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d AND f ELECTRONS IN A qp-QUANTIZED CUBICAL FIELD

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A procedure for qp-quantizing a crystal-field potential V with an arbitrary symmetry G is developed. Such a procedure is applied to the case where V involves cubic components ($G = O$) of the degrees 4 and 6. This case corresponds to d and f electrons in a qp-quantized cubical potential. It is shown that the qp-quantization of the considered cubical potential is equivalent to a symmetry breaking of type $O \to D_4$. A general conjecture about this symmetry breaking phenomenon is given.

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1. Introduction and preliminaries

The theory of quantum algebras and quantum groups, or more specifically, of *quantized universal enveloping algebras* or *Hopf's bi-algebras* [1–6] and *compact matrix pseudo-groups* [7, 8], is presently the object of numerous applications to physics and mathematics. Quantum algebras can be realized in terms of q-boson (or, more generally, qp-boson [9, 10]) operators. The various physical applications of q-boson (or qp-boson) operators and of quantum algebras/groups may be classified in four classes [11].

1. In any problem involving ordinary bosons, or ordinary harmonic oscillators, or ordinary angular momenta (orbital, spin, isospin, total, ... angular momenta), one may think of replacing them by corresponding q-deformed objects. If the limiting case where $q \to 1$ describes the problem in a reasonable way, one may expect that the case where q is close to 1 can describe some fine structure effects. In this approach, the parameter q is a fitting parameter. The main question in this approach is to find a physical interpretation of the parameter q. Along this vein, we have the following applications: (i) Application of q-deformed harmonic oscillators and of $su_q(1,1)$ to vibrational spectroscopy of molecules and nuclei. (ii) Application of the algebras $su_q(2)$ and $u_q(2)$ to (vibrational-)rotational spectroscopy

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of molecules and nuclei. (iii) Use of q-bosons for describing the interaction between radiation and matter. (iv) Application to statistical mechanics of a q-boson gas [12].

2. A second series of applications concerns the more general situation where a physical problem is well described by a given Lie algebra g. One may then consider to associate a q-quantized universal enveloping algebra $U_q(g)$ to the Lie algebra g. Here again, the case where q is close to 1 may serve to describe fine structure effects. Symmetries described by the Lie algebras are thus replaced by quantum algebra symmetries. As an illustration, we may go from the $g = so(4)$ symmetry of the Kepler–Coulomb system to the $su_q(2) \oplus su_q(2)$ symmetry [13]. When going from $so(4)$ to $su_q(2) \oplus su_q(2)$, we can generate a splitting of the non-relativistic (discrete) energy spectrum which mimics the spectrum afforded by relativistic quantum mechanics. (In this example, the parameter q can be related to the fine structure constant α.)

A common characteristic of the applications of type 1 and 2 is that q (or q and p) are parameters close to 1 either in $\mathcal{R}$ or S^1.

3. A third series arises by allowing the deformation parameters (q and p) not to be restricted to values close to 1. (This series includes the case where q and/or p are roots of unity.) Completely unexpected models may result from this approach. (See for example Ref. [14].)

4. Finally, a fourth series concerns more fundamental applications (more fundamental in the sense not being subjected to fitting procedures). In this respect, we may mention applications to anyonic statistics, gauge theories, conformal field theories, and deformations of space-time structures. (See Refs. [15–17] for a deformation of the Lorentz and Poincaré groups.)

In the present work, we give an application of type 2 for which the Lie algebra g is, grosso modo, replaced by a finite group. More precisely, the problem which we want to face may be introduced as follows. Given a harmonic function V (i.e., $\Delta V = 0$) defined on $L^2(\mathcal{R}^3)$ and invariant under a (finite) point group G (i.e., $G \subset O(3)$), it is possible to map $V(u)$, where u stands for the Cartesian coordinates (x, y, z), onto an operator $T(\mathcal{J})$ defined in the enveloping algebra of the Lie group $SU(2)$. This may be achieved by means of replacements of type $u \to \mathcal{J}_u$ $(u = x, y, z)$ with convenient symmetrizations (cf., the method of operator equivalents introduced by Stevens in the spectroscopy of transition ions in crystals [18]). As a well-known result, the spectrum of $T(\mathcal{J})$ on a space $\{\varepsilon(j) = |jm) \ : \ m = -j, -j+1, \ldots, j\}$ of constant angular momentum j (where $|jm)$ is a common eigenstate of the angular momentum operators $\mathcal{J}^2$ and $\mathcal{J}_z$) exhibits the degeneracies afforded by the group G or its double group G^* ($G = G^*/Z_2$). In other words, each sublevel arising from the diagonalization of $T(\mathcal{J})$ on the space $\varepsilon(j)$ is characterized by an irreducible representation class (IRC) of G or G^*. Then, a natural problem arises: what happens when one makes a q-quantization of $T(\mathcal{J})$ by replacing the generators $\mathcal{J}_u$ of $su(2)$ by the generators J_u of the quantum algebra $U_q(su(2))$?

