Point group invariants in the $U_{qp}(u(2))$ quantum algebra picture $^1, ^2$

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Some consequences of a $qp$-quantization of a point group invariant developed in the enveloping algebra of $SU(2)$ are examined in the present note. A set of open problems concerning such invariants in the $U_{qp}(u(2))$ quantum algebra picture is briefly discussed.

On examine quelques unes des conséquences d’une $qp$-quantification d’un invariant sous un groupe ponctuel donné développé dans l’algèbre enveloppante de $SU(2)$. On discute une série de problèmes ouverts concernant de tels invariants dans l’image de l’algèbre quantique $U_{qp}(u(2))$.

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1. Introduction

Potentials invariant under a point symmetry subgroup $G$ of the three-dimensional rotation group $O(3)$ play an important rôle in molecular physics and in the physics of crystals. In particular, $G$-invariant operators that can be expanded in the enveloping algebra of the two-dimensional special unitary group $SU(2)$ are of central importance in luminescence spectroscopy and electron paramagnetic resonance of transition ions in crystalline environments as well as in rotational spectroscopy of molecules and, to a less extent, of nuclei (see for instance refs. 1-3). The determination of operators $V_G(J_u)$ that are polynomials in the generators $J_u = J_x, J_y, J_z$ of the group $SU(2)$ and invariant under a (finite) group $G$ may be achieved by means of the method of operator equivalents, as first developed by Stevens (1) in the framework of crystal-field theory (see also refs. 2-5). Furthermore, group theoretical methods, based on the use of the so-called Molien generating function, have been developed by several people (6-12), involving Sharp and some of his colleagues, for obtaining an integrity basis of operators $V_G(J_u)$.

According to Wigner theorem, the spectrum of $V_G(J_u)$ may be characterized by representation classes of $G$. More precisely, in the absence of accidental degeneracies, the eigenvalues $W(j, \Gamma)$ arising from the diagonalization of $V_G(J_u)$ on a subspace $\varepsilon (j) = \{|jm\} : m = -j, -j+1, \ldots, j \}$ of constant angular momentum $j$ can be, at least partially, labelled by irreducible representation classes (IRC’s) $\Gamma$ of $G$ or of its spinor group $G^*$ ($G = G^*/Z_2$). (The vector $|jm\}$ is a common eigenstate of the angular momentum operators $\mathcal{J}^2 = \mathcal{J}_x^2 + \mathcal{J}_y^2 + \mathcal{J}_z^2$ and $\mathcal{J}_z$.)

It is the aim of this short paper to examine, from the point of view of spectral analysis, some of the consequences of replacing the Lie algebra $su(2)$ of the group $SU(2)$ by a $qp$-quantized universal enveloping algebra $U_{qp}(u(2))$. More specifically, we want to address here the following question. What happens when we replace in $V_G(J_u)$ each
basis element $\mathcal{J}_u$ of $su(2)$ by the corresponding basis element $J_u$ of the quantum algebra $U_{qp}(u(2))$? We shall not answer the latter question in the general case where $V_G(\mathcal{J}_u)$ is arbitrary. We shall rather investigate two particular cases of deformed invariants and shall try to extrapolate some general tendency.

The mathematical and physical motivations for investigating more general deformed invariants of the type $V_G(J_u \mapsto J_u)$, in the $qp$-quantized universal enveloping algebra $U_{qp}(u(2))$, are strongly connected. From a mathematical point of view, we may wonder whether the spectrum of $V_G(J_u)$ exhibits the degeneracies afforded by $G$. This is another way to address the questions what is the relation between the finite group $G$ and the quantum algebra $U_{qp}(u(2))$ and what is the relation between $G$ and the deformed invariants. We suspect that the replacement of $V_G(J_u)$ by $V_G(J_u)$ yields some symmetry breaking, a fact that is certainly interesting from a physical viewpoint (we have in mind some applications to electron paramagnetic resonance and to the Jahn-Teller effect).

