further modifications, we try removing the large centre-of-mass

( $E^*/m > 3$ ) points in fit (iii). In fits (iv) and (v) we introduce parameters  $r_0$  or  $r_2$  to capture any additional curvature in the energy dependence of the phase shifts. However, we find that these additional parameters are poorly constrained and lead to weaker  $\chi_r^2$  values. Hence we conclude that the best description of our lattice results is that of fit (iii), with a restriction to the lower-energy spectra and fitting just a single parameter in each partial wave,  $\ell = 0, 2, 4$ .

TABLE II. Fitted parameters.

Fit	$\{3_E\}$	$\{E^*/m > 3\}$	$N_{\text{data}}$	$a_{0,2,4}$	$r_0$	$r_2$
i	✓	✓	10	✓	×	×
ii	×	✓	9	✓	×	×
iii	×	×	7	✓	×	×
iv	×	✓	9	✓	✓	×
v	×	✓	9	✓	×	✓

TABLE III. Fitted parameters.

Fit	$a_0$	$r_0$	$a_2$	$r_2 \times 10^6$	$a_4$	$\chi^2$	$\chi_r^2$
i	-0.690(53)	—	-0.0111(84)	—	-0.0200(41)	36.2	5.2
ii	-0.691(65)	—	-0.0092(64)	—	-0.0208(43)	15.5	2.6
iii	-0.683(65)	—	-0.0602(58)	—	-0.0118(48)	7.2	1.8
iv	-0.65(11)	0.7(19)	-0.0091(90)	—	-0.0208(67)	15.4	3.1
v	-0.691(53)	—	-0.0092(96)	0.5(51)	-0.0208(67)	15.5	3.9

The fitted spectra for fit (iii) are displayed by the red lines in Fig. 4. For this fit, we also show additional predicted finite-volume spectra for this parameterisation by the blue lines. From the fit parameters in Table III, we see a clear signal for a  $G$ -wave interaction. This gets somewhat stronger for the other fit forms considered, however at the expense of a reduced fit quality. For the preferred fit, we show the corresponding phase shifts in Fig. 5.

#### IV. SUMMARY AND OUTLOOK

In this paper, we introduce a new extended operator to extract the spectra of irreducible representations at rest and in moving systems. In coordinate space, the two-particle operator projects onto an irrep by summing appropriately over a spherical shell. The method is straightforward to implement as a generalisation of conventional point sources, and hence offers an alternative for cases where stochastic momentum sources are impractical.

For the numerical investigation in this work, we studied the isospin-2  $\pi\pi$  system at a range of total momenta, on a  $24^3 \times 48$  volume with a lattice spacing of  $a = 0.071$  fm and  $m_\pi \approx 900$  MeV. The correlation functions of various irreps with a total momentum-squared ranging from 0 to 3 have been studied, with 13 plateaus—10 of which were considered as viable ground-state candidates. These discrete finite volume spectra have then been analysed

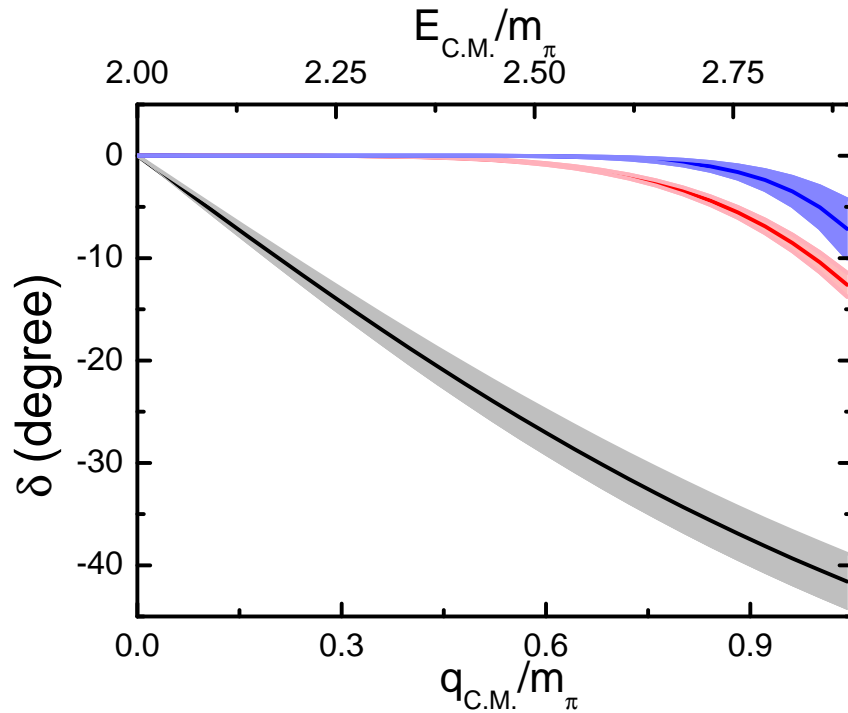


FIG. 5. The phase shifts from the fit parameterisation (iii), as described in the text. The black, red and blue curves are for the  $S$ -,  $D$ - and  $G$ -wave phase shifts. Note the top and bottom horizontal axes provide the total energy and the corresponding on-shell momentum, respectively, in the CM system.

with the Lüscher quantisation condition. Using a simple effective range expansion of the phase shifts, we identify  $S$ -,  $D$ - and  $G$ -wave interactions.

In the future, this method can also be readily extended to particles with spin, particularly for the two baryon system. Including a basis of operators at different hadronic separations would allow for a variational analysis to be performed, and thereby allow for a determination of the excited energy levels on the lattice. This would correspond to an analogue of mapping out the quantum mechanical coordinate-space wave function.

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## Appendix A: Octahedral Group ( $O_h$ ) and Its Little Groups

### 1. The 48 elements of $O_h$ group

The cubic group ( $O$ ) has 24 elements indicated as  $R_i$  ( $i = 1-24$ ) which correspond to 24 rotations,  $\hat{R}_i$  as listed in Table IV. Starting with one vector  $\boldsymbol{\delta}_1 \equiv (q_1, q_2, q_3)$ , one can then construct 23 vectors via  $\hat{R}_i$  ( $i = 2-24$ ) ( $\hat{R}_1$  is the identity operator) as follows:

$$\boldsymbol{\delta}_i = \hat{R}_i \boldsymbol{\delta}_1, \quad (\text{A1})$$

In Table IV, the 24 vectors  $\boldsymbol{\delta}_i$  are all listed. The  $O_h$  group can be recognized as the product of the  $O$  group and the  $C_2 = \{e, \hat{\sigma}\}$  group, *i.e.*,  $O_h = O \otimes C_2$ . Then the other 24 operators belonging to  $O_h$  group rather than  $O$  group will be  $\hat{R}_{i+24} = \hat{\sigma} \hat{R}_i$ , and correspondingly,  $\boldsymbol{\delta}_{i+24} = -\boldsymbol{\delta}_i$ .

### 2. The Classes and Irreps of $O_h$ group

There are 48 elements in the  $O_h$  group and they can be partitioned into 10 different classes. There are ten irreps,  $A_1^\pm(1)$ ,  $A_2^\pm(1)$ ,  $E^\pm(2)$ ,  $T_1^\pm(3)$ , and  $T_2^\pm(3)$ , where the numbers in the parentheses are the dimensions of these irreps. The character table of the cubic group is shown in Table V.

### 3. Regular Representation

Using the  $O_h$  group, a scalar function  $\phi(\boldsymbol{\delta})$  can be extended to 48 functions as follows

$$\phi_R(\boldsymbol{\delta}) = \hat{P}_R \phi(\boldsymbol{\delta}) = \phi(\hat{R}^{-1} \boldsymbol{\delta}). \quad (\text{A2})$$

Under the group action, they should transform as

$$\hat{P}_R \phi_{R'}(\boldsymbol{\delta}) = \sum_{R''} \phi_{R''}(\boldsymbol{\delta}) \left( \bar{B}(\hat{R}) \right)_{R'', R'} = \hat{P}_R \hat{P}_{R'} \phi(\boldsymbol{\delta}) = \hat{P}_{RR'} \phi(\boldsymbol{\delta}) = \phi(\hat{R}'^{-1} \hat{R}^{-1} \boldsymbol{\delta}) = \phi_{RR'}(\boldsymbol{\delta}).$$

Here  $\bar{B}(\hat{R})$  is the representation matrix of  $\hat{R}$  for the regular representation. The dimension of the regular representation is the same as the order of the group.

### 4. From Regular Representation to Irreps

The regular representation of any non-trivial group is reducible. So  $\bar{B}$  can be made block diagonal according to the irreps of  $O_h$  via a unitary transformation matrix  $\bar{S}$  as follows

$$\bar{S}^{-1} \bar{B}(\hat{R}) \bar{S} = 1\bar{A}_1^\pm(\hat{R}) \oplus 1\bar{A}_2^\pm(\hat{R}) \oplus 2\bar{E}^\pm(\hat{R}) \oplus 3\bar{T}_1^\pm(\hat{R}) \oplus 3\bar{T}_2^\pm(\hat{R}) \equiv \bar{A}(\hat{R}) \quad (\text{A3})$$

TABLE IV. For the  $O$  group, 24 vectors  $\delta_i$  and operators  $R_i$  ( $i = 1-24$ ) are listed.  $\delta_1^\top \equiv (q_1, q_2, q_3)$  and  $R_1 \equiv E$  which is the identity.  $R_i$  includes the rotation axis and angle.

