Angular Momentum on the Lattice: The Case of Non-Zero Linear Momentum

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Abstract

The irreducible representations (IRs) of the double cover of the Euclidean group with parity in three dimensions are subduced to the corresponding cubic space group. The reduction of these representations gives the mapping of continuum angular momentum states to the lattice in the case of non-zero linear momentum. The continuous states correspond to lattice states with the same momentum and continuum rotational quantum numbers decompose into those of the IRs of the little group of the momentum vector on the lattice. The inverse mapping indicates degeneracies that will appear between levels of different lattice IRs in the continuum limit, recovering the continuum angular momentum multiplets. An example of this inverse mapping is given for the case of the "moving" isotropic harmonic oscillator.

I. INTRODUCTION

A question of great interest in lattice QCD is how rotational states on the lattice correspond to states of definite angular momentum in the continuum limit. To find this correspondence, we find the mapping of continuum states to lattice irreducible representations (IRs) and invert it. This problem has been discussed in several contexts previously – in solid state physics, the "cubic harmonics" are formed by a projection of the continuum spherical harmonics onto the lattice, *e.g.* [1]. In lattice QCD, the reduction of continuum states to the hypercubic lattice was given by Mandula *et al.* [2, 3], and the reduction of the full continuum symmetry group (including Poincaré, color, flavor, and baryon number symmetries) to the lattice for the case of staggered fermions was given by Golterman and Smit [4, 5] and expanded to include non-zero momentum by Kilcup and Sharpe [6].

We are interested in the classes of lattice actions with unbroken flavor symmetries (*i.e.* Wilson and overlap). In particular, we focus on the IRs of the symmetry group of the lattice Hamiltonian. Johnson [7] considered the mapping of continuum SU(2) states to the octahedral group and its double cover, and Basak *et al.* [8, 9] considered the inclusion of parity in these groups. We expand on this work to include non-zero momentum. This extension will be needed to apply group theory methods to the calculation of matrix elements for hadrons and electromagnetic currents on the lattice [10].

The continuum spacetime symmetries of the QCD action are given by the Poincaré group, $\mathcal{P}$. The spatial symmetries of the QCD Hamiltonian correspond to a subgroup of $\mathcal{P}$ which is the semidirect product of the group of orthogonal transformations in three dimensions and the group of translations, $\mathcal{T}^3 \rtimes \mathrm{O}(3)$ (pure time inversion is also a symmetry element, but its addition is trivial since it commutes with all other group elements). On the lattice, the symmetry group is $\mathcal{T}_{lat}^3 \rtimes \mathrm{O}_h$, where the rotational group is reduced to a subgroup of $\mathrm{O}(3)$ with only a finite number of rotations and reflections, and where the subgroup of $\mathcal{T}^3$ contains only lattice translations. Throughout this paper we consider the double covers of the rotational groups since the double valued IRs correspond to fermionic states in the continuum [7]. We denote the continuous group $\mathcal{G} = \mathcal{T}^3 \rtimes \mathrm{O}^{\mathrm{D}}(3)$ and the discrete group $\mathcal{T}_{lat}^3 \rtimes \mathrm{O}_h^{\mathrm{D}}$, where the superscript D denotes the double cover.

We construct the IRs of these groups from the normal subgroups of translations by the method of little groups. We then subduce a representation of $\mathcal{T}_{lat}^3 \rtimes \mathrm{O}_h^{\mathrm{D}}$ by restricting the IRs

of $\mathcal{G}$ to the subgroup of lattice elements. Using the orthogonality properties of characters, we reduce the subduced representations into the IRs of the lattice group. As in the zero momentum case, many continuous states are mapped to each angular momentum state on the lattice. This presents complications in finding the inverse mapping, which is our actual interest. The ambiguities associated with this inverse mapping are demonstrated for the simple case of the moving harmonic oscillator.

II.   THE SYMMETRY GROUPS AND THEIR REPRESENTATIONS

A.   The discrete group, $\mathcal{T}^3_{lat} \rtimes O^D_h$

The group of proper rotations of a cube in three dimensions is the octahedral group, O. We are also interested in its double cover, O^D, and we consider the inclusion of parity by forming the group $O^D_h = O^D \times C_2$, where C_2 consists of the identity and a parity element I_s, corresponding to inversion of all three coordinate axes through the origin. The inclusion of parity is straightforward because I_s commutes with all proper rotations in three dimensions. Throughout this paper we adopt the Mulliken convention for the labeling of finite groups.