2. A two-parameter quantum algebra

We begin with those aspects of the quantum algebra $U_{qp}(u(2))$, recently introduced in ref. 13, that are of relevance for section 3. Loosely speaking, the two-parameter quantum algebra $U_{qp}(u(2))$ is spanned by the operators $J_x$, $J_y$, $J_z$ and $J_0$ acting on the space $\mathcal{E} = \bigoplus_{j} \mathcal{E}(j)$ and satisfying the commutation relations

$$[J_0, J_x] = [J_0, J_y] = [J_0, J_z] = 0$$

$$[J_x, J_y] = \frac{i}{2} (q^{-1} - q) [2J_z]_{qp}$$

$$[J_y, J_z] = i J_x, \quad [J_z, J_x] = i J_y$$

In this paper, we use the notation

$$[X]_{qp} = \frac{q^X - p^X}{q - p}$$

[2]
for both operators (X acts on the Hilbert space ε) and numbers (X belongs to the field of complex numbers). By introducing \( s = \ln q \) and \( r = \ln p \), eq. [2] can be rewritten in the useful form

\[
[X]_{qp} = \frac{\sinh(X \frac{s+r}{2})}{\sinh(X \frac{s-r}{2})} \exp \left[ \left( X - 1 \right) \frac{s + r}{2} \right]
\]  

[3]

which is easy to handle when \( p = q^{-1} \rightarrow 1 \).

The Hopf algebraic structure of \( U_{qp}(u(2)) \) needs the introduction of a coproduct, an antipode and a counit (see ref. 13 for details). In the particular case \( p = q^{-1} \) (or \( r = -s \)), the operators \( J_x, J_y \) and \( J_z \) span the well-known quantum algebra \( U_q(su(2)) \) described by many authors (see for example refs. 14 and 15). In addition, in the limiting case \( p = q^{-1} = 1 \), the quantum algebra \( U_{qp}(u(2)) \) gives back the Lie algebra \( u(2) \). Equation [1] indicates that the permutational symmetry of \( (x, y, z) \) is broken when going from \( u(2) \) to \( U_{qp}(u(2)) \).

The action on the space \( \varepsilon \) of the generators \( J_\pm = J_x \pm i J_y, J_3 = J_z \) and \( J_0 \) of \( U_{qp}(u(2)) \) is given by (see ref. 13)

\[
J_\pm |jm\rangle = \sqrt{|j \mp m\rangle_{qp} [j \pm m + 1]_{qp} |j, m \pm 1\rangle}
\]

[4]

\[
J_3 |jm\rangle = m |jm\rangle, \quad J_0 |jm\rangle = j |jm\rangle
\]

Note that \( J_+ \) turns out to be the adjoint of \( J_- \) if \( s - r \) and \( s + r \) are real numbers or if \( s - r \) is a pure imaginary number and \( s + r \) a real number.

To close this section, let us mention that the operator

\[
C_2(U_{qp}(u(2))) = J_x^2 + J_y^2 + \frac{1}{2} [2]_{qp} (qp)^{J_3 - J_z} ([J_z]_{qp})^2
\]

[5]

is an invariant, abbreviated as \( J^2 \) in the following, for \( U_{qp}(u(2)) \) in the sense that it commutes with each of the generators \( J_x, J_y, J_z \) and \( J_0 \). This invariant has the eigenvalues \( [j]_{qp} [j + 1]_{qp} \). In the limiting case \( p = q^{-1} = 1 \), note that the operator \( C_2(U_{qp}(u(2))) \) can be identified with the Casimir operator \( C_2(su(2)) = J^2 \) of \( su(2) \).
3. Point group invariants

We are now in a position to look at two examples for $V_G(J_u \mapsto J_u)$. The first example is devoted to the limiting situation where $G \equiv O(3)$. In this situation, the simplest operator $V_{O(3)}(J_u)$ is the second-order polynomial

$$\phi^2_{\text{axial}} = J_x^2 + J_y^2 + J_z^2 \quad [6]$$

In the limiting case $p = q^{-1} = 1$, the operator $\phi^2_{\text{axial}}$ is clearly $O(3)$-invariant since it coincides then with the Casimir operator $\mathcal{J}^2$ of $su(2)$. For generic $q$ and $p$, we suspect from eq. [1] that $\phi^2_{\text{axial}}$ is only axially invariant rather than being fully rotationally invariant. This may be easily proved by looking for the eigenvalues of $\phi^2_{\text{axial}}$ on the subspace $\varepsilon(j)$. We obtain

$$W_2(j, \Gamma_{|m|}) = \frac{1}{2}([j - m]_{qp}[j + m + 1]_{qp} + [j + m]_{qp}[j - m + 1]_{qp}) + m^2 \quad [7]$$

with $m = -j, -j + 1, \cdots, j$. (Of course, $W_2(j, \Gamma_{|m|}) \mapsto j(j + 1)$ when $p = q^{-1} \rightarrow 1$.) The eigenvalues [7] are $m$-dependent and invariant under the interchange $m \leftrightarrow -m$. The spectrum of $\phi^2_{\text{axial}}$ thus consists of $j + \frac{1}{2}$ doublets if $j$ is half of an odd integer and of one singlet and $j$ doublets if $j$ is an integer. It can be described with the help of the IRC's $\Gamma_{|m|}$ of the axial group $C_{\infty v}$. (In molecular physics notations, the IRC's of $C_{\infty v}$ are $\Gamma_0 = A_1$ for $j$ even, $\Gamma_0 = A_2$ for $j$ odd and $\Gamma_{|m|} = E_{|m|}$ for $m \neq 0$.) As a net result, the $qp$-quantization of the operator $V_{O(3)}(J_u) = \mathcal{J}^2$, via the replacement $J_u \mapsto J_u$, leads to a symmetry breaking characterized by the chain $O(3) \supset C_{\infty v}$.