We conjecture that the spectrum of $T(\mathcal{J})$ on $\varepsilon(j)$ exhibits the degeneracies of a subgroup H or H^* of the group G or G^* according to whether j is an integer or half of an odd integer. In this sense, a q-quantization yields a symmetry breaking, a fact already noted in Ref. [13].

It is the aim of this paper to give a proof of this conjecture in the special case where G is the octahedral group O (isomorphic with S_4) and $\varepsilon(j)$ corresponds to some subspaces arising from d^N and f^N (atomic) configurations. We shall show that, in that case, the group H is the tetragonal group D_4. In more physical words, we shall see that d and f electrons in a qp-quantized cubical potential are equivalent to d and f electrons in an ordinary tetragonal potential, respectively.

The rest of this paper is organized in the following way. In Sec. 2, we give those basic aspects of the two-parameter quantum algebra $U_{qp}(u(2))$ which are of relevance for the problem tackled in the present work. Section 3 is devoted to the qp-quantization of the cubical invariants of the degrees 4 and 6. Section 4 deals with the diagonalization of the obtained qp-quantized operators in subspaces of interest for d and f electrons in solids. Perspectives are examined in Sec. 5.

2. The quantum algebra $U_{qp}(u(2))$

From the generators $\mathcal{J}_- = \mathcal{J}_x - \mathrm{i}\mathcal{J}_y$, $\mathcal{J}_3 = \mathcal{J}_z$, $\mathcal{J}_0$ and $\mathcal{J}_+ = \mathcal{J}_x + \mathrm{i}\mathcal{J}_y$ of the ordinary Lie algebra $u(2)$, let us define the operators

$$J_- = \sigma(\mathcal{J}_3, \mathcal{J}_0)\, \mathcal{J}_-, \quad J_3 = \mathcal{J}_3, \quad J_0 = \mathcal{J}_0, \quad J_+ = \mathcal{J}_+\, \sigma(\mathcal{J}_3, \mathcal{J}_0), \tag{1}$$

where the operator-valued factor σ reads

$$\sigma(\mathcal{J}_3, \mathcal{J}_0) = \sqrt{[\mathcal{J}_0 - \mathcal{J}_3]_{qp}[\mathcal{J}_0 + \mathcal{J}_3 + 1]_{qp}}\, \frac{1}{\sqrt{(\mathcal{J}_0 - \mathcal{J}_3)(\mathcal{J}_0 + \mathcal{J}_3 + 1)}}. \tag{2}$$

The qp-deformed operators $[X]_{qp}$ in (2) are given by

$$[X]_{qp} = \frac{q^X - p^X}{q - p}, \tag{3}$$

where q and p are fixed (complex) numbers such that the operators J_- and J_+ satisfy $J_+ = J_-^\dagger$. (Both the operators of type $\mathcal{J}$ and J in (1) act on the Hilbert space $\varepsilon = \oplus_j \varepsilon(j)$ and the basis vectors $|jm)$ of ε are common eigenstates of the operators $\mathcal{J}_3$ and $\mathcal{J}^2 = \mathcal{J}_x^2 + \mathcal{J}_y^2 + \mathcal{J}_z^2$.) Then, it can be shown that the action of the operators of type J on ε is characterized by

$$\begin{aligned} J_-|jm) &= \sqrt{[j+m]_{qp}[j-m+1]_{qp}}\,|j, m-1), \\ J_3|jm) &= m|jm), \quad J_0|jm) = j|jm), \\ J_+|jm) &= \sqrt{[j-m]_{qp}[j+m+1]_{qp}}\,|j, m+1), \end{aligned} \tag{4}$$

where the qp-numbers $[x]_{qp}$ in (4) are defined through (3) by replacing the operator X by the (real) number x. Then, it is a simple matter of straightforward calculation to show that the commutation relations of the J_α ($\alpha = -, 3, 0, +$) operators are

$$\begin{aligned} &[J_0, J_3] = 0, \qquad [J_0, J_+] = 0, \qquad [J_0, J_-] = 0, \\ &[J_3, J_-] = -J_-, \qquad [J_3, J_+] = +J_+, \qquad [J_+, J_-] = (qp)^{J_0 - J_3}\, [2J_3]_{qp}, \end{aligned} \tag{5}$$

a result presented, with some details, in Ref. [11].