Class	$R_i$	Axis-Angle	Euler Angle	$\delta_i^\top$
$E$	$R_1$	Any $0^\circ$	$(0^\circ, 0^\circ, 0^\circ)$	$(q_1, q_2, q_3)$
$8C'_3$	$R_2$	$(1, 1, 1) -120^\circ$	$(90^\circ, 90^\circ, 180^\circ)$	$(q_2, q_3, q_1)$
	$R_3$	$(1, 1, 1) +120^\circ$	$(0^\circ, 90^\circ, 90^\circ)$	$(q_3, q_1, q_2)$
	$R_4$	$(-1, 1, 1) -120^\circ$	$(180^\circ, 90^\circ, 90^\circ)$	$(-q_3, -q_1, q_2)$
	$R_5$	$(-1, 1, 1) +120^\circ$	$(90^\circ, 90^\circ, 0^\circ)$	$(-q_2, q_3, -q_1)$
	$R_6$	$(-1, -1, 1) -120^\circ$	$(-90^\circ, 90^\circ, 0^\circ)$	$(q_2, -q_3, -q_1)$
	$R_7$	$(-1, -1, 1) +120^\circ$	$(180^\circ, 90^\circ, -90^\circ)$	$(-q_3, q_1, -q_2)$
	$R_8$	$(1, -1, 1) -120^\circ$	$(0^\circ, 90^\circ, -90^\circ)$	$(q_3, -q_1, -q_2)$
	$R_9$	$(1, -1, 1) +120^\circ$	$(-90^\circ, 90^\circ, 180^\circ)$	$(-q_2, -q_3, q_1)$
	$6C_4$	$R_{10}$	$(1, 0, 0) -90^\circ$	$(90^\circ, 90^\circ, -90^\circ)$
$R_{11}$		$(1, 0, 0) +90^\circ$	$(-90^\circ, 90^\circ, 90^\circ)$	$(q_1, -q_3, q_2)$
$R_{12}$		$(0, 1, 0) -90^\circ$	$(180^\circ, 90^\circ, 180^\circ)$	$(-q_3, q_2, q_1)$
$R_{13}$		$(0, 1, 0) +90^\circ$	$(0^\circ, 90^\circ, 0^\circ)$	$(q_3, q_2, -q_1)$
$R_{14}$		$(0, 0, 1) -90^\circ$	$(-90^\circ, 0^\circ, 0^\circ)$	$(q_2, -q_1, q_3)$
$R_{15}$		$(0, 0, 1) +90^\circ$	$(90^\circ, 0^\circ, 0^\circ)$	$(-q_2, q_1, q_3)$
$6C''_2$	$R_{16}$	$(0, 1, 1) -180^\circ$	$(90^\circ, 90^\circ, 90^\circ)$	$(-q_1, q_3, q_2)$
	$R_{17}$	$(0, -1, 1) -180^\circ$	$(-90^\circ, 90^\circ, -90^\circ)$	$(-q_1, -q_3, -q_2)$
	$R_{18}$	$(1, 1, 0) -180^\circ$	$(-90^\circ, 180^\circ, 0^\circ)$	$(q_2, q_1, -q_3)$
	$R_{19}$	$(1, -1, 0) -180^\circ$	$(90^\circ, 180^\circ, 0^\circ)$	$(-q_2, -q_1, -q_3)$
	$R_{20}$	$(1, 0, 1) -180^\circ$	$(0^\circ, 90^\circ, 180^\circ)$	$(q_3, -q_2, q_1)$
	$R_{21}$	$(-1, 0, 1) -180^\circ$	$(180^\circ, 90^\circ, 0^\circ)$	$(-q_3, -q_2, -q_1)$
$3C^2_4$	$R_{22}$	$(1, 0, 0) -180^\circ$	$(180^\circ, 180^\circ, 0^\circ)$	$(q_1, -q_2, -q_3)$
	$R_{23}$	$(0, 1, 0) -180^\circ$	$(0^\circ, 180^\circ, 0^\circ)$	$(-q_1, q_2, -q_3)$
	$R_{24}$	$(0, 0, 1) -180^\circ$	$(180^\circ, 0^\circ, 0^\circ)$	$(-q_1, -q_2, q_3)$

The number before the irrep indicates the occurrence of that irrep. At last you will find  $48 = 2(1^2 + 1^2 + 2^2 + 3^2 + 3^2)$ . And the matrix  $\bar{A}$  can be written as:

$$\bar{A}_{i\Gamma n, i'\Gamma' n'}(\hat{R}) = \delta_{i'i} \delta_{\Gamma'\Gamma} \bar{\Gamma}_{n, n'}(\hat{R}), \quad (\text{A4})$$

where  $\Gamma$  is the name of the irrep, and  $i$  shows how many times it appears, for example  $i = 1, 2, 3$  for  $T_1^\pm$  and  $T_2^\pm$ , and  $i = 1, 2$  for  $E$ , and  $i = 1$  for  $A_1^\pm$  and  $A_2^\pm$ ; and  $n$  indicates the order of the irrep  $\Gamma$ . The matrix  $\bar{\Gamma}(\hat{R})$  is the matrix representation of element  $\hat{R}$  in the irrep  $\Gamma$ . Because  $O_h$  is a finite group, the matrices  $\bar{\Gamma}$  can be chosen to be unitary.

As shown in Eq.(A3), the matrices  $\bar{B}(\hat{R})$  show the rotations of 48 scalar functions  $\phi$ . Then matrices  $\bar{A}$  also have 48 scalar functions satisfied:

$$\hat{P}_R \Phi_{i, \Gamma, n}(\boldsymbol{\delta}) = \sum_{i', \Gamma', n'} \Phi_{i', \Gamma', n'}(\boldsymbol{\delta}) \left( \bar{A}(\hat{R}) \right)_{i' \Gamma' n', i \Gamma n}. \quad (\text{A5})$$

The transformation matrix  $\bar{S}$  can connect  $\Phi_R$  and  $\Phi_{i, \Gamma, n}$  as follows:

$$\Phi_{i, \Gamma, n} = \sum_R \phi_R \bar{S}_{R, i \Gamma n}. \quad (\text{A6})$$

The row index of  $\bar{S}$  is the name of the elements of the cubic group, and the column index is the same as the indices of  $\Phi$ ,  $(i, \Gamma, n)$ .

On the other hand, from Eq.(A3, A5, A6), we have:

$$\begin{aligned} \hat{P}_R \Phi_{i, \Gamma, n} &= \sum_{n'} \Phi_{i, \Gamma, n'} \bar{\Gamma}_{n' n}(\hat{R}) = \sum_{R'} \sum_{n'} \phi_{R'} \bar{S}_{R' i \Gamma n'} \bar{\Gamma}_{n' n}(\hat{R}) \\ &= \hat{P}_R \sum_{R'} \phi_{R'} \bar{S}_{R', i \Gamma n} = \sum_{R'} \phi_{RR'} \bar{S}_{R', i \Gamma n}, \end{aligned} \quad (\text{A7})$$

Then we have:

$$\sum_{R'} \sum_{n'} \phi_{R'} \bar{S}_{R' i \Gamma n'} \bar{\Gamma}_{n' n}(\hat{R}) = \sum_{R'} \phi_{RR'} \bar{S}_{R', i \Gamma n}, \quad (\text{A8})$$

$$\bar{S}_{R, i \Gamma n} = \sum_m C_{i \Gamma m} \bar{\Gamma}_{m, n}(R^{-1}). \quad (\text{A9})$$

$$C_{i \Gamma m} = \bar{S}_{I, i \Gamma m} \quad (\text{A10})$$

The  $C_{i \Gamma m}$  satisfy the orthogonality relations:

$$\frac{l_\Gamma}{G} \delta_{i, i'} = \sum_m C_{i \Gamma m} C_{i' \Gamma m}^*, \quad (\text{A11})$$

$$\frac{l_\Gamma}{G} \delta_{m, m'} = \sum_i C_{i \Gamma m} C_{i \Gamma m'}^*. \quad (\text{A12})$$

where  $G$  and  $l_\Gamma$  are the orders of  $O_h$  group and irrep  $\Gamma$ , respectively.



## 5. The inner product of $\Phi_R$ and $\Phi_{(i,\Gamma,n)}$

We use the Dirac symbol for the inner product of  $\Phi_R$  and  $\Phi_{(i,\Gamma,n)}$ . The normalization is given by:

$$\delta_{R,R'} = \langle \Phi_R | \Phi_{R'} \rangle, \quad (\text{A13})$$

$$\delta_{i,i'} \delta_{\Gamma,\Gamma'} \delta_{n,n'} = \langle \Phi_{i,\Gamma,n} | \Phi_{i',\Gamma',n'} \rangle, \quad (\text{A14})$$

If we have some operator,  $\hat{H}$ , which is invariant under the rotation, such as the Hamiltonian operator, through Eq.(A6,A9,A12), we have:

$$\begin{aligned} \sum_i \langle \Phi_{i,\Gamma,n} | \hat{H} | \Phi_{i,\Gamma',n'} \rangle &= \sum_i \sum_{R,R'} \bar{S}_{R,i\Gamma n}^* \langle \phi_R | \hat{H} | \phi_{R'} \rangle \bar{S}_{R',i\Gamma' n'} \\ &= \sum_i \sum_{R,R'} \sum_{m,m'} C_{i\Gamma m}^* \bar{\Gamma}_{m,n}^*(R^{-1}) \langle \phi_{R'^{-1}R} | \hat{H} | \phi_I \rangle C_{i\Gamma' m'} \bar{\Gamma}_{m',n'}(R'^{-1}) \\ &= \sum_i \sum_{\tilde{R},R'} \sum_{m,m'} C_{i\Gamma m}^* \bar{\Gamma}_{m,n}^*(\tilde{R}^{-1}R'^{-1}) \langle \phi_{\tilde{R}} | \hat{H} | \phi_I \rangle C_{i\Gamma' m'} \bar{\Gamma}_{m',n'}(R'^{-1}) \\ &= \sum_i \sum_{\tilde{R}} \langle \phi_{\tilde{R}} | \hat{H} | \phi_I \rangle \sum_{m,m'} C_{i\Gamma m}^* C_{i\Gamma' m'} \sum_l \delta_{n,n'} \delta_{\Gamma,\Gamma'} \delta_{l,m'} \bar{\Gamma}_{m,l}^*(\tilde{R}^{-1}) \\ &= \sum_i \sum_{\tilde{R}} \langle \phi_{\tilde{R}} | \hat{H} | \phi_I \rangle \sum_m C_{i\Gamma m}^* C_{i\Gamma m} \frac{G}{l_\Gamma} \delta_{\Gamma,\Gamma'} \delta_{n,n'} \bar{\Gamma}_{m',m}(\tilde{R}) \\ &= \delta_{\Gamma,\Gamma'} \delta_{n,n'} \sum_{\tilde{R}} \left( \frac{G}{l_\Gamma} \sum_{m,m'} \sum_i C_{i\Gamma m'} \bar{\Gamma}_{m',m}(\tilde{R}) C_{i\Gamma m}^* \right) \langle \phi_{\tilde{R}} | \hat{H} | \phi_I \rangle \\ &= \delta_{\Gamma,\Gamma'} \delta_{n,n'} \sum_{\tilde{R}} \left( \frac{G}{l_\Gamma} \sum_{m,m'} \frac{l_\Gamma}{G} \delta_{m,m'} \bar{\Gamma}_{m',m}(\tilde{R}) \right) \langle \phi_{\tilde{R}} | \hat{H} | \phi_I \rangle \\ &= \delta_{\Gamma,\Gamma'} \delta_{n,n'} \sum_{\tilde{R}} \left( \chi^\Gamma(\tilde{R}) \right) \langle \phi_{\tilde{R}} | \hat{H} | \phi_I \rangle \end{aligned} \quad (\text{A15})$$

At last, we find

$$\sum_i \langle \Phi_{i,\Gamma,n} | \hat{H} | \Phi_{i,\Gamma',n'} \rangle = \delta_{\Gamma,\Gamma'} \delta_{n,n'} \sum_R \chi^\Gamma(R) \langle \phi_R | \hat{H} | \phi_I \rangle, \quad (\text{A16})$$

where  $\chi_{\tilde{R}}^\Gamma$  is the character of element  $\hat{R}$  in the  $\Gamma$  irrep. The character tables for  $O_h$  group and the little group are listed in Table V.

## 6. The rotation operator in the little group

The  $O_h$  group is discussed in detail in the above sections, and it is the symmetry group in the rest frame, i.e.,  $\mathbf{p} = 0$ . In the nonzero momentum system, the symmetry group becomes the subgroup of  $O_h$ , named as the little group. In each little group, the rotations satisfying  $\hat{R}\mathbf{p} = \mathbf{p}$  will survive. Therefore, for the moving system, one just needs to keep the surviving rotations and do the same procedure as that in the rest frame. All the rotations for different momentum with  $|\mathbf{p}| = 1, 2, 3$  are listed in Table VI.