The second example of operator $V_G(J_u \mapsto J_u)$ is concerned with the octahedral group $G \equiv O$. Let us take for $V_G(J_u)$ the fourth-order polynomial

$$\phi^4_{\text{trig}} = \frac{\Delta}{180} \left\{ 5\sqrt{2}[J_z(J_+^3 + J_-^3) + (J_+^3 + J_-^3)J_z] - 35J_z^4 - 25J_z^2 + 30J_z^2J_z^2 + 6J_z^4 - 3J_z^4 \right\} \quad [8]$$
where $\Delta$ is a positive parameter. (The parameter $\Delta$ has a well-known significance in the spectroscopy of $d^N$ ions in cubical symmetry, see below.) In the limiting case $p = q^{-1} = 1$, the operator $\phi^4_{1\text{ri}}$ can be shown to be invariant under the octahedral group $O$. For generic $q$ and $p$, the diagonalization of $\phi^4_{1\text{ri}}$ on a manifold $\varepsilon(j)$ does not lead generally to a spectrum of the type of the one afforded by the group $O$. As an illustration, the diagonalization of $\phi^4_{1\text{ri}}$ on the subspace $\varepsilon(2)$ yields two doublets

$$W(2, \langle ET_2 \rangle E)_+ = \frac{1}{2} \left[ \alpha + \beta + \sqrt{(\alpha - \beta)^2 + 4\gamma^2} \right]$$

$$W(2, \langle ET_2 \rangle E)_- = \frac{1}{2} \left[ \alpha + \beta - \sqrt{(\alpha - \beta)^2 + 4\gamma^2} \right]$$

and one singlet

$$W_4(2, \langle T_2 \rangle A_1) = \frac{1}{60} \Delta d (2 - d)$$

In eqs. [9, 10], we have put

$$\alpha = + \frac{1}{540} \Delta \left( 20d \sqrt{[4]_{qp}} - 780 + 198d - 9d^2 \right)$$

$$\beta = - \frac{1}{540} \Delta \left( 20d \sqrt{[4]_{qp}} + 1380 - 288d + 9d^2 \right)$$

$$\gamma = + \frac{\sqrt{2}}{108} \Delta \left( d \sqrt{[4]_{qp}} - 120 + 18d \right)$$

with $d = [2]_{qp}[3]_{qp}$. The degeneracy of the spectrum [9, 10] is characteristic of the dihedral group $D_3$, a trigonal subgroup of the group $O$. The eigenvalues in [9, 10] are labelled by the IRC’s $A_1$ and $E$ of the group $D_3$. We have also indicated in [9, 10], within $\langle \rangle$, the parent IRC’s $T_2$ and $E, T_2$ of the group $O$ for the trigonal levels of symmetry $A_1$ and $E$, respectively. In the limiting case $p = q^{-1} = 1$, we get

$$W_4(2, \langle ET_2 \rangle E)_+ = + \frac{3}{5} \Delta, \quad W_4(2, \langle ET_2 \rangle E)_- = - \frac{2}{5} \Delta, \quad W_4(2, \langle T_2 \rangle A_1) = - \frac{2}{5} \Delta$$

The trigonal levels [9, 10] thus reduce to the cubical levels $W_4(2, E) = +(3/5)\Delta$ and $W_4(2, T_2) = -(2/5)\Delta$ of cubical symmetry $E$ and $T_2$, respectively. (Observe that $\Delta = \ldots$)
\[ W_4(2, E) - W_4(2, T_2). \] In other words, passing from the limiting case where \( p = q^{-1} = 1 \) to the case where \( q \) and \( p \) are arbitrary, produces a level splitting

\[ E \rightarrow E, \quad T_2 \rightarrow A_1 \oplus E \]  

[13]
corresponding to the chain of groups \( O \supset D_3 \).

4. Concluding remarks

Five concluding remarks may be drawn from the results of sections 2 and 3.