Equations (5) define the two-parameter quantum algebra $U_{qp}(u(2))$. The latter algebra may be endowed with a triangular Hopf algebraic structure [11]. Furthermore, it is to be pointed out that the generators of the two-parameter algebra $U_{qp}(u(2))$ may be realized in terms of qp-bosons [11]. Finally, it should be noted that, in the particular case $p = q^{-1}$, the generators J_-, J_3 and J_+ span the familiar one-parameter quantum algebra $U_q(su(2))$ introduced by various authors [1–8] in the early days of the theory of quantum algebras.

As an essential result to be used besides Eqs. (4) in Sec. 3, it can be proved that the operator

$$J^2 = \frac{1}{2}(J_+J_- + J_-J_+) + \frac{[2]}{2}(qp)^{J_0 - J_3}([J_3]_{qp})^2 \tag{6}$$

is an $U_{qp}(u(2))$ invariant in the sense that it commutes with each of the generators J_-, J_3, J_0 and J_+. The eigenvalues of J^2 can be calculated to be

$$\frac{q^{2j+1} - q^j p^{j+1} - q^{j+1}p^j + p^{2j+1}}{(q-p)^2} \equiv [j]_{qp}\,[j+1]_{qp} \tag{7}$$

with $2j \in \mathcal{N}$, a result compatible with the well-known one corresponding to the limiting case $p = q^{-1} = 1$.

3. qp-quantized cubical potentials

We want to qp-quantize cubical (for instance, octahedral and tetrahedral) potentials of interest for d and f electrons in crystalline environments. Thus, we shall start from the cubical invariants of the degrees 4 and 6 (degree 4 for d electrons, degrees 4 and 6 for f electrons). We shall work in a cubical basis adapted to the chain of groups $SO(3) \supset O \supset D_4 \supset D_2$, i.e., oriented with respect to a C_4 axis. (The groups O, D_4 and D_2 are the octahedral group, the dihedral group of order 4 and the dihedral group of order 2, respectively.)

We begin with the cubical invariant of the degree 4

$$\phi^4_{\rm cub} = \sqrt{\frac{7}{12}}\, y_0^{(4)} + \sqrt{\frac{5}{24}}\left(y_{-4}^{(4)} + y_4^{(4)}\right), \tag{8}$$

where $y_q^{(k)}$ stands for a solid harmonic $r^k Y_{kq}(\theta, \varphi)$. Clearly $\phi^4_{\rm cub}$ satisfies the Laplace equation. By passing from the spherical coordinates (r, θ, φ) to the Cartesian coordinates (x, y, z), we obtain that $\phi^4_{\rm cub}$ is proportional to

$$V_4 = x^4 + y^4 + z^4 - \frac{3}{5}(x^2 + y^2 + z^2)^2. \tag{9}$$

Under the replacement $u \to \mathcal{J}_u$ $(u = x, y, z)$, with appropriate symmetrizations to take into account the noncommutativity of the (ordinary) angular momentum operators $\mathcal{J}_u$, the function V_4 can be changed into an operator equivalent. This yields an operator denoted as $T_{4A_1A_1A}(\mathcal{J})$ in the notation of Ref. [19]. (The triplet A_1A_1A indicates that the latter operator transforms as the identity IRC's A_1, A_1 and A of the groups O, D_4 and D_2, respectively.) The qp-quantization of $T_{4A_1A_1A}(\mathcal{J})$ is obtained by simply replacing the operators of type $\mathcal{J}$ by the corresponding operators of type J defined by (1). From the expression for $T_{4A_1A_1A}(\mathcal{J})$ (see Ref. [19]) we get

$$T_{4A_1A_1A}(J) = \frac{1}{8}\sqrt{\frac{5}{6}}(J_+^4 + J_-^4)$$

$$+\frac{1}{4}\sqrt{\frac{1}{30}}(35J_z^4+25J_z^2-30J_z^2J^2-6J^2+3J^4), \tag{10}$$

where the operators of type J are generators of the quantum algebra $U_{qp}(u(2))$ rather than generators of the Lie algebra $su(2)$.