TABLE V. Character table of  $O_h$ ,  $C_{4\nu}$ ,  $C_{2\nu}$  and  $C_{3\nu}$  for  $|\mathbf{p}L/2\pi|^2 = 0, 1, 2,$  and  $3,$  respectively.

$O_h$	$\Gamma/\text{Class}$	$I$	$8C'_3$	$6C_4$	$6C'_4$	$3C_4^2$	$\hat{\pi}$	$8C'_3 \times \hat{\pi}$	$6C_4 \times \hat{\pi}$	$6C'_4 \times \hat{\pi}$	$3C_4^2 \times \hat{\pi}$
	$A_1^\pm$	1	1	1	1	1	$\pm 1$	$\pm 1$	$\pm 1$	$\pm 1$	$\pm 1$
	$A_2^\pm$	1	1	-1	-1	1	$\pm 1$	$\pm 1$	$\mp 1$	$\mp 1$	$\pm 1$
	$E^\pm$	2	-1	0	0	2	$\pm 2$	$\mp 1$	0	0	$\pm 2$
	$T_1^\pm$	3	0	-1	1	-1	$\pm 3$	0	$\mp 1$	$\pm 1$	$\mp 1$
	$T_2^\pm$	3	0	1	-1	-1	$\pm 3$	0	$\pm 1$	$\mp 1$	$\mp 1$
$C_{4\nu}$	$\Gamma/\text{Class}$	$I$	$2C_4$	$2C'_2 \times \hat{\pi}$	$2C_2 \times \hat{\pi}$	$C'_2$					
	$A_1$	1	1	1	1	1					
	$A_2$	1	1	-1	-1	1					
	$B_1$	1	-1	-1	1	1					
	$B_2$	1	-1	1	-1	1					
	$E$	2	0	0	0	-2					
$C_{2\nu}$	$\Gamma/\text{Class}$	$I$	$C'_2$	$C'_2 \times \hat{\pi}$	$C_2 \times \hat{\pi}$						
	$A_1$	1	1	1	1						
	$A_2$	1	1	-1	-1						
	$B_1$	1	-1	1	-1						
	$B_2$	1	-1	-1	1						
$C_{3\nu}$	$\Gamma/\text{Class}$	$I$	$2C_3$	$3C'_2 \times \hat{\pi}$							
	$A_1$	1	1	1							
	$A_2$	1	1	-1							
	$E$	2	-1	0							

## Appendix B: Lüscher's quantisation condition

The Lüscher formalism provides a model-independent relationship between the phase shifts and the energy levels, assuming exponentially-suppressed finite-volume effects can be safely neglected. In this section, we give the relationship between the spectra of irreps considered in this work and the phase shifts up to  $\ell = 4$ . We have confirmed that the partial waves  $\ell = 0$  and  $\ell = 2$  agree with previous results reported in Ref. [31]. The general quantisation condition equation is summarised by:

$$\det[M_{ln,l'n'}^{\Gamma,\mathbf{p}}(q(\Gamma)) - \delta_{l,l'}\delta_{n,n'} \cot \delta_l(q(\Gamma))] = 0, \quad (\text{B1})$$

where  $\Gamma$ ,  $\mathbf{p}$ ,  $l(l')$  and  $n(n')$  indicate the irrep, total momentum, angular momentum and the  $n$ -th  $\Gamma$  appearing in the representation of this angular momentum, respectively.  $q(\Gamma)$  is the on-shell momentum of the energy level of irrep  $\Gamma$  in the C.M. system.

TABLE VI. The rotation for the each class in the  $O_h$  group,  $C_{4\nu}$ ,  $C_{2\nu}$  and  $C_{3\nu}$  for  $|\mathbf{p}| = 0, 1, 2$  and 3, respectively.

$O_h$	$\mathbf{p}/\text{Class}$	$I$	$8C'_3$	$6C_4$	$6C'_4$	$3C_4^2$	$\hat{\pi}$	$8C'_3 \times \hat{\pi}$	$6C_4 \times \hat{\pi}$	$6C'_4 \times \hat{\pi}$	$3C_4^2 \times \hat{\pi}$
	(0, 0, 0)	$\hat{R}_1$	$\hat{R}_{2-9}$	$\hat{R}_{10-15}$	$\hat{R}_{16-21}$	$\hat{R}_{22-24}$	$\hat{R}_{25}$	$\hat{R}_{26-33}$	$\hat{R}_{33-38}$	$\hat{R}_{39-44}$	$\hat{R}_{45-48}$
$C_{4\nu}$	$\mathbf{p}/\text{Class}$	$I$	$2C_4$	$2C'_2 \times \hat{\pi}$	$2C_2 \times \hat{\pi}$	$C_2$					
	(0, 0, $\pm 1$ )	$\hat{R}_1$	$\hat{R}_{14, 15}$	$\hat{R}_{42, 43}$	$\hat{R}_{46, 47}$	$\hat{R}_{24}$					
	(0, $\pm 1$ , 0)	$\hat{R}_1$	$\hat{R}_{12, 13}$	$\hat{R}_{44, 45}$	$\hat{R}_{46, 48}$	$\hat{R}_{23}$					
	( $\pm 1$ , 0, 0)	$\hat{R}_1$	$\hat{R}_{10, 11}$	$\hat{R}_{40, 41}$	$\hat{R}_{47, 48}$	$\hat{R}_{22}$					
$C_{2\nu}$	$\mathbf{p}/\text{Class}$	$I$	$C'_2$	$C'_2 \times \hat{\pi}$	$C_2 \times \hat{\pi}$						
	( $\pm 1$ , $\pm 1$ , 0)	$\hat{R}_1$	$\hat{R}_{18}$	$\hat{R}_{43}$	$\hat{R}_{48}$						
	( $\pm 1$ , 0, $\pm 1$ )	$\hat{R}_1$	$\hat{R}_{20}$	$\hat{R}_{45}$	$\hat{R}_{47}$						
	(0, $\pm 1$ , $\pm 1$ )	$\hat{R}_1$	$\hat{R}_{16}$	$\hat{R}_{41}$	$\hat{R}_{46}$						
	(0, $\pm 1$ , $\mp 1$ )	$\hat{R}_1$	$\hat{R}_{17}$	$\hat{R}_{40}$	$\hat{R}_{46}$						
	( $\pm 1$ , $\mp 1$ , 0)	$\hat{R}_1$	$\hat{R}_{21}$	$\hat{R}_{44}$	$\hat{R}_{47}$						
	( $\pm 1$ , 0, $\mp 1$ )	$\hat{R}_1$	$\hat{R}_{19}$	$\hat{R}_{42}$	$\hat{R}_{48}$						
$C_{3\nu}$	$\mathbf{p}/\text{Class}$	$I$	$2C_3$	$3C'_2 \times \hat{\pi}$							
	( $\pm 1$ , $\pm 1$ , $\pm 1$ )	$\hat{R}_1$	$\hat{R}_{2, 3}$	$\hat{R}_{41, 43, 45}$							
	( $\pm 1$ , $\pm 1$ , $\mp 1$ )	$\hat{R}_1$	$\hat{R}_{6, 7}$	$\hat{R}_{40, 43, 44}$							
	( $\pm 1$ , $\mp 1$ , $\pm 1$ )	$\hat{R}_1$	$\hat{R}_{8, 9}$	$\hat{R}_{40, 42, 45}$							
	( $\mp 1$ , $\pm 1$ , $\pm 1$ )	$\hat{R}_1$	$\hat{R}_{4, 5}$	$\hat{R}_{41, 42, 44}$							

The matrix  $M$  is calculated from:

$$M_{ln, l'n'}^{\Gamma, \mathbf{p}}(q(\Gamma)) = \sum_{m, m'} C_{l, m}^{\Gamma, \alpha, n*} C_{l', m'}^{\Gamma, \alpha, n'} M_{lm, l'm'}^{\mathbf{p}}(q(\Gamma)), \quad (\text{B2})$$

$$M_{lm, l'm'}^{\mathbf{p}}(q(\Gamma)) = (-1)^l \sum_{j=|l-l'|}^{l+l'} \sum_{s=-j}^j i^j \sqrt{2j+1} \omega_{js}^{\mathbf{d}=\mathbf{p}L/2\pi} (\tilde{q} = q(\Gamma)L/2\pi) C_{lm, js, l'm'}, \quad (\text{B3})$$

$$\omega_{js}^{\mathbf{d}}(\tilde{q}) = \frac{1}{\pi^{3/2} \sqrt{2j+1}} \frac{Z_{js}^{\mathbf{d}}(1, \tilde{q})^{-1}}{\gamma \tilde{q}^{j+1}}, \quad (\text{B4})$$

where the index  $\alpha$  is an index denoting the dimension of the irrep  $\Gamma$ .  $\gamma$  is the Lorentz factor

$$\gamma = \frac{W}{E_{C.M.}} = \frac{\sqrt{\mathbf{p}^2 + E_{C.M.}^2}}{E_{C.M.}}, \quad (\text{B5})$$

where  $E_{C.M.} = 2\sqrt{q^2 + m_\pi^2}$  is the energy level in the C.M. system.

The factor  $C_{lm,js,l'm'}$  is related to the Wigner 3-j symbols as follows,

$$C_{lm,js,l'm'} = (-1)^{m'} i^{l-j+l'} \sqrt{(2l+1)(2j+1)(2l'+1)} \begin{pmatrix} l & j & l' \\ m & s & -m' \end{pmatrix} \begin{pmatrix} l & j & l' \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{B6})$$

Now we only need to know the coefficients  $C_{l,m}^{\Gamma,\alpha,n}$  in Eq. (B2). We give these values in Table VII for the moving system, while for the rest frame, the matrices  $M_{ln,l'n'}^{\Gamma,\mathbf{p}}(q(\Gamma))$  can be read from Ref. [26]. It is worth mentioning that in our calculation we average over all momenta with fixed  $|\mathbf{p}|$ . Since the spectra of them are the same, we choose one case to list each  $C_{l,m}^{\Gamma,\alpha,n}$ . Finally, Eq. (B1) for each case are listed in the following.