For $\mathcal{T}^3_{lat} \rtimes O^D_h$, we can then write the group elements $\{R_i, \mathbf{n}\}$, where R_i denotes a rotation in one of the lattice rotation groups discussed above, followed by a lattice translation by $\mathbf{n}$. The subgroup of translations, $\mathcal{T}^3_{lat}$, is normal, so we can easily use this subgroup to induce the IRs of the full group [1, 11]. The IRs of $\mathcal{T}^3_{lat}$ are labeled by a vector of real numbers, $\mathbf{k}$, where the k_i lie in an interval of length 2π. For an IR of $\mathcal{T}^3_{lat}$ labeled by $\mathbf{k}$, we form the little group, which consists of the R_j in O^D_h such that $R_j \mathbf{k} = \mathbf{k}$. We also form the star of $\mathbf{k}$, which is the set of vectors $\mathbf{k}_p = R_p \mathbf{k}$ for all R_p in the rotation group. The IRs of $\mathcal{T}^3_{lat} \rtimes O^D_h$ are then labeled by $\mathbf{k}$ and a label α denoting an irreducible representation of the little group of $\mathbf{k}$. After summing over the diagonal elements, we find the characters:

$$\chi^{(\mathbf{k},\alpha)}(R_j, \mathbf{n}) = \sum_{\mathbf{k}_q} \chi^\alpha(R_j) e^{-i\mathbf{k}_q \cdot \mathbf{n}} \tag{1}$$

where the sum is taken over only the subset $\mathbf{k}_q$ of the star vectors $\mathbf{k}_p$ such that R_j is in the little group of $\mathbf{k}_q$. Also, $\chi^\alpha(R_j)$ is the character in the representation α of the little group and in general can depend on the particular point in the star. We see that representations labeled by $\mathbf{k}$ in the same star are equivalent, so we label the inequivalent irreducible representations,

TABLE I: Little groups for the possible lattice momenta. Dic_n denotes the dicyclic group of order $4n$.

$(0,0,0)$	O_h	O_h^{D}
$(n,0,0)$	C_{4v}	Dic_4
$(n,n,0)$	C_{2v}	Dic_2
(n,n,n)	C_{3v}	Dic_3
$(n,m,0)$	C_2	C_4
(n,n,m)	C_2	C_4
(n,m,p)	C_1	C_2

$\Gamma^{(|\mathbf{k}|,\alpha)}$, by a star given by $|\mathbf{k}|$ and an IR of the little group labeled by α. Care must be taken to distinguish between IRs labeled by $\mathbf{k}$ in different stars but with the same length, *e.g.* $\mathbf{k} = (2,2,1)$ and $\mathbf{k} = (3,0,0)$.

To use the above formula, we will need to know the characters of the little group for a given $\mathbf{k}$. If $\mathbf{k} = (0,0,0)$, then the little group is the full rotation group, O_h^{D}, and the results for this case are well-known. If $\mathbf{k}$ is non-zero, then the little group becomes a subgroup of O_h^{D}. The possible little groups for the rotation group O_h^{D} are given in Tab. I. Since we are interested in the covering group $SU(2) \times Z_2$, we find that the double covers of the little groups are dicyclic groups [12]. The character tables for the double covers of the little groups can be calculated using the $J^P = \frac{1}{2}^-$ representation of $SU(2) \times Z_2$ to determine the multiplication tables [13].

B.   The continuous group, $\mathcal{G}$

We can construct the characters for the irreducible representations of the continuous group $\mathcal{G}$ analogously. Translations are again a normal subgroup and their IRs are labeled by $\mathbf{k}$, but there is no longer a restriction on the values of the k_i. Every non-zero vector $\mathbf{k}$ now has a little group of the same form, which consists of rotations in the plane orthogonal to $\mathbf{k}$ and reflections through planes containing $\mathbf{k}$. This little group, known as $C_{\infty v}$, is isomorphic to the group $O(2)$ of all orthogonal matrices in two dimensions (as usual we consider the double covers). We induce a representation of $\mathcal{G}$ from the subgroup of translations, and we

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TABLE II: The character table for the double cover of $C_{\infty v}$. E denotes the identity, $R(\theta)$ is any proper rotation by θ, and σ_v is any reflection through the axis given by $\mathbf{k}$.

m_j	E	$R(\theta)$	σ_v
0^+	1	1	1
0^-	1	1	-1
$m_j \geq \frac{1}{2}$	2	$2\cos m_j\theta$	0

construct basis vectors labeled by the star of $\mathbf{k}$, and by $m_j = 0^+, 0^-, \frac{1}{2}, 1, ...$, which labels the IR of the little group ($C_{\infty v}$ has two one dimensional IRs labeled as $m_j = 0^+, 0^-$. All other IRs are two dimensional and are labeled by a positive integer or half-integer). Here, the star of $\mathbf{k}$ is all vectors of length $|\mathbf{k}|$. A general irreducible representation of $\mathcal{G}$ is then labeled as $E^{(|\mathbf{k}|,m_j)}$. Physically, m_j denotes the projection of the total angular momentum, j, along $\mathbf{k}$.