Similarly, from the cubical invariant of the degree 6

$$\phi^6_{\rm cub}=\sqrt{\frac{1}{8}}y_0^{(6)}-\sqrt{\frac{7}{16}}\left(y_{-4}^{(6)}+y_4^{(6)}\right), \tag{11}$$

we can generate the qp-quantized operator

$$\begin{aligned}T_{6A_1A_1A}(J)=&-\frac{1}{16}\sqrt{\frac{21}{22}}J_+^4(11J_z^2+44J_z+50-J^2)\\&-\frac{1}{16}\sqrt{\frac{21}{22}}J_-^4(11J_z^2-44J_z+50-J^2)\\&+\frac{1}{16}\sqrt{\frac{2}{231}}(231J_z^6+735J_z^4-315J_z^4J^2\\&+294J_z^2-525J_z^2J^2+105J_z^2J^4-60J^2+40J^4-5J^6)\end{aligned} \tag{12}$$

in terms of the generators of $U_{qp}(u(2))$.

4. qp-quantized energy levels

4.1. The case of d electrons

We shall diagonalize the operator

$$X_4=8\sqrt{\frac{6}{5}}a_4T_{4A_1A_1A}(J)\quad\text{with}\quad a_4\in\mathcal{R} \tag{13}$$

on the subspace $\varepsilon(\ell=2)$. We shall take the basis vectors of $\varepsilon(2)$ in the form

$$|2\Gamma(O)\Gamma(D_4)\Gamma(D_2))=\sum_{m=-2}^{+2}|2m)(2m|2\Gamma(O)\Gamma(D_4)\Gamma(D_2)), \tag{14}$$

where $\Gamma(G)$ stands for an IRC of the group $G=O$, or D_4 or D_2. In the detail, we have

$$\begin{aligned}&|2EA_1A)=|20),\\&|2EB_1A)=\sqrt{1/2}|22)+\sqrt{1/2}|2-2),\\&|2T_2B_2B_1)=\sqrt{1/2}|22)-\sqrt{1/2}|2-2),\\&|2T_2EB_2)=\mathrm{i}\sqrt{1/2}|21)-\mathrm{i}\sqrt{1/2}|2-1),\\&|2T_2EB_3)=-\sqrt{1/2}|21)-\sqrt{1/2}|2-1).\end{aligned} \tag{15}$$

The eigenvalues $W_4(2\Gamma(D_4))$ of X_4, in units of a_4, are

$$W_4(2A_1)=\frac{6}{5}d(-2+d)\qquad\text{(singlet)},$$

$$W_4(2B_1) = +[4]! + 6\left(44 - \frac{42}{5}d + \frac{1}{5}d^2\right) \qquad \text{(singlet)},$$

$$W_4(2B_2) = -[4]! + 6\left(44 - \frac{42}{5}d + \frac{1}{5}d^2\right) \qquad \text{(singlet)},$$

$$W_4(2E) = 6\left(4 - \frac{12}{5}d + \frac{1}{5}d^2\right) \qquad \text{(doublet)}, \tag{16}$$

where we have used the shorthand notation $[4]! = [2]_{qp}[3]_{qp}[4]_{qp}$ and $d = [2]_{qp}[3]_{qp}$.

In the limiting situation where $p = q^{-1} = 1$, we have $[4]! = 24$ and $d = 6$ so that Eq. (16) gives back the well-known octahedral levels, viz., one doublet of symmetry $\Gamma(O) = E$ (of energy 144/5) and one triplet of symmetry $\Gamma(O) = T_2$ (of energy $-96/5$). When going from $p = q^{-1} = 1$ to arbitrary values of q and p, we have a splitting of the levels of symmetry $\Gamma(O) = E$ and T_2. For arbitrary values of q and p, we obtain levels completely characterized by IRC's of the group D_4. The $O \to D_4$ level splitting is described by

$$E \to A_1 \oplus B_1, \quad T_2 \to B_2 \oplus E. \tag{17}$$

In other parlance, the energy levels for d electrons in a qp-quantized cubical potential exhibit the same degeneracies as the ones for d electrons in an ordinary tetragonal potential.