For the  $A_1$  irrep in the rest frame,  $\mathbf{d} = \mathbf{p}L/2\pi = \mathbf{0}$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_0 + \omega_{00}^{\mathbf{d}} & \frac{6\sqrt{21}}{7}\omega_{40}^{\mathbf{d}} \\ \frac{6\sqrt{21}}{7}\omega_{40}^{\mathbf{d}} & -\cot \delta_4 + \omega_{00}^{\mathbf{d}} + \frac{324}{143}\omega_{40}^{\mathbf{d}} + \frac{80}{11}\omega_{60}^{\mathbf{d}} + \frac{560}{143}\omega_{80}^{\mathbf{d}} \end{pmatrix}. \quad (\text{B7})$$

For the  $E$  irrep in the rest frame,  $\mathbf{d} = \mathbf{0}$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_2 + \omega_{00}^{\mathbf{d}} + \frac{18}{7}\omega_{40}^{\mathbf{d}} & -\frac{120\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} - \frac{30\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} \\ -\frac{120\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} - \frac{30\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} & -\cot \delta_4 + \omega_{00}^{\mathbf{d}} + \frac{324}{1001}\omega_{40}^{\mathbf{d}} - \frac{64}{11}\omega_{60}^{\mathbf{d}} + \frac{392}{143}\omega_{80}^{\mathbf{d}} \end{pmatrix}. \quad (\text{B8})$$

For the  $T_2$  irrep in the rest frame,  $\mathbf{d} = \mathbf{0}$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_2 + \omega_{00}^{\mathbf{d}} - \frac{12}{7}\omega_{40}^{\mathbf{d}} & -\frac{60\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} - \frac{40\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} \\ -\frac{60\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} - \frac{40\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} & -\cot \delta_4 + \omega_{00}^{\mathbf{d}} - \frac{162}{77}\omega_{40}^{\mathbf{d}} + \frac{20}{11}\omega_{60}^{\mathbf{d}} \end{pmatrix}. \quad (\text{B9})$$

For the  $A_1$  irrep in the moving frame with  $|\mathbf{p}L/2\pi| = 1$ , we choose  $\mathbf{d} = \mathbf{p}L/2\pi = (0, 0, 1)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_0 + \omega_{00}^{\mathbf{d}} & -\sqrt{5}\omega_{20}^{\mathbf{d}} & \frac{3}{\sqrt{2}}\omega_{40}^{\mathbf{d}} + 3\omega_{44}^{\mathbf{d}} & -\frac{3}{\sqrt{2}}\omega_{40}^{\mathbf{d}} + 3\omega_{44}^{\mathbf{d}} \\ -\sqrt{5}\omega_{20}^{\mathbf{d}} & -\cot \delta_2 + M_{21,21}^{A_1,\mathbf{p}} & M_{21,41}^{A_1,\mathbf{p}} & M_{21,42}^{A_1,\mathbf{p}} \\ \frac{3}{\sqrt{2}}\omega_{40}^{\mathbf{d}} + 3\omega_{44}^{\mathbf{d}} & M_{21,41}^{A_1,\mathbf{p}} & -\cot \delta_4 + M_{41,41}^{A_1,\mathbf{p}} & M_{41,42}^{A_1,\mathbf{p}} \\ -\frac{3}{\sqrt{2}}\omega_{40}^{\mathbf{d}} + 3\omega_{44}^{\mathbf{d}} & M_{21,41}^{A_1,\mathbf{p}} & M_{41,42}^{A_1,\mathbf{p}} & -\cot \delta_4 + M_{42,42}^{A_1,\mathbf{p}} \end{pmatrix} \quad (\text{B10})$$

where

$$\begin{aligned}
M_{21,21}^{A_1,\mathbf{p}} &= \omega_{00}^{\mathbf{d}} + \frac{10}{7}\omega_{20}^{\mathbf{d}} + \frac{18}{7}\omega_{40}^{\mathbf{d}}, \\
M_{21,41}^{A_1,\mathbf{p}} &= -\frac{3\sqrt{10}}{7}\omega_{20}^{\mathbf{d}} + \frac{12\sqrt{5}}{11}\omega_{44}^{\mathbf{d}} - \frac{15}{11}\omega_{64}^{\mathbf{d}} - \frac{30\sqrt{10}}{77}\omega_{40}^{\mathbf{d}} - \frac{15\sqrt{10}}{22}\omega_{60}^{\mathbf{d}}, \\
M_{21,42}^{A_1,\mathbf{p}} &= +\frac{3\sqrt{10}}{7}\omega_{20}^{\mathbf{d}} + \frac{12\sqrt{5}}{11}\omega_{44}^{\mathbf{d}} - \frac{15}{11}\omega_{64}^{\mathbf{d}} + \frac{30\sqrt{10}}{77}\omega_{40}^{\mathbf{d}} + \frac{15\sqrt{10}}{22}\omega_{60}^{\mathbf{d}}, \\
M_{41,41}^{A_1,\mathbf{p}} &= +\omega_{00}^{\mathbf{d}} - \frac{20}{77}\omega_{20}^{\mathbf{d}} + \frac{1296}{1001}\omega_{40}^{\mathbf{d}} + \frac{8}{11}\omega_{60}^{\mathbf{d}} + \frac{497}{286}\omega_{80}^{\mathbf{d}} + \frac{162\sqrt{2}}{143}\omega_{44}^{\mathbf{d}} \\
&\quad - \frac{12\sqrt{10}}{11}\omega_{64}^{\mathbf{d}} + \frac{42}{13}\sqrt{\frac{5}{22}}\omega_{84}^{\mathbf{d}} + 21\sqrt{\frac{5}{286}}\omega_{88}^{\mathbf{d}}, \\
M_{41,42}^{A_1,\mathbf{p}} &= -\frac{120}{77}\omega_{20}^{\mathbf{d}} - \frac{162}{1001}\omega_{40}^{\mathbf{d}} - \frac{12}{11}\omega_{60}^{\mathbf{d}} - \frac{483}{286}\omega_{80}^{\mathbf{d}} + 21\sqrt{\frac{5}{286}}\omega_{88}^{\mathbf{d}}, \\
M_{42,42}^{A_1,\mathbf{p}} &= +\omega_{00}^{\mathbf{d}} - \frac{20}{77}\omega_{20}^{\mathbf{d}} + \frac{1296}{1001}\omega_{40}^{\mathbf{d}} + \frac{8}{11}\omega_{60}^{\mathbf{d}} + \frac{497}{286}\omega_{80}^{\mathbf{d}} - \frac{162\sqrt{2}}{143}\omega_{44}^{\mathbf{d}} \\
&\quad + \frac{12\sqrt{10}}{11}\omega_{64}^{\mathbf{d}} - \frac{42}{13}\sqrt{\frac{5}{22}}\omega_{84}^{\mathbf{d}} + 21\sqrt{\frac{5}{286}}\omega_{88}^{\mathbf{d}}.
\end{aligned}$$

For the  $B_1$  irrep in the moving frame with  $|\mathbf{pL}/2\pi| = 1$ , we choose  $\mathbf{d} = \mathbf{pL}/2\pi = (0, 0, 1)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_2 + \omega_{00}^{\mathbf{d}} - \frac{10}{7}\omega_{00}^{\mathbf{d}} + \frac{3}{7}\omega_{40}^{\mathbf{d}} + 6\sqrt{\frac{5}{14}}\omega_{44}^{\mathbf{d}} & M_{21,41}^{B_1,\mathbf{p}} \\ M_{21,41}^{B_1,\mathbf{p}} & -\cot \delta_4 + M_{41,41}^{B_1,\mathbf{p}} \end{pmatrix}. \quad (\text{B11})$$

where

$$\begin{aligned}
M_{21,41}^{B_1,\mathbf{p}} &= -\frac{5\sqrt{3}}{7}\omega_{20}^{\mathbf{d}} + \frac{90\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} - \frac{5\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} + \frac{6\sqrt{210}}{77}\omega_{44}^{\mathbf{d}} - \frac{5\sqrt{42}}{11}\omega_{64}^{\mathbf{d}}, \\
M_{41,41}^{B_1,\mathbf{p}} &= +\omega_{00}^{\mathbf{d}} + \frac{40}{77}\omega_{20}^{\mathbf{d}} - \frac{81}{91}\omega_{40}^{\mathbf{d}} - 2\omega_{60}^{\mathbf{d}} + \frac{196}{143}\omega_{80}^{\mathbf{d}} + \frac{243}{143}\sqrt{\frac{10}{7}}\omega_{44}^{\mathbf{d}} \\
&\quad + \frac{6\sqrt{14}}{11}\omega_{64}^{\mathbf{d}} + \frac{42}{13}\sqrt{\frac{14}{11}}\omega_{84}^{\mathbf{d}}.
\end{aligned}$$

For the  $B_2$  irrep in the moving frame with  $|\mathbf{pL}/2\pi| = 1$ , we choose  $\mathbf{d} = \mathbf{pL}/2\pi = (0, 0, 1)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_2 + \omega_{00}^{\mathbf{d}} - \frac{10}{7}\omega_{00}^{\mathbf{d}} + \frac{3}{7}\omega_{40}^{\mathbf{d}} - \frac{3\sqrt{70}}{7}\omega_{44}^{\mathbf{d}} & M_{21,41}^{B_2,\mathbf{p}} \\ M_{21,41}^{B_2,\mathbf{p}} & -\cot \delta_4 + M_{41,41}^{B_2,\mathbf{p}} \end{pmatrix}. \quad (\text{B12})$$

where

$$\begin{aligned}
M_{21,41}^{B_2,\mathbf{p}} &= +\frac{5\sqrt{3}}{7}\omega_{20}^{\mathbf{d}} - \frac{90\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} + \frac{5\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} + \frac{6\sqrt{210}}{77}\omega_{44}^{\mathbf{d}} - \frac{5\sqrt{42}}{11}\omega_{64}^{\mathbf{d}}, \\
M_{41,41}^{B_2,\mathbf{p}} &= +\omega_{00}^{\mathbf{d}} + \frac{40}{77}\omega_{20}^{\mathbf{d}} - \frac{81}{91}\omega_{40}^{\mathbf{d}} - 2\omega_{60}^{\mathbf{d}} + \frac{196}{143}\omega_{80}^{\mathbf{d}} - \frac{243}{143}\sqrt{\frac{10}{7}}\omega_{44}^{\mathbf{d}} \\
&\quad - \frac{6\sqrt{14}}{11}\omega_{64}^{\mathbf{d}} - \frac{42}{13}\sqrt{\frac{14}{11}}\omega_{84}^{\mathbf{d}}.
\end{aligned}$$

For the  $E$  irrep in the moving frame with  $|\mathbf{p}L/2\pi| = 1$ , we choose  $\mathbf{d} = \mathbf{p}L/2\pi = (0, 0, 1)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_2 + \omega_{00}^{\mathbf{d}} + \frac{5}{7}\omega_{20}^{\mathbf{d}} - \frac{12}{7}\omega_{40}^{\mathbf{d}} & M_{21,41}^{E,\mathbf{p}} & M_{21,41}^{E,\mathbf{p}*} \\ M_{21,41}^{E,\mathbf{p}*} & -\cot \delta_4 + M_{41,41}^{E,\mathbf{p}} & M_{41,42}^{E,\mathbf{p}} \\ M_{21,41}^{E,\mathbf{p}} & M_{41,42}^{E,\mathbf{p}*} & -\cot \delta_4 + M_{41,41}^{E,\mathbf{p}} \end{pmatrix}. \quad (\text{B13})$$

where

$$\begin{aligned} M_{21,41}^{E,\mathbf{p}} &= -\frac{5\sqrt{3}}{7}\omega_{20}^{\mathbf{d}} - \frac{15\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} + \frac{10\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} - i\frac{3\sqrt{30}}{11}\omega_{44}^{\mathbf{d}} - i\frac{10\sqrt{6}}{11}\omega_{64}^{\mathbf{d}}, \\ M_{41,41}^{E,\mathbf{p}} &= +\omega_{00}^{\mathbf{d}} + \frac{25}{77}\omega_{20}^{\mathbf{d}} - \frac{486}{1001}\omega_{40}^{\mathbf{d}} + \frac{8}{11}\omega_{60}^{\mathbf{d}} - \frac{224}{143}\omega_{80}^{\mathbf{d}}, \\ M_{41,42}^{E,\mathbf{p}} &= +\frac{60}{77}\omega_{20}^{\mathbf{d}} + \frac{1215}{1001}\omega_{40}^{\mathbf{d}} - \frac{9}{11}\omega_{60}^{\mathbf{d}} - \frac{168}{143}\omega_{80}^{\mathbf{d}} + i\frac{81\sqrt{10}}{143}\omega_{44}^{\mathbf{d}} + i\frac{3\sqrt{2}}{11}\omega_{64}^{\mathbf{d}} - i\frac{84}{13}\sqrt{\frac{2}{11}}\omega_{84}^{\mathbf{d}}. \end{aligned}$$