We are interested in subducing a representation of the cubic space group by considering the IRs of $\mathcal{G}$ restricted to the subgroup of elements which are in the lattice group. As before, we are only interested in the characters of the (generally reducible) representations of the space group subduced from $\mathcal{G}$. For these elements, we compute the characters by summing only over the diagonal matrix elements in the IRs of $\mathcal{G}$ which correspond to lattice vectors $\mathbf{k}$. The character of this subduced representation for a general group element $\{R_i, \mathbf{n}\}$ is then given as:

$$\chi^{(\mathbf{k},\alpha)}(R_i, \mathbf{n}) = \chi^{(m_j)}(R_i) \sum_{\mathbf{k}_q} e^{-i\mathbf{k}_q \cdot \mathbf{n}} \tag{2}$$

where, as in the discrete case, the sum is only taken over the vectors $\mathbf{k}_q$ of length $|\mathbf{k}|$ on the lattice such that R_i leaves $\mathbf{k}_q$ invariant. The characters $\chi^{(m_j)}$ of a rotation R_i of magnitude θ are given in Tab. II. In the special case $\mathbf{k} = 0$, the star contains only one point, and the little group is just $O^D(3)$. Therefore the representations $E^{(0,m_j)} = D^{(j,\pi)}$, which are just the familiar representations of $SU(2) \times C_2$ labeled by $j = 0, \frac{1}{2}, 1, ...$ and a parity $\pi = \pm 1$.

III. THE REDUCTION OF STATES

By the orthogonality properties of characters for finite groups, the multiplicity, m, that an irreducible representation of $\mathcal{T}_{lat}^3 \rtimes O_h^D$ labeled by $(|\mathbf{k}|, \alpha)$ is contained in a subduced

representation of $\mathcal{G}$ labeled by $(|\mathbf{k}'|, m_j)$ is given by:

$$m = \frac{1}{g} \sum_a \chi^{(|\mathbf{k}|, \alpha)}(G_a)^* \chi^{(|\mathbf{k}'|, m_j)}(G_a) \tag{3}$$

where the sum is taken over all group elements G_a, and g is the order of the group. The groups $\mathcal{G}$ and $\mathcal{T}_{lat}^3 \rtimes O_h^D$ allow arbitrarily large translations, so we cannot apply Eq. (3) directly, but must consider the 3-torus formed by the boundary conditions $\mathbf{r} + \mathbf{N} = \mathbf{r}$ for all vectors $\mathbf{r}$ and some constant vector $\mathbf{N} = (N, N, N)$. The boundary conditions limit the allowed values of $\mathbf{k}$ to $k_i = 2\pi \frac{n_i}{N}$, where $n_i < N$ is an integer. For simplicity, we denote the vectors $\mathbf{k}$ on the finite lattice as simply the integers (n_1, n_2, n_3), and introduce a factor of $2\pi/N$ in the exponential of Eq. (1). We then apply Eq. (3) using the characters given in Eqs. (1) and (2), modified for use on the torus. For finite lattices, we find that the projection formula reduces to the projection of the continuous rotation group to the little group given by $\mathbf{k}$, independent of the lattice size. We also find that representations labeled by different stars are orthogonal. Therefore, the reduction of an arbitrary IR of $\mathcal{G}$ labeled by $(\mathbf{k}, m_j)$ contains IRs of the discrete group labeled by $\mathbf{k}$, and by α which correspond to the reduction of $O^D(2)$ to the little group. These reductions for the various little groups of O_h^D and $m_j = 0, \frac{1}{2}, ..., 3$ are given in Tab. III. As an example, we see that if $\mathbf{k} = (1, 0, 0)$ and $m_j = 2$, then $E^{(1,0,0),2} = \Gamma^{(1,0,0),B_1} \oplus \Gamma^{(1,0,0),B_2}$.

