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ANGULAR MOMENTUM ON A LATTICE

R.C. Johnson

CERN - Geneva

and

Durham University, England *)

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Reduction of SU_2 with respect to the double cover of the rotation group of the cube shows how spin is realized on a cubic lattice. Only spins 0, $1/2$, 1, $3/2$ are described by single representations of the cube group. Higher spins are described by two or more such representations. Implications for lattice dynamical calculations are discussed.

*) Permanent address; after 1st April 1982.

The group of rotational symmetries of a cube is the "angular momentum" group for the cubic lattice. It is the well-known¹⁾ crystallographic point group $\mathbf{O}$ (octahedral group) and is of course a finite subgroup of the continuum rotation group SO_3 .

As is familiar, SO_3 has the infinite sequence of vector irreducible representations (IRs) labelled by integer angular momentum $j = 0, 1, 2, \dots$ plus the interleaving sequence of ray IRs for half-odd-integer angular momentum $j = 1/2, 3/2, 5/2, \dots$, together being the vector IRs of its double cover SU_2 .

The cube group $\mathbf{O}$, however, has only five vector IRs and three further ray IRs, corresponding to the eight vector IRs of ${}^2\mathbf{O}$, its double cover.

That is, only a handful of different possibilities exist for rotational classification of lattice energy eigenstates. So the question arises: exactly how do these correspond to angular momentum in the continuum limit?

The question is currently interesting because of lattice QCD calculations of hadron states and attempts to include fermions²⁾.

Some part of the answer, for integer j , is evidently well known³⁾, and more can be extracted from the solid-state literature⁴⁾. This note summarizes the complete answer, including fermions, and comments on its implications.

$\mathbf{O}$ has 24 elements in five conjugacy classes, and is isomorphic to the full tetrahedral group T_d (rotations plus reflections of a regular tetrahedron), and to the permutation group of four objects, S_4 - permutations of the tetrahedron's vertices or the cube's body diagonals.

If the origin of Cartesian co-ordinates x, y, z is at the cube's centre with the axes parallel to its edges, then the elements of $\mathbf{O}$ are:

I : identity:

$3C_2$: π rotations about three co-ordinate axes;

$8C_3$: $\pm 2\pi/3$ rotations about four body diagonals, e.g. $x = y = z$;

$6C_4$: $\pm\pi/2$ rotations about three co-ordinate axes;

$6C'_2$: π rotations about axes parallel to six face diagonals, e.g., $x = y, z = 0$.

${}^2\mathbf{O}$ is constructed by adding a negative identity J for $\pm 2\pi$ rotations. Then from the C_3 and C_4 classes of $\mathbf{O}$ come two new classes of elements of ${}^2\mathbf{O}$, of order six and eight. Thus the 48 elements of ${}^2\mathbf{O}$ divide into eight conjugacy classes.

The five standard vector IRs of $\mathbf{O}$, called A_1, A_2, E, T_1, T_2 - collectively $\mathcal{V}$, say - have respective dimensions 1, 1, 2, 3, 3. A_1 is the identity representation, and T_1 rotates the geometrical vector (x, y, z) . A sign change of matrices in classes C_4 and C'_2 connects A_1 to A_2 and T_1 to T_2 .

The three further IRs of ${}^2\mathbf{0}$ (ray IRs of $\mathbf{0}$) - call them G_1, G_2, H , and collectively $\mathcal{R}$ - must have even dimension, and only 2, 2, 4 fits. G_1 and G_2 are mutually linked like A_1 and A_2 , T_1 and T_2 .

Table 1 gives characters of the eight vector plus ray IRs of $\mathbf{0}$, and with these at hand the calculations are straightforward. The traces of SU_2 matrices for spin j and rotation angle θ are given by

$$\chi_{\theta}^{(j)} = \frac{\sin[(j+\frac{1}{2})\theta]}{\sin[\theta/2]}, \quad (1)$$

so characters of SU_2 matrices for the operators of $\mathbf{0}$ and ${}^2\mathbf{0}$ are written down at once (see Table 1). Then their content of IRs $\mathcal{U}$ (for $J = 0, 1, 2, \dots$) or $\mathcal{R}$ (for $j = 1/2, 3/2, 5/2, \dots$) is projected out using standard results¹⁾ on orthogonality of characters. That is, the multiplicity $m_j^{(r)}$ of an IR r for spin j is given by

$$m_j^{(r)} = \frac{1}{g} \sum_k n_k \chi_k^{(r)} \chi_k^{(j)},$$

where there are n_k elements in class k with character $\chi_k^{(r)}$, and $g = \sum_k n_k$.

