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LETTER TO THE EDITOR

Tensor operators and the trace metric

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Abstract. The traditional unit tensor operators are shown to be orthonormal vectors in a trace metric approach. The operator equivalents of crystal field theory are used as models of the tensor operators which act as generators in Lie group theory.

1. Introduction

Many of the Lie groups used in physics are most easily defined and visualized in terms of matrices (eg SU_3 is the group of 3×3 complex unitary matrices with determinant $+1$). The infinitesimal generators of the group then arise naturally when we consider group elements in the neighbourhood of the identity element, which is a unit matrix. These generators form a Lie algebra under the commutation operation. An alternative approach (Judd 1963) is to use unit tensor operators of the rotation group O(3), and to construct families of these operators which are 'closed' with respect to the commutation operation. The connection between the two approaches is as follows, for the illustrative case of U_3 (Killingbeck 1975); the matrices of the eight tensor operators of type T_0^0, T_1^m, T_2^m within the $L=1$ manifold are (when suitably scaled) the matrix generators of the group U_3 of 3×3 matrices. This simple point can cause confusion if not clearly noted; for example, in Judd's book (1963) the symbols $V_q^{(k)}$ which appear throughout chapter 5 are perhaps better regarded as matrices than as operators. Equation (5.14) of that book resembles an operator identity, whereas it is a tensor operator commutation rule which holds only for certain operands. We can illustrate this as follows. The major feature of the operators used is that they are diagonal in total angular momentum and in other quantum numbers. We can satisfy this by using as models the operator equivalents which are popular in crystal field theory (eg Stevens 1952). The simple operators L_+^2 and L_-^2 will serve to represent operators of types T_2^2 and T_2^{-2}; we quickly find the following identities within the manifolds $L=2$ and $L=1$:

$$5[L_+^2, L_-^2] \equiv \begin{cases} 84L_z - 8(5L_z^3 - 17L_z) & (L=2) \qquad (1) \\ 20L_z & (L=1). \qquad (2) \end{cases}$$

These results show that there is a T_3^0 component in the operator commutator, but that this is ineffective if the restricted $L=1$ manifold alone is used. The present letter is 'inter-disciplinary' in that it uses the operator equivalents of solid state theory to explore a few points in Lie group theory; it also uses a trace metric approach, which should be useful to workers in several areas of theoretical physics. In § 2, we derive a useful sum rule which characterizes the unit tensor operators, and give a few examples of these operators. In § 3 we introduce the trace metric, show its relation to the tensor operator theory, and illustrate its usefulness by means of a few examples. Section 4 treats some ideas from Lie group theory, and § 5 gives the trace metric approach to the group G_2. Our intention is to report these useful techniques briefly so that other workers may be encouraged to develop and apply them.

2. Unit tensor operators

The basic theory scattered through the papers of Racah is neatly summarized in Judd's book (1963). The unit tensor operators of the theory are diagonal in L, and have the following matrix elements, obtained by combining equations (2.27) and (5.13) of Judd:

$$\langle LM|T_n^m|LM'\rangle = (-1)^{L-M}\begin{pmatrix} L & n & L \\ -M & m & M' \end{pmatrix}(2n+1)^{1/2} \tag{3}$$

$$= (-1)^{3L+n-M}\begin{pmatrix} L & L & n \\ -M & M' & m \end{pmatrix}(2n+1)^{1/2}. \tag{4}$$

To obtain (4), we use the permutation symmetry properties of the $3j$-symbol, and using the well-known orthogonality sum rule for the $3j$-symbols gives us

$$\sum_{M,M'} |\langle LM|T_n^m|LM'\rangle|^2 = 1. \tag{5}$$

This useful result will fix the form of our operators to within a phase factor. For example, if we set $T_1 = AL$, we find from (5)

$$1 = A^2 \sum_{M=-L}^{+L} M^2 = \tfrac{1}{3}L(L+1)(2L+1)A^2 \tag{6}$$

which is in accord with Judd (1963) and Wadzinski (1969). Setting $T_2^0 = B[3L_z^2 - L(L+1)]$ gives

$$1 = \tfrac{1}{5}(2L-1)L(L+1)(2L+1)(2L+3)B^2 \tag{7}$$

and so on. It is easier to get the form of the operator for a specific L value than to take a general L. For example, the operator equivalent for T_3^0 is $5L_z^3 - 17L_z$ within the $L = 2$ manifold, as already used in equation (1). We set $T_3^0 = C(2)(5L_z^3 - 17L_z)$ and obtain

$$1 = 2(F(1) + F(2))(C(2))^2 = 360(C(2))^2 \tag{8}$$

where we set $F(M) = (5M^3 - 17M)^2$. The L dependence of the coefficients for higher rank operators T_n^m is as would be anticipated from equations (6) and (7), by adding factors at each end of the product.