If $\mathbf{k} = 0$, one reduces $O^D(3)$ to O_h^D. These results can be read off those given by Johnson [7] using the result that IRs of $O^D(3)$ with positive parity, $\pi = +1$, correspond to the "gerade" IRs (*e.g.* A_{1g}) of O_h^D only, and those with $\pi = -1$ correspond to the "ungerade" IRs (*e.g.* A_{1u}) only [8, 14].

IV. THE MOVING HARMONIC OSCILLATOR

We can now apply these results to a physical problem – the isotropic harmonic oscillator potential moving at some constant (non-relativistic) velocity. The solution for such a moving potential is known in the continuum [15], and the wavefunctions are simply products of a translational piece and the wavefunctions of the stationary potential. Accordingly, the energies just pick up an extra contribution due to the translational energy of the center of mass, and the continuum spectrum is $E_{n,v} = \frac{1}{2}mv^2 + E_n$ for translation at a constant velocity, v, and the energies of the stationary oscillator, E_n. In Cartesian coordinates, the

TABLE III: Reduction of the double cover of O(2) to the possible little groups. The double covers of the little groups include the single valued IRs of the corresponding little groups in O_h and double valued IRs corresponding to fermionic continuum IRs.

m_j	Dic_4	Dic_3	Dic_2	C_4	C_2
0^+	A_1	A_1	A_1	A	A
0^-	A_2	A_2	A_2	B	A
$\frac{1}{2}$	E_1	E_1	E	E	$2B$
1	E_2	E_2	$B_1 \oplus B_2$	$A \oplus B$	$2A$
$\frac{3}{2}$	E_3	$B_1 \oplus B_2$	E	E	$2B$
2	$B_1 \oplus B_2$	E_2	$A_1 \oplus A_2$	$A \oplus B$	$2A$
$\frac{5}{2}$	E_3	E_1	E	E	$2B$
3	E_2	$A_1 \oplus A_2$	$B_1 \oplus B_2$	$A \oplus B$	$2A$
$\frac{7}{2}$	E_1	E_1	E	E	$2B$
4	$A_1 \oplus A_2$	E_2	$A_1 \oplus A_2$	$A \oplus B$	$2A$

Hamiltonian for the stationary harmonic oscillator potential is just the sum of three 1-D oscillators in each of the coordinate directions. These coordinate pieces commute, so the Schrödinger equation is variable separable, the wavefunctions are just products of the 1-D wavefunctions, and the energies are just sums of the 1-D energies. Thus, the familiar continuum levels are evenly spaced and have alternating parities given as $(-1)^n$.

On an N^3 lattice, the Hamiltonian is still the sum of three commuting pieces, where each piece is now an $N \times N$ matrix. Using the finite difference approximation for the momentum, $p_x^2 = -\hbar^2(\delta_{x+1,x'} + \delta_{x-1,x'} - 2\delta_{x,x'})/a^2$, where a is the lattice spacing, then on a 3^3 lattice, we find three 1-D levels with energies denoted as E_0, E_1, and E_2 in order of increasing energy, and where $E_1 - E_0 > E_2 - E_1$. Unlike the continuum, the energies are not evenly spaced, and they have parities $+, +, -$ respectively. The energies of the 3-D oscillator on the lattice are then given as $E_n = E_{n_x} + E_{n_y} + E_{n_z}$ for $n_i = 0, 1, 2$.

We now consider the inverse mapping of these lattice oscillator states into continuum states of some angular momentum. This inversion presents difficulty because as in Tab. III, many continuum states are mapped to each discrete state. For $E_{|\mathbf{k}|,n}$ with $\mathbf{k} = 0$, this inverse mapping was found by Johnson [7]. We consider this mapping in the case of a non-trivial

TABLE IV: (a) The reduction of O(2) to the little group C_{4v}, which are obtained from Tab. III by taking the single valued representations of Dic_4 on the integer values of m_j. (b) The reduction of the lattice oscillator states to C_{4v} along with the parities of the states, which correspond to the parities in the continuum limit.