Table 2 gives consequent results up to $j = 5$, and continuation is routine. Only angular momenta $j = 0, 1/2, 1$ and $3/2$ correspond to single IRs of both SU_2 and ${}^2\mathbf{0}$. Higher spins $j \geq 2$ are described by two or more different IRs of the cube group. No reason appears why reduced rotational symmetry alone could lead to species multiplication of lattice fermions⁵⁾.

A specific question arising in the context of lattice QCD calculations of the hadron spectrum^{2),3),6)} is: what is the spin content of a lattice energy eigenstate transforming as a single IR of $\mathbf{0}$?

From Table 3, etc., the answer is:

- $A_1 \rightarrow (j = 0, 4, 6, 8, \dots),$
- $A_2 \rightarrow (j = 3, 6, 7, 9, \dots),$
- $E \rightarrow (j = 2, 4, 5, 6, \dots),$
- $T_1 \rightarrow (j = 1, 3, 4, 5 \text{ (twice)}, \dots),$
- $T_2 \rightarrow (j = 2, 3, 4, 5, \dots),$
- $G_1 \rightarrow (j = 1/2, 7/2, 9/2, 11/2, \dots)$
- $G_2 \rightarrow (j = 5/2, 7/2, 11/2, 13/2 \text{ (twice)}, \dots),$
- $H \rightarrow (j = 3/2, 5/2, 7/2, 9/2 \text{ (twice)}, \dots).$

Ascribing a definite spin to a single lattice state is therefore not possible without further dynamical information.

However, presumably few would quarrel with bosonic and fermionic ground states in representations A_1 and G_1 being identified as spins 0 and 1/2 respectively.

Perhaps also a low-mass T_1 state could be $j = 1$ - but if in the continuum limit hitherto distant A_2 and T_2 levels moved to coalesce with it, then $j = 3$ would be there too, or instead. Similarly the interpretation of H as $j = 3/2$ alone is uncertain if G_2 could move in to make $j = 5/2$.

Is an E state spin 2? Maybe, if T_2 is nearby; yes if they coincide in the continuum limit - but without going to the limit the mass M is not well defined. The best that can be done is to take

$$M(j=2) = \text{Some average of } \{ M(E), M(T_2) \},$$

where what should be used for averaging is quite vague. For higher spins, where more representations of $\mathbf{0}$ contribute, mass predictions are correspondingly harder, even if all the IRs needed can be found.

Some illustration of possible ambiguities is given by the spectrum of a three-dimensional isotropic simple harmonic oscillator on a cubic lattice. Energy levels are sums of excitations in each of the three directions, and wave functions are simple products. On an n^3 lattice, each of the three pieces of the Hamiltonian $p^2 + x^2$ is an $n \times n$ matrix, irrespective of the choice of momentum operator p , and so gives n energy levels. Because of restriction to a finite lattice these levels are generally by no means equally spaced. The spectrum is a jumble of states of degeneracies at least 1, 3 and 6, corresponding to the non-accidental degeneracy of $E_a + E_b + E_c = \text{fixed}$, with a, b, c ($= 1, 2, \dots, n$ independently) either all the same, or with two the same, or all different. Both six-fold and three-fold levels project onto IRs $\mathcal{U}$ of $\mathbf{0}$ in four different ways (according to their parity content), and the non-degenerate levels are either A_1 or A_2 .

Table 3 gives the spectrum for a case $n = 3$. The oscillator has 10 levels, corresponding to the lowest 7 of the continuum system, which has equal spacing. The first two levels here (111, 211) are clearly $j = 0$ and $j = 1$ respectively. The next two together (122+311), which coincide in the continuum, are needed to make the $j = 0, j = 2$ tower. But even with this knowledge, since E and T_2 are split apart, on the lattice the energy of $j = 2$ is not defined.