For the  $A_1$  irrep in the moving frame with  $|\mathbf{p}L/2\pi| = \sqrt{2}$ , we choose  $\mathbf{d} = \mathbf{p}L/2\pi = (1, 1, 0)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_0 + \omega_{00}^{\mathbf{d}} & -\sqrt{5}\omega_{20}^{\mathbf{d}} & \sqrt{10}\omega_{22}^{\mathbf{d}} & 3(\omega_{44}^{\mathbf{d}} + \omega_{42}^{\mathbf{d}}) & 3(\omega_{44}^{\mathbf{d}} - \omega_{42}^{\mathbf{d}}) & 3\omega_{40}^{\mathbf{d}} \\ -\sqrt{5}\omega_{20}^{\mathbf{d}} & -\cot \delta_2 + M_{21,21}^{A_1,\mathbf{p}} & M_{21,22}^{A_1,\mathbf{p}} & M_{21,41}^{A_1,\mathbf{p}} & M_{21,41}^{A_1,\mathbf{p}*} & M_{21,43}^{A_1,\mathbf{p}} \\ -\sqrt{10}\omega_{22}^{\mathbf{d}} & M_{21,41}^{A_1,\mathbf{p}*} & M_{22,21}^{A_1,\mathbf{p}} - \cot \delta_2 & M_{22,41}^{A_1,\mathbf{p}} & -M_{22,41}^{A_1,\mathbf{p}*} & M_{22,43}^{A_1,\mathbf{p}} \\ 3(\omega_{44}^{\mathbf{d}} - \omega_{42}^{\mathbf{d}}) & M_{21,41}^{A_1,\mathbf{p}*} & M_{22,41}^{A_1,\mathbf{p}*} & M_{41,41}^{A_1,\mathbf{p}} - \cot \delta_4 & M_{41,42}^{A_1,\mathbf{p}} & M_{41,43}^{A_1,\mathbf{p}} \\ 3(\omega_{44}^{\mathbf{d}} + \omega_{42}^{\mathbf{d}}) & M_{21,41}^{A_1,\mathbf{p}} & -M_{22,41}^{A_1,\mathbf{p}} & M_{41,42}^{A_1,\mathbf{p}*} & M_{41,41}^{A_1,\mathbf{p}} - \cot \delta_4 & M_{41,43}^{A_1,\mathbf{p}*} \\ 3\omega_{40}^{\mathbf{d}} & M_{21,43}^{A_1,\mathbf{p}*} & M_{22,43}^{A_1,\mathbf{p}*} & M_{41,43}^{A_1,\mathbf{p}*} & M_{41,43}^{A_1,\mathbf{p}} & M_{43,43}^{A_1,\mathbf{p}} - \cot \delta_4 \end{pmatrix}, \quad (\text{B14})$$

where

$$\begin{aligned}
M_{21,21}^{A_1, \mathbf{P}} &= \omega_{00}^{\mathbf{d}} + \frac{10}{7}\omega_{20}^{\mathbf{d}} + \frac{18}{7}\omega_{40}^{\mathbf{d}}, \\
M_{21,22}^{A_1, \mathbf{P}} &= \frac{10\sqrt{2}}{7}\omega_{22}^{\mathbf{d}} - \frac{3\sqrt{30}}{7}\omega_{42}^{\mathbf{d}}, \\
M_{21,41}^{A_1, \mathbf{P}} &= -\frac{5\sqrt{10}}{7}\omega_{22}^{\mathbf{d}} - \frac{24\sqrt{5}}{77}\omega_{42}^{\mathbf{d}} - \frac{2\sqrt{210}}{11}\omega_{62}^{\mathbf{d}} + \frac{12\sqrt{5}}{11}\omega_{44}^{\mathbf{d}} - \frac{15}{11}\omega_{64}^{\mathbf{d}}, \\
M_{21,43}^{A_1, \mathbf{P}} &= -\frac{6\sqrt{5}}{77}\omega_{20}^{\mathbf{d}} - \frac{60\sqrt{5}}{77}\omega_{40}^{\mathbf{d}} - \frac{15}{11}\omega_{60}^{\mathbf{d}}, \\
M_{22,22}^{A_1, \mathbf{P}} &= \omega_{00}^{\mathbf{d}} - \frac{10}{7}\omega_{20}^{\mathbf{d}} + \frac{3}{7}\omega_{40}^{\mathbf{d}} - 6\sqrt{\frac{5}{14}}\omega_{44}^{\mathbf{d}}, \\
M_{22,41}^{A_1, \mathbf{P}} &= +\frac{5\sqrt{6}}{14}\omega_{20}^{\mathbf{d}} - \frac{45\sqrt{6}}{77}\omega_{40}^{\mathbf{d}} + \frac{5\sqrt{6}}{22}\omega_{60}^{\mathbf{d}} + \frac{5\sqrt{7}}{7}\omega_{22}^{\mathbf{d}} - \frac{6\sqrt{105}}{77}\omega_{42}^{\mathbf{d}} + \frac{\sqrt{10}}{22}\omega_{62}^{\mathbf{d}} \\
&\quad + \frac{6\sqrt{105}}{77}\omega_{44}^{\mathbf{d}} - \frac{5\sqrt{21}}{11}\omega_{64}^{\mathbf{d}} - \frac{15}{\sqrt{22}}\omega_{66}^{\mathbf{d}}, \\
M_{22,43}^{A_1, \mathbf{P}} &= -\frac{\sqrt{10}}{7}\omega_{22}^{\mathbf{d}} + \frac{90\sqrt{6}}{77}\omega_{42}^{\mathbf{d}} - \frac{10\sqrt{7}}{11}\omega_{62}^{\mathbf{d}}, \\
M_{41,41}^{A_1, \mathbf{P}} &= \omega_{00}^{\mathbf{d}} - \frac{50}{77}\omega_{20}^{\mathbf{d}} + \frac{243}{2002}\omega_{40}^{\mathbf{d}} - \frac{13}{11}\omega_{60}^{\mathbf{d}} + \frac{203}{286}\omega_{80}^{\mathbf{d}} - \frac{243}{143}\sqrt{\frac{5}{14}}\omega_{44}^{\mathbf{d}} \\
&\quad - \frac{3\sqrt{14}}{11}\omega_{64}^{\mathbf{d}} - \frac{42}{13}\sqrt{\frac{7}{22}}\omega_{84}^{\mathbf{d}} + 21\sqrt{\frac{5}{286}}\omega_{88}^{\mathbf{d}}, \\
M_{41,42}^{A_1, \mathbf{P}} &= -\frac{90}{77}\omega_{20}^{\mathbf{d}} + \frac{2025}{2002}\omega_{40}^{\mathbf{d}} + \frac{9}{11}\omega_{60}^{\mathbf{d}} - \frac{189}{286}\omega_{80}^{\mathbf{d}} - \frac{10}{11}\sqrt{\frac{6}{7}}\omega_{22}^{\mathbf{d}} \\
&\quad + \frac{243}{143}\sqrt{\frac{10}{7}}\omega_{42}^{\mathbf{d}} - \frac{4\sqrt{15}}{11}\omega_{62}^{\mathbf{d}} + \frac{21\sqrt{5}}{143}\omega_{82}^{\mathbf{d}} + \frac{243}{143}\sqrt{\frac{5}{14}}\omega_{44}^{\mathbf{d}} + \frac{3\sqrt{14}}{11}\omega_{64}^{\mathbf{d}}, \\
&\quad + \frac{42}{13}\sqrt{\frac{7}{22}}\omega_{84}^{\mathbf{d}} + 4\sqrt{\frac{3}{11}}\omega_{66}^{\mathbf{d}} - 7\sqrt{\frac{21}{143}}\omega_{86}^{\mathbf{d}} + 21\sqrt{\frac{5}{286}}\omega_{88}^{\mathbf{d}}, \\
M_{41,43}^{A_1, \mathbf{P}} &= +\frac{30\sqrt{15}}{77}\omega_{22}^{\mathbf{d}} + \frac{81}{91}\omega_{42}^{\mathbf{d}} - \frac{105\sqrt{14}}{143}\omega_{62}^{\mathbf{d}} + \frac{162}{143}\omega_{44}^{\mathbf{d}} - \frac{12\sqrt{5}}{11}\omega_{64}^{\mathbf{d}} + \frac{21}{13}\sqrt{\frac{5}{11}}\omega_{84}^{\mathbf{d}}, \\
M_{43,43}^{A_1, \mathbf{P}} &= \omega_{00}^{\mathbf{d}} + \frac{100}{77}\omega_{20}^{\mathbf{d}} + \frac{1458}{1001}\omega_{40}^{\mathbf{d}} + \frac{20}{11}\omega_{60}^{\mathbf{d}} + \frac{490}{143}\omega_{80}^{\mathbf{d}}.
\end{aligned}$$

For the  $A_2$  irrep in moving frame with  $|\mathbf{p}L/2\pi| = \sqrt{2}$ , we choose  $\mathbf{d} = \mathbf{p}L/2\pi = (1, 1, 0)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_0 + M_{21,21}^{A_2, \mathbf{P}} & M_{21,41}^{A_2, \mathbf{P}} & -M_{21,41}^{A_2, \mathbf{P}*} \\ M_{21,41}^{A_2, \mathbf{P}*} & -\cot \delta_4 + M_{41,41}^{A_2, \mathbf{P}} & M_{41,42}^{A_2, \mathbf{P}} \\ -M_{21,41}^{A_2, \mathbf{P}} & M_{41,42}^{A_2, \mathbf{P}*} & -\cot \delta_4 + M_{41,41}^{A_2, \mathbf{P}} \end{pmatrix}, \quad (\text{B15})$$