H.O. states	Parity	C_{4v} content
$|000\rangle$	$+$	A_1
$|100\rangle$	$+$	$2A_1 \oplus B_1$
$|200\rangle$	$-$	$A_1 \oplus E$
$|110\rangle$	$+$	$2A_1 \oplus B_1$
$|210\rangle$	$-$	$A_1 \oplus B_1 \oplus 2E$
$|220\rangle$	$+$	$B_2 \oplus E$
$|111\rangle$	$+$	A_1
$|211\rangle$	$-$	$A_1 \oplus E$
$|221\rangle$	$+$	$B_2 \oplus E$
$|222\rangle$	$-$	B_2

(b)

m_j	C_{4v} content
0^+	A_1
0^-	A_2
1	E
2	$B_1 \oplus B_2$
3	E
4	$A_1 \oplus A_2$

(a)

momentum, $\mathbf{k} = (1,0,0)$ with little group C_{4v} in O_h. We see the degenerate states are labeled by the vectors $\mathbf{k}'$ in the star of $\mathbf{k}$ and the set of oscillator states $|n_x n_y n_z\rangle$ with energy E_n for some fixed n. The characters of the degenerate states as basis vectors for the representations of $\mathcal{T}_{lat}^3 \rtimes O_h$ are then found, and the reduction of the oscillator states to the IRs of the space group is given in Tab. V(b). For simplicity, we omit the translation labels in the table as the oscillator states trivially contain only IRs labeled by $\mathbf{k} = (1,0,0)$. Thus, the first row of the table indicates that the moving oscillator state labeled by $\mathbf{k} = (1,0,0)$ and $|n_x n_y n_z\rangle = |000\rangle$ contains the irreducible representation $\Gamma^{(1,0,0),A_1}$ of $\mathcal{T}_{lat}^3 \rtimes O_h$. In the following, we speak only of the rotational states, but the translational component is implicit.

By comparison with the reduction of O(2) to C_{4v}, as given in Tab. V(a), we see that the ground state $|000\rangle$ is the lowest state containing A_1 and corresponds to $m_j = 0^+$. The next state, $|100\rangle$ with C_{4v} content $2A_1 \oplus B_1$, has positive parity and corresponds to

the $m_j = 0^2, 1, 2$ doublet in the continuum (in the continuous case, the degenerate states $|200\rangle_{cont}$ and $|110\rangle_{cont}$ form a doublet with $j = 0, 2$. For the projection along some axis, this gives $m_j = 0$ and $m_j = 0, 1, 2$). The states $|220\rangle$ and $|221\rangle$ both have positive parity and the correct C_{4v} content to partner it, but the lower energy state $|220\rangle$ is the correct partner. Without knowledge of the continuum states, this assignment would be unclear. The state $|200\rangle$ has negative parity and is the lowest energy $A_1 \oplus E$ state, and it corresponds to $m_j = 0, 1$ (i.e. $j = 1$). On this small lattice, the symmetric boundary conditions have moved this level above part of the $j = 0, 2$ doublet. The states $|110\rangle$ and $|210\rangle$ with respective partners $|221\rangle$ and $|222\rangle$ are parts of the continuum multiplets $j = 0, 2, 4$ and $j = 1, 3$, but the multiplets are not complete due to the small size of the lattice. Angular momentum assignments for higher energy states are increasingly difficult, and rely heavily upon knowledge of the continuum states.

The results found for the moving oscillator correspond to those found in the case of $\mathbf{k} = 0$ since the moving states of the oscillator have the same angular momentum content as the states of the stationary oscillator. However, states are now labeled only by the projection of j along $\mathbf{k}$. Thus, states labeled by $m_j = 0, 1, ..., j$ lie in different IRs and contribute to any state with a given j. With non-zero $\mathbf{k}$, the rotation group is some subgroup of O_h, and thus has fewer irreducible representations. This leads to even more ambiguity in the inverse mapping as the continuum states are mapped into fewer rotational states on the lattice.

V. CONCLUSION

We have expanded upon the results for the mapping of angular momentum states to the lattice and demonstrated the inverse mapping for a system moving with non-zero linear momentum. Due to the semidirect product structure of the groups we induce representations of the groups from the subgroups of translations. Since arbitrarily large translations are allowed, we consider the projection of states on finite lattices and take the limit as the number of lattices sites grows arbitrarily large. We find that the continuum states are mapped to states with the same momentum vector, with the continuum rotational states decomposing into the states in the little group of the momentum vector.

In the example of the moving harmonic oscillator potential, we have seen that, without additional information, the inverse mapping of lattice states to continuum states is difficult

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for anything but the lowest angular momentum states. In the continuum case these ambiguities increase for non-zero momentum because continuum states are mapped to fewer rotational states on the lattice. In addition, states are now labeled by the projection of j along the direction of motion, so states with the same j but different projections m_j belong to different irreducible representations.

VI.   ACKNOWLEDGEMENTS

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