The operators L_+^n, L_-^n, are proportional to the unit tensor operators T_n^n; T_n^{-n}, and this fact will be used in the later discussion. We should indicate briefly how the more complicated operator equivalents of type T_n^0 can be found without any use of classical Legendre polynomials, since this makes the techniques of this paper completely self-contained. One procedure is to set down the expansion

$$T_3^0 \propto [L_z^3 + AL(L+1)L_z + BL_z] \tag{9}$$

and choose A and B so that the operator has zero matrix elements for the manifolds

$L = \frac{1}{2}$ and $L = 1$. This gives $B = \frac{1}{5}$, $A = -\frac{3}{5}$; if we wish to make even fewer assumptions about the form of T_3^0, we can use the trace metric technique, as explained in the next section.

3. The trace metric

If we consider a set of bounded linear operators acting within a finite-dimensional space, then we can add the operators and form linear combinations of them in an obvious way. This gives us a linear space, which becomes an inner product space if we use the trace metric, ie we set

$$A \,.\, B = \mathrm{Tr}(A^{\dagger}B). \tag{10}$$

This enables us to use all the traditional apparatus of quantum mechanical linear space theory, but with operators instead of wavefunctions as the elements of the space. We wish to specialize to the case of tensor operators T_n^m acting within the $2L+1$ dimensional space of states $|LM\rangle$. We can express the result (5) in the form

$$\mathrm{Tr}(T_n^{m\dagger}T_n^m) = 1. \tag{11}$$

This shows that the unit tensor operators as defined by Judd, following Racah, are unit vectors in the trace metric approach, but this fact does not seem to have been exploited in the published literature. The unit tensor operators are actually orthonormal, since only T_0^0 has non-zero trace, and zero resultant angular momentum is only produced by coupling two equal angular momenta.

Corio (1968) has already used the trace metric concept in connection with the calculation of operator equivalents, but we adopt a different tactic here. To find T_3^0 we set down the expansion

$$L_z^3 = aT_3^0 + bL_z \tag{12}$$

and take the inner product with L_z (in a general L space). We find

$$\mathrm{Tr}\, L_z^4 = b\, \mathrm{Tr}\, L_z^2. \tag{13}$$

This kind of calculation involves the formulae for the sums of powers of the first L integers, but we can also use the convenient trace tables of Ambler *et al* (1962). We find $b = \frac{1}{5}(3L^2+3L-1)$ which when re-inserted in (12) gives us a T_3^0 component proportional to $5L_z^3 + [1-3L(L+1)]L_z$. As an example involving a particular L value, we can find the T_4^0 operator equivalent in the $L = 2$ manifold. We set

$$L_z^4 = aT_4^0 + b(L_z^2 - 2) + c \tag{14}$$

(using the correct $L = 2$ form for the T_2^0 operator). We find

$$\mathrm{Tr}\, L_z^4 = c \tag{15}$$

$$\mathrm{Tr}(L_z^6 - 2L_z^4) = b\, \mathrm{Tr}(L_z^4 - 4L_z^2 + 4). \tag{16}$$

The final result is $c = \frac{34}{5}$, $b = \frac{31}{7}$, giving a T_4^0 component proportional to $35L_z^4 - 155L_z^2 + 72$.