where

$$\begin{aligned}
M_{21,21}^{A_2, \mathbf{P}} &= \omega_{00}^{\mathbf{d}} + \frac{5}{7}\omega_{20}^{\mathbf{d}} - \frac{12}{7}\omega_{40}^{\mathbf{d}} + i\frac{\sqrt{30}}{7}\left(\sqrt{5}\omega_{22}^{\mathbf{d}} + 2\sqrt{3}\omega_{42}^{\mathbf{d}}\right), \\
M_{21,41}^{A_2, \mathbf{P}} &= -\frac{5\sqrt{3}}{7}\omega_{20}^{\mathbf{d}} - \frac{15\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} + \frac{10\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} + \frac{5\sqrt{2}}{14}\left(i + \sqrt{7}\right)\omega_{22}^{\mathbf{d}} \\
&\quad + \frac{3}{11}\sqrt{\frac{15}{14}}\left(5 - i\frac{9}{\sqrt{7}}\right)\omega_{42}^{\mathbf{d}} - \frac{4\sqrt{5}}{11}\left(1 + i\sqrt{7}\right)\omega_{62}^{\mathbf{d}} + i\frac{3\sqrt{30}}{11}\omega_{44}^{\mathbf{d}} + i\frac{10\sqrt{6}}{11}\omega_{64}^{\mathbf{d}}, \\
M_{41,41}^{A_2, \mathbf{P}} &= +\omega_{00}^{\mathbf{d}} + \frac{25}{77}\omega_{20}^{\mathbf{d}} - \frac{486}{1001}\omega_{40}^{\mathbf{d}} + \frac{8}{11}\omega_{60}^{\mathbf{d}} - \frac{224}{143}\omega_{80}^{\mathbf{d}} + i\frac{25\sqrt{6}}{77}\omega_{22}^{\mathbf{d}} \\
&\quad + i\frac{243\sqrt{10}}{1001}\omega_{42}^{\mathbf{d}} + i\frac{\sqrt{105}}{11}\omega_{62}^{\mathbf{d}} + i\frac{42\sqrt{35}}{143}\omega_{82}^{\mathbf{d}} - i\sqrt{\frac{21}{11}}\omega_{66}^{\mathbf{d}} - i14\sqrt{\frac{3}{143}}\omega_{86}^{\mathbf{d}}, \\
M_{41,42}^{A_2, \mathbf{P}} &= -\frac{60}{77}\omega_{20}^{\mathbf{d}} - \frac{1215}{1001}\omega_{40}^{\mathbf{d}} + \frac{9}{11}\omega_{60}^{\mathbf{d}} + \frac{168}{143}\omega_{80}^{\mathbf{d}} + \frac{5\sqrt{6}}{77}\left(3\sqrt{7} - i5\right)\omega_{22}^{\mathbf{d}} \\
&\quad + \frac{81\sqrt{10}}{1001}\left(-\sqrt{7} - i3\right)\omega_{42}^{\mathbf{d}} + \frac{\sqrt{15}}{11}\left(-6 - i\sqrt{7}\right)\omega_{62}^{\mathbf{d}} + \frac{42\sqrt{5}}{143}\left(2 - i\sqrt{7}\right)\omega_{82}^{\mathbf{d}} \\
&\quad + i\frac{81\sqrt{10}}{143}\omega_{44}^{\mathbf{d}} + i\frac{3\sqrt{2}}{11}\omega_{64}^{\mathbf{d}} - i\frac{84}{13}\sqrt{\frac{2}{11}}\omega_{84}^{\mathbf{d}} - i\sqrt{\frac{21}{11}}\omega_{66}^{\mathbf{d}} - i14\sqrt{\frac{3}{143}}\omega_{86}^{\mathbf{d}}.
\end{aligned}$$

For the  $B_1$  irrep in the moving frame with  $|\mathbf{p}L/2\pi| = \sqrt{2}$ , we choose  $\mathbf{d} = \mathbf{p}L/2\pi = (1, 1, 0)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_0 + M_{21,21}^{B_1, \mathbf{P}} & M_{21,41}^{B_1, \mathbf{P}} & -M_{21,41}^{B_1, \mathbf{P}*} \\ M_{21,41}^{B_1, \mathbf{P}*} & -\cot \delta_4 + M_{41,41}^{B_1, \mathbf{P}} & M_{41,42}^{B_1, \mathbf{P}} \\ -M_{21,41}^{B_1, \mathbf{P}} & M_{41,42}^{B_1, \mathbf{P}*} & -\cot \delta_4 + M_{41,41}^{B_1, \mathbf{P}} \end{pmatrix}, \quad (\text{B16})$$

where

$$\begin{aligned}
M_{21,21}^{B_1, \mathbf{P}} &= \omega_{00}^{\mathbf{d}} + \frac{5}{7}\omega_{20}^{\mathbf{d}} - \frac{12}{7}\omega_{40}^{\mathbf{d}} - i\frac{\sqrt{30}}{7}\left(\sqrt{5}\omega_{22}^{\mathbf{d}} + 2\sqrt{3}\omega_{42}^{\mathbf{d}}\right) \\
M_{21,41}^{B_1, \mathbf{P}} &= -\frac{5\sqrt{3}}{7}\omega_{20}^{\mathbf{d}} - \frac{15\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} + \frac{10\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} + \frac{5\sqrt{2}}{14}\left(-i + \sqrt{7}\right)\omega_{22}^{\mathbf{d}} \\
&\quad + \frac{3}{11}\sqrt{\frac{15}{14}}\left(5 + i\frac{9}{\sqrt{7}}\right)\omega_{42}^{\mathbf{d}} - \frac{4\sqrt{5}}{11}\left(1 - i\sqrt{7}\right)\omega_{62}^{\mathbf{d}} - i\frac{3\sqrt{30}}{11}\omega_{44}^{\mathbf{d}} - i\frac{10\sqrt{6}}{11}\omega_{64}^{\mathbf{d}}, \\
M_{41,41}^{B_1, \mathbf{P}} &= +\omega_{00}^{\mathbf{d}} + \frac{25}{77}\omega_{20}^{\mathbf{d}} - \frac{486}{1001}\omega_{40}^{\mathbf{d}} + \frac{8}{11}\omega_{60}^{\mathbf{d}} - \frac{224}{143}\omega_{80}^{\mathbf{d}} - i\frac{25\sqrt{6}}{77}\omega_{22}^{\mathbf{d}} \\
&\quad - i\frac{243\sqrt{10}}{1001}\omega_{42}^{\mathbf{d}} - i\frac{\sqrt{105}}{11}\omega_{62}^{\mathbf{d}} - i\frac{42\sqrt{35}}{143}\omega_{82}^{\mathbf{d}} + i\sqrt{\frac{21}{11}}\omega_{66}^{\mathbf{d}} + i14\sqrt{\frac{3}{143}}\omega_{86}^{\mathbf{d}}, \\
M_{41,42}^{B_1, \mathbf{P}} &= -\frac{60}{77}\omega_{20}^{\mathbf{d}} - \frac{1215}{1001}\omega_{40}^{\mathbf{d}} + \frac{9}{11}\omega_{60}^{\mathbf{d}} + \frac{168}{143}\omega_{80}^{\mathbf{d}} + \frac{5\sqrt{6}}{77}\left(3\sqrt{7} + i5\right)\omega_{22}^{\mathbf{d}} \\
&\quad + \frac{81\sqrt{10}}{1001}\left(-\sqrt{7} + i3\right)\omega_{42}^{\mathbf{d}} + \frac{\sqrt{15}}{11}\left(-6 + i\sqrt{7}\right)\omega_{62}^{\mathbf{d}} + \frac{42\sqrt{5}}{143}\left(2 + i\sqrt{7}\right)\omega_{82}^{\mathbf{d}} \\
&\quad - i\frac{81\sqrt{10}}{143}\omega_{44}^{\mathbf{d}} - i\frac{3\sqrt{2}}{11}\omega_{64}^{\mathbf{d}} + i\frac{84}{13}\sqrt{\frac{2}{11}}\omega_{84}^{\mathbf{d}} + i\sqrt{\frac{21}{11}}\omega_{66}^{\mathbf{d}} + i14\sqrt{\frac{3}{143}}\omega_{86}^{\mathbf{d}}.
\end{aligned}$$



For the  $B_2$  irrep in the moving frame with  $|\mathbf{p}L/2\pi| = \sqrt{2}$ , we choose  $\mathbf{d} = \mathbf{p}L/2\pi = (1, 1, 0)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_0 + M_{21,21}^{B_2, \mathbf{P}} & M_{21,41}^{B_2, \mathbf{P}} & M_{21,41}^{B_2, \mathbf{P}^*} \\ M_{21,41}^{B_2, \mathbf{P}^*} & -\cot \delta_4 + M_{41,41}^{B_2, \mathbf{P}} & M_{41,42}^{B_2, \mathbf{P}} \\ M_{21,41}^{B_2, \mathbf{P}} & M_{41,42}^{B_2, \mathbf{P}^*} & -\cot \delta_4 + M_{41,41}^{B_2, \mathbf{P}} \end{pmatrix}, \quad (\text{B17})$$

where

$$\begin{aligned} M_{21,21}^{B_2, \mathbf{P}} &= \omega_{00}^{\mathbf{d}} - \frac{10}{7}\omega_{20}^{\mathbf{d}} + \frac{3}{7}\omega_{40}^{\mathbf{d}} + 6\sqrt{\frac{5}{14}}\omega_{44}^{\mathbf{d}}, \\ M_{21,41}^{B_2, \mathbf{P}} &= -\frac{5\sqrt{6}}{14}\omega_{20}^{\mathbf{d}} + \frac{45\sqrt{6}}{77}\omega_{40}^{\mathbf{d}} - \frac{5\sqrt{6}}{22}\omega_{60}^{\mathbf{d}} - \frac{5}{\sqrt{7}}\omega_{22}^{\mathbf{d}} \\ &\quad + \frac{6\sqrt{105}}{77}\omega_{42}^{\mathbf{d}} - \frac{\sqrt{10}}{22}\omega_{62}^{\mathbf{d}} + \frac{6\sqrt{105}}{77}\omega_{44}^{\mathbf{d}} - \frac{5\sqrt{21}}{11}\omega_{64}^{\mathbf{d}} - \frac{15}{\sqrt{22}}\omega_{66}^{\mathbf{d}}, \\ M_{41,41}^{B_2, \mathbf{P}} &= +\omega_{00}^{\mathbf{d}} - \frac{50}{77}\omega_{20}^{\mathbf{d}} + \frac{243}{2002}\omega_{40}^{\mathbf{d}} - \frac{13}{11}\omega_{60}^{\mathbf{d}} + \frac{203}{286}\omega_{80}^{\mathbf{d}} \\ &\quad + \frac{243}{143}\sqrt{\frac{5}{14}}\omega_{44}^{\mathbf{d}} + \frac{3\sqrt{14}}{11}\omega_{64}^{\mathbf{d}} + \frac{42}{13}\sqrt{\frac{7}{22}}\omega_{84}^{\mathbf{d}} - 21\sqrt{\frac{5}{286}}\omega_{88}^{\mathbf{d}}, \\ M_{41,42}^{B_2, \mathbf{P}} &= +\frac{90}{77}\omega_{20}^{\mathbf{d}} - \frac{2025}{2002}\omega_{40}^{\mathbf{d}} - \frac{9}{11}\omega_{60}^{\mathbf{d}} + \frac{189}{286}\omega_{80}^{\mathbf{d}} + \frac{10}{11}\sqrt{\frac{6}{7}}\omega_{22}^{\mathbf{d}} - \frac{243}{143}\sqrt{\frac{10}{7}}\omega_{42}^{\mathbf{d}} \\ &\quad + \frac{4\sqrt{5}}{11}\omega_{62}^{\mathbf{d}} - \frac{21\sqrt{5}}{143}\omega_{82}^{\mathbf{d}} + \frac{243}{143}\sqrt{\frac{5}{14}}\omega_{44}^{\mathbf{d}} + \frac{3\sqrt{14}}{11}\omega_{64}^{\mathbf{d}} \\ &\quad + \frac{42}{13}\sqrt{\frac{7}{22}}\omega_{84}^{\mathbf{d}} + 4\sqrt{\frac{3}{11}}\omega_{66}^{\mathbf{d}} - 7\sqrt{\frac{21}{143}}\omega_{86}^{\mathbf{d}} + 21\sqrt{\frac{5}{286}}\omega_{88}^{\mathbf{d}}. \end{aligned}$$