Likewise the next two (222+123) should go to make up $j = 1$ plus $j = 3$. But besides splitting them apart, the small size of the lattice does not allow sufficient additional degrees of freedom - no 411 state. These, and higher levels more so, are just shadows of their continuum counterparts, without knowledge of which it would be impossible to discover their angular momentum assignments.

The oscillator example illustrates vividly the remarks made above - beyond perhaps the very lowest states unambiguous mass and spin assignments are a matter of guesswork without examining the continuum limit. This is normally an impossible dream.

What can be concluded ?

Group theory shows how to put spin onto a cubic lattice. With a simple example to drive home the point it also warns against too careless conclusions about masses and spins of states calculated there. In particular, mass predictions of at least $j > 1$ mesons/glueballs⁶⁾ must have large uncertainties. If baryons are calculated, then perhaps a nucleon mass may be credible, but masses of N^* states, etc., could be wildly inaccurate.

Table 1

Characters of IRs of $\mathbf{O}$ and ${}^2\mathbf{O}$. Values of θ are given to calculate traces of corresponding SU_2 matrices via Eq. (1).

(a) Vector IRs $\mathcal{V}$ of $\mathbf{O}$.

	I	$3C_2$	$8C_3$	$6C_4$	$6C'_2$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	2	-1	0	0
T_1	3	-1	0	1	-1
T_2	3	-1	0	-1	1
θ	2π	π	$2\pi/3$	$\pi/2$	π

(b) Additional ray IRs $\mathcal{R}$ of $\mathbf{O}$ - vector IRs of ${}^2\mathbf{O}$.

	I	J	$6C_4$	$8C_3$	$8C_6$	$6C_8$	$6C_8$	$12C'_4$
G_1	2	-2	0	-1	1	$-\sqrt{2}$	$\sqrt{2}$	0
G_2	2	-2	0	-1	1	$\sqrt{2}$	$-\sqrt{2}$	0
H	4	-4	0	1	-1	0	0	0
θ	4π	2π	π	$4\pi/3$	$2\pi/3$	$3\pi/2$	$\pi/2$	π

Table 2

Reduction of SU_2 matrices
to IRs of ${}^2\mathbf{O}$

j = 0	A_1
1/2	G_1
1	T_1
3/2	H
2	E, T_2
5/2	G_2, H
3	A_2, T_1, T_2
7/2	G_1, G_2, H
4	A_1, E, T_1, T_2
9/2	$G_1, 2H$
5	$E, 2T_1, 2T_2$

Table 3

Spectrum of an isotropic simple harmonic oscillator on a 3^3 lattice, in order of increasing energy, assuming that $E_2 - E_1 < E_3 - E_2 < 2(E_2 - E_1)$ - where the second inequality avoids the extra complication of level crossing.

Quantum numbers	Degeneracy	$\mathbf{O}$ Content
111	1	A_1
211	3	T_1
122	3	T_2
311	3	A_1, E
222	1	A_2
123	6	T_1, T_2
322	3	T_2
133	3	A_1, E
233	3	T_1
333	1	A_1

REFERENCES

- 1) W. Miller, "Symmetry Groups and their Applications", Academic Press, N.Y., (1972).
- 2) H. Hamber and G. Parisi, Phys. Rev. Lett. 47 (1981) 1792;
E. Marinari, H. Hamber and G. Parisi, Phys. Rev. Lett. 47 (1981) 1795; 314;
H. Hamber, E. Marinari, G. Parisi and C. Rebbi, Phys. Lett. 108B (1982)
A. Hasenfratz, Z. Kunszt, P. Hasenfratz and C.B. Lang, CERN preprint TH.3220 (1981).
- 3) J.M. Drouffe and C. Itzykson, Phys. Rep. 38C (1978) 133.
- 4) S.L. Altmann and A.P. Cracknell, Rev. Mod. Phys. 37 (1965) 19.
- 5) L.H. Karsten and J. Smit, Nucl. Phys. B183 (1981) 103;
H.B. Nielson and M. Ninomiya, Nucl. Phys. B185 (1981) 20;
L.H. Karsten, Phys. Lett. 104B (1981) 315.
- 6) M. Falcioni, E. Marinari, M.L. Paciello, G. Parisi, F. Rapuano, B. Taglienti and Zhang Yi-cheng, preprint ROM 81-277 (Dec. 1981).