4. Generators for SU_2

We now use the trace metric technique to explore the relationship between different approaches to Lie group theory. We consider the two-dimensional isotropic harmonic oscillator, with Hamiltonian

$$H = P_x^2 + P_y^2 + x^2 + y^2. \tag{17}$$

We can introduce the operator $\eta(x) = P_x + \mathrm{i}x$, and form $\eta^\dagger(x)$, $\eta(y)$ and $\eta^\dagger(y)$. Any linear combination of operators of type $\eta^\dagger\eta$ will commute with H. We can form combinations with definite rotational properties, eg

$$\eta^\dagger(x)\eta(y) - \eta^\dagger(y)\eta(x) = 2\mathrm{i}(xP_y - yP_x) = 2\mathrm{i}L_z \tag{18}$$

$$(\eta^\dagger(x) \pm \mathrm{i}\eta^\dagger(y))(\eta(x) \pm \mathrm{i}\eta(y)) = (P_x^2 - P_y^2) + (x^2 - y^2) \pm 2\mathrm{i}(P_xP_y + xy). \tag{19}$$

The symmetry operator (18) is of T_1^0 tensor operator type, while taking real and imaginary parts of (19) gives us T_2^2 and T_2^{-2} operators. The interesting point here is that these three tensor operators give a genuinely *closed* system under operator commutation, even though the commutator of two T_2 operators might be expected to have a T_3 component (it is identically zero in this case). The three operators give abstract commutation rules which are just those of ordinary angular momentum theory, and produce the dynamical symmetry group SU_2 for the system.

To obtain the SU_2 matrix generators, we know that the operators $L_z, L_\pm$ in the $L = 1$ basis will suffice, but we could ask whether it is possible to follow the physical system more closely and use T_1^0, $T_2^{\pm 2}$ operators. These operators will only give closed commutators within a restricted manifold; we take $L = 1$. We set

$$[L_+^2, L_-^2] \equiv AT_3^0 + BL_z \tag{20}$$

and find (for $L = 1$)

$$\mathrm{Tr}(L_z[L_+^2, L_-^2]) = 8 = B\,\mathrm{Tr}\,L_z^2 = 2B \tag{21}$$

and $A = 0$ (as required by selection rules). We also have $[L_z, L_+^2] = 2L_+^2$. Putting these results together we find that the three operators $\frac{1}{2}L_z$, $\frac{1}{2}L_+^2$, $\frac{1}{2}L_-^2$ give the same commutation rules within the $L = 1$ manifold as do L_z, L_+, L_-, respectively. For the case of the three-dimensional isotropic harmonic oscillator, the dynamical symmetry group contains a set of operators of type T_2^m, T_1^m, T_0^0, closed under commutation (Killingbeck 1975). The relevant group is U_3, and the generators can be alternatively obtained by using T_2^m, T_1^m and T_0^0 tensor operators of O(3), restricted to the manifold $L = 1$. If the two-dimensional isotropic oscillator is anharmonic, then the dynamical symmetry group becomes smaller. The operator L_z drops out, and only the operator $H_x - H_y$ remains if we set the Hamiltonian equal to $H_x + H_y$. These two operators belong to the definite reps B_2 and A_1 of the group C_{4v}. In general, if an operator X belongs to the dynamical symmetry group, and if the Hamiltonian has some geometrical symmetry group with elements G_J, then $G_J^{-1}XG_J$ will belong to the dynamical symmetry group. We thus expect the dynamical symmetry operators to fill complete rep families of G (eg the three-dimensional harmonic oscillator has complete T_2, T_1 and T_0 families of symmetry operators; if the oscillator is anharmonic, we expect complete families of octahedral group rep types).

5. The Lie group G_2

We consider now the $L = 3$ manifold, and investigate the commutators of two T_5 type tensor operators. We take the following representative case:

$$[L_+^5, L_-^5] \equiv AT_5^0 + BT_3^0 + CT_1^0. \tag{22}$$

To extract the T_3^0 part we use the trace metric:

$$\mathrm{Tr}(T_3^0[L_+^5, L_-^5]) = B\,\mathrm{Tr}(T_3^{0\dagger}T_3^0). \tag{23}$$

The trace on the right-hand side is positive; that on the left equals

$$2\langle 33|L_+^5L_-^5|33\rangle(\langle 33|T_3^0|33\rangle + \langle 32|T_3^0|32\rangle). \tag{24}$$

Using the operator equivalent for T_3^0, we find that the term in parentheses equals zero. This gives us a very simple proof of the closure of the T_5 and T_1 families under commutation, which is basic to the theory of the group G_2 (Judd 1963). If we wish to use the *nj* symbolism, we have to use the equality of two 3*j*-symbols rather than the vanishing of a 6*j*-symbol.

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