For the  $A_1$  irrep in the moving frame with  $|\mathbf{p}L/2\pi| = \sqrt{3}$ , we choose  $\mathbf{d} = \mathbf{p}L/2\pi = (1, 1, 1)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_0 + \omega_{00}^{\mathbf{d}} & \sqrt{30}\omega_{22}^{\mathbf{d}} & \frac{6\sqrt{21}}{7}\omega_{40}^{\mathbf{d}} & 3\sqrt{3}(1-i)\omega_{42}^{\mathbf{d}} \\ -\sqrt{30}\omega_{22}^{\mathbf{d}} & -\cot \delta_2 + M_{21,21}^{A_1, \mathbf{P}} & M_{21,41}^{A_1, \mathbf{P}} & M_{21,42}^{A_1, \mathbf{P}} \\ \frac{6\sqrt{21}}{7}\omega_{40}^{\mathbf{d}} & M_{21,41}^{A_1, \mathbf{P}^*} & M_{41,41}^{A_1, \mathbf{P}} - \cot \delta_2 & M_{41,42}^{A_1, \mathbf{P}} \\ 3\sqrt{3}(-1-i)\omega_{42}^{\mathbf{d}} & M_{21,42}^{A_1, \mathbf{P}^*} & M_{41,42}^{A_1, \mathbf{P}^*} & M_{42,42}^{A_1, \mathbf{P}} - \cot \delta_4 \end{pmatrix}, \quad (\text{B18})$$

where

$$\begin{aligned}
M_{21,21}^{A_1,\mathbf{p}} &= \omega_{00}^{\mathbf{d}} - \frac{12}{7}\omega_{40}^{\mathbf{d}} - i\frac{10\sqrt{6}}{7}\omega_{22}^{\mathbf{d}} - i\frac{12\sqrt{10}}{7}\omega_{42}^{\mathbf{d}}, \\
M_{21,41}^{A_1,\mathbf{p}} &= +2\sqrt{\frac{10}{7}}\omega_{22}^{\mathbf{d}} + \frac{30}{11}\sqrt{\frac{6}{7}}\omega_{42}^{\mathbf{d}} - \frac{260}{99}(1-i)\omega_{63}^{\mathbf{d}} - \frac{100}{9}\sqrt{\frac{5}{11}}\omega_{66}^{\mathbf{d}}, \\
M_{21,42}^{A_1,\mathbf{p}} &= -\frac{20}{77}(1+i)\omega_{22}^{\mathbf{d}} - \frac{30\sqrt{6}}{77}(1-i)\omega_{40}^{\mathbf{d}} - \frac{39\sqrt{15}}{77}(1+i)\omega_{42}^{\mathbf{d}} + \frac{20\sqrt{6}}{11}(1-i)\omega_{60}^{\mathbf{d}} \\
&\quad + \frac{64\sqrt{70}}{99}\omega_{63}^{\mathbf{d}} + \frac{20}{9}\sqrt{\frac{14}{11}}(1+i)\omega_{66}^{\mathbf{d}}, \\
M_{41,41}^{A_1,\mathbf{p}} &= \omega_{00}^{\mathbf{d}} + \frac{324}{143}\omega_{40}^{\mathbf{d}} + \frac{80}{11}\omega_{60}^{\mathbf{d}} + \frac{560}{143}\omega_{80}^{\mathbf{d}}, \\
M_{41,42}^{A_1,\mathbf{p}} &= -\frac{10}{11}\sqrt{\frac{15}{7}}(1-i)\omega_{22}^{\mathbf{d}} - \frac{81}{11}\sqrt{\frac{1}{7}}(1-i)\omega_{42}^{\mathbf{d}} - i\frac{80}{33}\sqrt{\frac{2}{3}}\omega_{63}^{\mathbf{d}} - \frac{4}{3}\sqrt{\frac{10}{33}}(1-i)\omega_{66}^{\mathbf{d}} \\
&\quad + \frac{8}{11}\sqrt{\frac{210}{143}}(1-i)\omega_{86}^{\mathbf{d}} + i\frac{240}{11}\sqrt{\frac{7}{143}}\omega_{87}^{\mathbf{d}}, \\
M_{42,42}^{A_1,\mathbf{p}} &= \omega_{00}^{\mathbf{d}} - \frac{162}{77}\omega_{40}^{\mathbf{d}} + \frac{20}{11}\omega_{60}^{\mathbf{d}} - i\frac{65\sqrt{6}}{77}\omega_{22}^{\mathbf{d}} + i\frac{162\sqrt{10}}{1001}\omega_{42}^{\mathbf{d}} + \frac{20}{33}\sqrt{\frac{35}{3}}(1+i)\omega_{63}^{\mathbf{d}} \\
&\quad + i\frac{4}{3}\sqrt{\frac{77}{3}}\omega_{66}^{\mathbf{d}} + i\frac{7952}{143}\sqrt{\frac{3}{143}}\omega_{86}^{\mathbf{d}} + \frac{1008}{143}\sqrt{\frac{10}{143}}(1+i)\omega_{87}^{\mathbf{d}}.
\end{aligned}$$

For the  $E$  irrep in the moving frame with  $|\mathbf{p}L/2\pi| = \sqrt{3}$ , we choose  $\mathbf{d} = \mathbf{p}L/2\pi = (1, 1, 1)$ ,

$$0 = \det \begin{pmatrix} -\cot \delta_2 + M_{21,21}^{E,\mathbf{p}} & M_{21,22}^{E,\mathbf{p}} & M_{21,41}^{E,\mathbf{p}} & M_{21,42}^{E,\mathbf{p}} & M_{21,43}^{E,\mathbf{p}} \\ M_{21,22}^{E,\mathbf{p}*} & -\cot \delta_2 + M_{22,22}^{E,\mathbf{p}} & M_{22,41}^{E,\mathbf{p}} & M_{22,42}^{E,\mathbf{p}} & M_{22,43}^{E,\mathbf{p}} \\ M_{21,41}^{E,\mathbf{p}*} & M_{22,41}^{E,\mathbf{p}*} & -\cot \delta_4 + M_{41,41}^{E,\mathbf{p}} & M_{41,42}^{E,\mathbf{p}} & M_{41,43}^{E,\mathbf{p}} \\ M_{21,42}^{E,\mathbf{p}*} & M_{22,42}^{E,\mathbf{p}*} & M_{41,42}^{E,\mathbf{p}*} & -\cot \delta_4 + M_{42,42}^{E,\mathbf{p}} & M_{42,43}^{E,\mathbf{p}} \\ M_{21,43}^{E,\mathbf{p}*} & M_{22,43}^{E,\mathbf{p}*} & M_{41,43}^{E,\mathbf{p}*} & M_{42,43}^{E,\mathbf{p}*} & -\cot \delta_4 + M_{43,43}^{E,\mathbf{p}} \end{pmatrix},$$

where

$$\begin{aligned}
M_{21,21}^{E,\mathbf{p}} &= \omega_{00}^{\mathbf{d}} + \frac{18}{7}\omega_{40}^{\mathbf{d}}, \\
M_{21,22}^{E,\mathbf{p}} &= \frac{\sqrt{10}}{14}(1-i)(\sqrt{60}\omega_{22}^{\mathbf{d}} - 9\omega_{42}^{\mathbf{d}}), \\
M_{21,41}^{E,\mathbf{p}} &= +\frac{15\sqrt{2}}{14}(1-i)\omega_{22}^{\mathbf{d}} + \frac{12\sqrt{30}}{77}(1-i)\omega_{42}^{\mathbf{d}} - i\frac{32\sqrt{35}}{33}\omega_{63}^{\mathbf{d}} + \frac{10}{3}\sqrt{\frac{7}{11}}(1-i)\omega_{66}^{\mathbf{d}}, \\
M_{21,42}^{E,\mathbf{p}} &= \frac{30\sqrt{3}}{77}(-4\omega_{40}^{\mathbf{d}} - 7\omega_{60}^{\mathbf{d}}), \\
M_{21,43}^{E,\mathbf{p}} &= -\frac{5\sqrt{21}}{7}\omega_{22}^{\mathbf{d}} + \frac{18\sqrt{35}}{77}\omega_{42}^{\mathbf{d}} - \frac{4}{33}\sqrt{\frac{10}{3}}(1-i)\omega_{63}^{\mathbf{d}} - \frac{70}{3}\sqrt{\frac{2}{33}}\omega_{66}^{\mathbf{d}}, \\
M_{22,22}^{E,\mathbf{p}} &= \omega_{00}^{\mathbf{d}} + i\frac{5\sqrt{6}}{7}\omega_{22}^{\mathbf{d}} - \frac{12}{7}\omega_{40}^{\mathbf{d}} + i\frac{6\sqrt{10}}{7}\omega_{42}^{\mathbf{d}}, \\
M_{22,41}^{E,\mathbf{p}} &= -i\frac{10\sqrt{2}}{7}\omega_{22}^{\mathbf{d}} + \frac{60\sqrt{3}}{77}\omega_{40}^{\mathbf{d}} - i\frac{39\sqrt{30}}{154}\omega_{42}^{\mathbf{d}} - \frac{40\sqrt{3}}{11}\omega_{60}^{\mathbf{d}} + i\frac{32\sqrt{35}}{99}(1+i)\omega_{63}^{\mathbf{d}} + i\frac{20\sqrt{77}}{99}\omega_{66}^{\mathbf{d}}, \\
M_{22,42}^{E,\mathbf{p}} &= -\frac{10\sqrt{2}}{7}(1+i)\omega_{22}^{\mathbf{d}} + \frac{3\sqrt{30}}{7}(1+i)\omega_{42}^{\mathbf{d}} - \frac{4\sqrt{35}}{9}\omega_{63}^{\mathbf{d}} + i\frac{20}{9}\sqrt{\frac{7}{11}}(1+i)\omega_{66}^{\mathbf{d}}, \\
M_{22,43}^{E,\mathbf{p}} &= -\frac{9\sqrt{35}}{22}(1-i)\omega_{42}^{\mathbf{d}} + i\frac{32}{11}\sqrt{\frac{10}{3}}\omega_{63}^{\mathbf{d}} - 10\sqrt{\frac{2}{33}}(1-i)\omega_{66}^{\mathbf{d}}, \\
M_{41,41}^{E,\mathbf{p}} &= \omega_{00}^{\mathbf{d}} - \frac{162}{77}\omega_{40}^{\mathbf{d}} + \frac{20}{11}\omega_{60}^{\mathbf{d}} + i\frac{65\sqrt{6}}{154}\omega_{22}^{\mathbf{d}} - i\frac{81\sqrt{10}}{1001}\omega_{42}^{\mathbf{d}} - \frac{10}{33}\sqrt{\frac{35}{3}}(1+i)\omega_{63}^{\mathbf{d}} - i\frac{2}{3}\sqrt{\frac{77}{3}}\omega_{66}^{\mathbf{d}} \\
&\quad - i\frac{3976}{143}\sqrt{\frac{3}{143}}\omega_{86}^{\mathbf{d}} - \frac{504}{143}\sqrt{\frac{10}{143}}(1+i)\omega_{87}^{\mathbf{d}}, \\
M_{41,42}^{E,\mathbf{p}} &= -\frac{5\sqrt{6}}{7}(1+i)\omega_{22}^{\mathbf{d}} + \frac{405\sqrt{10}}{2002}(1+i)\omega_{42}^{\mathbf{d}} - \frac{16}{33}\sqrt{\frac{35}{3}}\omega_{63}^{\mathbf{d}} + \frac{4}{3}\sqrt{\frac{7}{33}}(1+i)\omega_{66}^{\mathbf{d}} \\
&\quad - \frac{238}{13}\sqrt{\frac{3}{143}}(1+i)\omega_{86}^{\mathbf{d}} - \frac{168}{13}\sqrt{\frac{10}{143}}\omega_{87}^{\mathbf{d}}, \\
M_{41,43}^{E,\mathbf{p}} &= -\frac{15\sqrt{7}}{22}(1-i)\omega_{22}^{\mathbf{d}} - i\frac{2\sqrt{10}}{3}\omega_{63}^{\mathbf{d}} - \frac{\sqrt{22}}{33}(1-i)\omega_{66}^{\mathbf{d}} - \frac{24}{11}\sqrt{\frac{14}{143}}(1-i)\omega_{86}^{\mathbf{d}} - i\frac{48}{11}\sqrt{\frac{105}{143}}\omega_{87}^{\mathbf{d}}, \\
M_{42,42}^{E,\mathbf{p}} &= \omega_{00}^{\mathbf{d}} + \frac{324}{1001}\omega_{40}^{\mathbf{d}} - \frac{64}{11}\omega_{60}^{\mathbf{d}} + \frac{392}{143}\omega_{80}^{\mathbf{d}}, \\
M_{42,43}^{E,\mathbf{p}} &= +\frac{30\sqrt{7}}{77}\omega_{22}^{\mathbf{d}} - \frac{243}{143}\sqrt{\frac{15}{7}}\omega_{42}^{\mathbf{d}} + \frac{16\sqrt{10}}{33}(1-i)\omega_{63}^{\mathbf{d}} + \frac{28}{3}\sqrt{\frac{2}{11}}\omega_{66}^{\mathbf{d}} \\
&\quad - \frac{1434}{143}\sqrt{\frac{14}{143}}\omega_{86}^{\mathbf{d}} + \frac{48}{143}\sqrt{\frac{105}{143}}(1-i)\omega_{87}^{\mathbf{d}}, \\
M_{43,43}^{E,\mathbf{p}} &= \omega_{00}^{\mathbf{d}} + \frac{162}{143}\omega_{40}^{\mathbf{d}} - \frac{4}{11}\omega_{60}^{\mathbf{d}} - \frac{448}{143}\omega_{80}^{\mathbf{d}} - i\frac{5\sqrt{6}}{22}\omega_{22}^{\mathbf{d}} - i\frac{81\sqrt{10}}{143}\omega_{42}^{\mathbf{d}} - \frac{26}{33}\sqrt{\frac{35}{3}}(1+i)\omega_{63}^{\mathbf{d}} \\
&\quad - i\frac{14}{3}\sqrt{\frac{7}{33}}\omega_{66}^{\mathbf{d}} + i\frac{1288}{143}\sqrt{\frac{3}{143}}\omega_{86}^{\mathbf{d}} + \frac{840}{143}\sqrt{\frac{10}{143}}(1+i)\omega_{87}^{\mathbf{d}}.
\end{aligned}$$