(i) As a trivial remark, we note that the Casimir invariant \( C_2(su(2)) = J^2 \) of the Lie algebra \( su(2) \) is also an invariant of the quantum algebra \( U_{qp}(u(2)) \); this may be easily checked from the commutation relations of \( J^2 \) with \( J_u \) \((u = x, y, z, 0)\). However, a \( qp \)-quantization of \( J^2 \) leads to an operator, the operator \( \phi_{axial}^2 \) of eq. [6], that is not an invariant of \( U_{qp}(u(2)) \). Such a \( qp \)-quantization yields a symmetry breaking described by the restriction of \( O(3) \) to its subgroup \( C_{\infty_v} \).

(ii) An incomplete reciprocal part of point (i) is as follows: the invariant operator \( C_2(U_{qp}(u(2))) = J^2 \) of the quantum algebra \( U_{qp}(u(2)) \) is also an invariant operator of the Lie algebra \( su(2) \).

(iii) In complement of points (i) and (ii), it is possible to show that the invariant \( J^2 \) of \( U_{qp}(u(2)) \) can be expressed by series involving the invariants \( J^2 \) and \( J_0 \) of the Lie algebra \( u(2) \) (see ref. 16). For instance, in the particular case where \( p = q^{-1} \) with \( q = \exp(i\varphi) \in S^1 \), we can prove that

\[ J^2 = \sum_{k=1}^{+\infty} a_k(\varphi) (J^2)^k \]  

[14]
where

\[ a_k(\varphi) = 2^{2k-1} \frac{1}{\sin^2 \varphi} \sum_{\ell=0}^{+\infty} (-1)^{k+\ell+1} \varphi^{2(k+\ell)} \frac{1}{[2(k+\ell)]!} \frac{(k+\ell)!}{k! \ell!} \]  

[15]
In terms of the spherical Bessel functions of the first kind \( j_{k-1} \), we have

\[
a_k(\varphi) = (-1)^{k-1} \frac{\varphi^2}{\sin^2 \varphi} \frac{(2\varphi)^{k-1}}{k!} j_{k-1}(\varphi)
\]

The transcription of eqs. [14, 16] in terms of eigenvalues gives the formula derived in ref. 17 in connection with rotational spectroscopy of nuclei. Note that the generalization of [14-16] to any doublet \((U_{qp}(g), g)\), \(g\) being a simple Lie algebra, is an open problem.

(iv) The \( qp \)-quantization of a \( G \)-invariant operator \( V_G(J_u) \), through the replacement \( J_u \rightarrow I_u \), produces an operator that is invariant under a subgroup \( H \) of \( G \) rather than being invariant under \( G \). A question then naturally arises: given a group \( G \), what \( G \supset H \) symmetry breaking do we obtain by performing a \( qp \)-quantization of an operator of type \( V_G(J_u) \) (see also ref. 18)? The answer is certainly not unique. Let us clarify the latter assertion. In the case of \( \phi_4 \text{trigo} \), we have obtained an \( O \supset D_3 \) symmetry breaking corresponding to \( H \equiv D_3 \). This comes from the fact that the operator \( V_O(J_u) \) implicitly considered in section 3 is a cubical invariant oriented according to a \( C_3 \) axis. Should we have considered an operator \( W_O(J_u) \) oriented according to a \( C_4 \) principal axis, equivalent to \( V_O(J_u) \) as far as their spectra are concerned, we would have obtained an \( O \supset D_4 \) symmetry breaking corresponding to the tetragonal subgroup \( H \equiv D_4 \) of \( O \) (cf. ref. 18). In this respect, it should be interesting to investigate the \( G \supset H \) symmetry breakings that we may obtain from the \( qp \)-quantization of the integrity basis for the operators \( V_G(J_u) \) derived in refs. 6-12.

(v) Finally, to find in a systematic way polynomials, in the generators \( J_u \) \((u = x, y, z, 0)\) of the quantum algebra \( U_{qp}(u(2)) \), that are invariant under a finite subgroup \( G \) of \( O(3) \) is an appealing problem. The generating function methods, applied in refs. 6-12 to the derivation of operators \( V_G(J_u) \), might be a key for solving this problem.

Points (i)-(v) pave the way for future investigations and we hope to return on these matters in a forthcoming paper.
To close this paper, it should be mentioned that multiparameter quantum algebras have been studied by many authors including Sudbery (19) and Fairlie and Zachos (20) among others (see also references in refs. 13 and 16). The main advantage of our version of the quantum algebra $U_{qp}(u(2))$ introduced in section 2 lies in the fact that the latter algebra is not equivalent to a one-parameter algebra as far as the eigenvalues of the Casimir operator [5] are concerned. The reader should consult ref. 16 where this fact has been successfully used to develop a model for rotational spectroscopy of nuclei.

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