TABLE VII. The relationship between angular momentum and irrep at momenta up to  $P^2 = 3P_0^2$ .

$\mathbf{p}$	$l$	$n$	$\Gamma$	$\alpha$	$C_{l,m}^{\Gamma,\alpha,n} l, m\rangle$	
(0, 0, 1)	0	1	$A_1$	1	$ 0, 0\rangle$	
	2	1	$A_1$	1	$ 2, 0\rangle$	
		1	$B_1$	1	$\frac{1}{\sqrt{2}}( 2, -2\rangle +  2, 2\rangle)$	
		1	$B_2$	1	$\frac{1}{\sqrt{2}}( 2, -2\rangle -  2, 2\rangle)$	
	1	$E$	1	1	$\frac{1}{\sqrt{2}}( 2, -1\rangle - i 2, 1\rangle)$	
		2			$\frac{1-i}{2}( 2, -1\rangle + i 2, 1\rangle)$	
	4	1	$A_1$	1	$\frac{1}{2}( 4, -4\rangle + \sqrt{2} 4, 0\rangle +  4, 4\rangle)$	
		2	$A_1$	1	$\frac{1}{2}( 4, -4\rangle - \sqrt{2} 4, 0\rangle +  4, 4\rangle)$	
	1	$A_2$	1	$\frac{1}{\sqrt{2}}(- 4, -4\rangle +  4, 4\rangle)$		
	1	$B_1$	1	$\frac{1}{\sqrt{2}}( 4, -2\rangle +  4, 2\rangle)$		
	1	$B_2$	1	$\frac{1}{\sqrt{2}}(- 4, -2\rangle +  4, 2\rangle)$		
	1	$E$	1	1	$\frac{1+i}{2\sqrt{2}}(- 4, -3\rangle +  4, -1\rangle - i 4, 1\rangle - i 4, 3\rangle)$	
		2			$\frac{1}{2}( 4, -3\rangle +  4, -1\rangle + i 4, 1\rangle - i 4, 3\rangle)$	
	2	$E$	1	1	$\frac{1+i}{2\sqrt{2}}( 4, -3\rangle +  4, -1\rangle - i 4, 1\rangle + i 4, 3\rangle)$	
		2			$\frac{1}{2}(- 4, -3\rangle +  4, -1\rangle + i 4, 1\rangle + i 4, 3\rangle)$	
	(1, 1, 0)	0	1	$A_1$	1	$ 0, 0\rangle$
		2	1	$A_1$	1	$ 2, 0\rangle$
			1	$A_1$	1	$\frac{1}{\sqrt{2}}( 2, -2\rangle -  2, 2\rangle)$
1		$A_2$	1	$\frac{1}{\sqrt{2}}( 2, -1\rangle - i 2, 1\rangle)$		
1		$B_1$	1	$\frac{1}{\sqrt{2}}( 2, -1\rangle + i 2, 1\rangle)$		
1		$B_2$	1	$\frac{1}{\sqrt{2}}( 2, -2\rangle +  2, 2\rangle)$		
4		1	$A_1$	1	$\frac{1}{2}( 4, -4\rangle -  4, -2\rangle +  4, 2\rangle +  4, 4\rangle)$	
		2	$A_1$	1	$\frac{1}{2}( 4, -4\rangle +  4, -2\rangle -  4, 2\rangle +  4, 4\rangle)$	
3		$A_1$	1	$ 4, 0\rangle$		
1		$A_2$	1	$\frac{1}{2}( 4, -3\rangle +  4, -1\rangle - i 4, 1\rangle + i 4, 3\rangle)$		
2		$A_2$	1	$\frac{1}{2}( 4, -3\rangle -  4, -1\rangle + i 4, 1\rangle + i 4, 3\rangle)$		
1		$B_1$	1	$\frac{1}{2}( 4, -3\rangle +  4, -1\rangle + i 4, 1\rangle - i 4, 3\rangle)$		
2		$B_1$	1	$\frac{1}{2}( 4, -3\rangle -  4, -1\rangle - i 4, 1\rangle - i 4, 3\rangle)$		
1		$B_2$	1	$\frac{1}{2}(- 4, -4\rangle +  4, -2\rangle +  4, 2\rangle +  4, 4\rangle)$		
2		$B_2$	1	$\frac{1}{2}( 4, -4\rangle +  4, -2\rangle +  4, 2\rangle -  4, 4\rangle)$		
(1, 1, 1)		0	1	$A_1$	1	$ 0, 0\rangle$
		2	1	$A_1$	1	$\frac{1}{\sqrt{6}}( 2, -2\rangle + (1-i) 2, -1\rangle + (1+i) 2, 1\rangle -  2, 2\rangle)$
			1	$E$	1	$\frac{1}{\sqrt{2}}( 2, -2\rangle +  2, 2\rangle)$
	2			$- 2, 0\rangle$		
	2	$E$	1	1	$\frac{1}{\sqrt{2}}( 2, -1\rangle - i 2, 1\rangle)$	
		2			$\frac{1}{\sqrt{6}}(-(1-i) 2, -2\rangle - i 2, -1\rangle +  2, 1\rangle + (1-i) 2, 2\rangle)$	
	4	1	$A_1$	1	$\frac{1}{2}\sqrt{\frac{5}{6}}( 4, -4\rangle + \sqrt{\frac{14}{5}} 4, 0\rangle +  4, 4\rangle)$	
		2	$A_1$	1	$\frac{1}{2}\left(-\sqrt{\frac{7}{6}} 4, -3\rangle + \frac{-1+i}{\sqrt{3}} 4, -2\rangle + \frac{-i}{\sqrt{6}} 4, -1\rangle + \frac{1}{\sqrt{6}} 4, 1\rangle + \frac{1-i}{\sqrt{3}} 4, 2\rangle + i\sqrt{\frac{7}{6}} 4, 3\rangle\right)$	
	3	$A_2$	1	$\frac{1}{2}\left(\frac{-1+i}{\sqrt{3}} 4, -4\rangle - \frac{i}{\sqrt{6}} 4, -3\rangle + \sqrt{\frac{7}{6}} 4, -1\rangle - i\sqrt{\frac{7}{6}} 4, 1\rangle + \frac{1}{\sqrt{6}} 4, 3\rangle + \frac{1-i}{\sqrt{3}} 4, 4\rangle\right)$		
	1	$E$	1	$\frac{1}{4}(-i\sqrt{7} 4, -3\rangle -  4, -1\rangle + i 4, 1\rangle + \sqrt{7} 4, 3\rangle)$		
	2	$E$	2	1	$\frac{1}{4}\left(\sqrt{\frac{7}{3}} 4, -3\rangle + \frac{4(-1+i)}{\sqrt{6}} 4, -2\rangle + \frac{i}{\sqrt{3}} 4, -1\rangle - \frac{1}{\sqrt{3}} 4, 1\rangle + \frac{4(1-i)}{\sqrt{6}} 4, 2\rangle - i\sqrt{\frac{7}{3}} 4, 4\rangle\right)$	
		2	$E$	1	$-\frac{1}{\sqrt{2}}( 4, -2\rangle +  4, 2\rangle)$	
	2			$\frac{1}{2}(\sqrt{\frac{7}{6}} 4, -4\rangle - \sqrt{\frac{5}{3}} 4, 0\rangle + \sqrt{\frac{7}{6}} 4, 4\rangle)$		
	3	$E$	1	1	$\frac{1}{\sqrt{3}}\left(- 4, -4\rangle - \frac{1-i}{4\sqrt{2}} 4, -3\rangle - \frac{\sqrt{7}(1+i)}{4\sqrt{2}} 4, -1\rangle + \frac{\sqrt{7}(-1+i)}{4\sqrt{2}} 4, 1\rangle - \frac{1+i}{4\sqrt{2}} 4, 3\rangle +  4, 4\rangle\right)$	
		2			$\frac{1+i}{4\sqrt{2}}( 4, -3\rangle - i\sqrt{7} 4, -1\rangle + \sqrt{7} 4, 1\rangle - i 4, 3\rangle)$	

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