From a more quantitative point of view, by putting

$$\overline{Dq} = \left(\frac{14}{5} + \frac{1}{12}[4]!\right)a_4, \quad \overline{Ds} = 12(6-d)a_4, \quad \overline{Dt} = \left(-4 + \frac{1}{6}[4]!\right)a_4, \tag{18}$$

the expressions (16) can be rewritten as

$$W_4(2A_1) = g + 6\overline{Dq} - 2\overline{Ds} - 3\overline{Dt},$$

$$W_4(2B_1) = g + 6\overline{Dq} + 2\overline{Ds} + 3\overline{Dt},$$

$$W_4(2B_2) = g - 4\overline{Dq} + 2\overline{Ds} - 4\overline{Dt},$$

$$W_4(2E) = g - 4\overline{Dq} - \overline{Ds} + 2\overline{Dt}, \tag{19}$$

where

$$g = \frac{6}{5}(96 - 22d + d^2)a_4 \tag{20}$$

is the center of gravity of the levels (16). The energies (19) are nothing but the energies for d electrons in an ordinary tetragonal potential (see Ref. [20]). In Eq. (19), the parameters $\overline{Dq}$ and $\overline{Dt}$ correspond to the tetragonal invariants of the degree 4, the parameter $\overline{Ds}$ corresponds to the tetragonal invariant of the degree 2, and the barycenter g corresponds to the tetragonal invariant of the degree 0.

4.2. The case of f electrons

In this case, we shall perform the diagonalization of X_4 (see (13)) and of

$$X_6 = 16\sqrt{\frac{22}{21}}a_6 T_{6A_1A_1A}(J) \quad \text{with} \quad a_6 \in \mathcal{R} \tag{21}$$

on the subspace $\varepsilon(\ell = 3)$. The relevant zeroth-order approximation state vectors, adapted to the chain $SO(3) \supset O \supset D_4 \supset D_2$, are here

$$|3A_2B_1A) = \sqrt{1/2}|32) - \sqrt{1/2}|3-2),$$

$$|3T_1A_2B_1) = -|30),$$

$$|3T_2B_2B_1) = \sqrt{1/2}|32) + \sqrt{1/2}|3-2),$$

$$|3T_1EB_2) = \mathrm{i}\sqrt{5/16}|33) + \mathrm{i}\sqrt{3/16}|31) + \mathrm{i}\sqrt{3/16}|3-1) + \mathrm{i}\sqrt{5/16}|3-3),$$

$$|3T_2EB_2) = \mathrm{i}\sqrt{3/16}|33) - \mathrm{i}\sqrt{5/16}|31) - \mathrm{i}\sqrt{5/16}|3-1) + \mathrm{i}\sqrt{3/16}|3-3),$$

$$|3T_1EB_3) = \sqrt{5/16}|33) - \sqrt{3/16}|31) + \sqrt{3/16}|3-1) - \sqrt{5/16}|3-3),$$

$$|3T_2EB_3) = \sqrt{3/16}|33) + \sqrt{5/16}|31) - \sqrt{5/16}|3-1) - \sqrt{3/16}|3-3), \quad (22)$$

in terms of the state vectors $|3m)$ adapted to the chain $SO(3) \supset SO(2)$.

For the operator X_4, we obtain (in units of a_4) three singlets of symmetry $\Gamma(D_4) = A_2$, B_1 and B_2

$$W_4(3A_2) = \frac{6}{5}f(-2+f),$$

$$W_4(3B_1) = -[5]! + 6\left(44 - \frac{42}{5}f + \frac{1}{5}f^2\right),$$

$$W_4(3B_2) = +[5]! + 6\left(44 - \frac{42}{5}f + \frac{1}{5}f^2\right), \quad (23)$$

and two doublets of symmetry $\Gamma(D_4) = E$

$$W_4(3E)_\pm = \frac{1}{2}\left[\alpha_4 + \beta_4 \pm \sqrt{(\alpha_4 - \beta_4)^2 + 4\gamma_4^2}\right], \quad (24)$$

where

$$\alpha_4 = +\frac{1}{4}\sqrt{15}\sqrt{[6]!}\sqrt{f} + 6\left(129 - \frac{62}{5}f + \frac{1}{5}f^2\right),$$

$$\beta_4 = -\frac{1}{4}\sqrt{15}\sqrt{[6]!}\sqrt{f} + 6\left(79 - \frac{42}{5}f + \frac{1}{5}f^2\right),$$

$$\gamma_4 = -\frac{1}{4}\sqrt{[6]!}\sqrt{f} + 6\sqrt{15}(25 - 2f). \quad (25)$$

In Eqs. (23) and (25), we have set $[5]! = [4]![5]_{qp}$, $[6]! = [5]![6]_{qp}$ and $f = [3]_{qp}[4]_{qp}$. The energies of the doublets result from the interaction via X_4 of the state vectors of symmetry T_1EB_2 and T_2EB_2 (or equivalently T_1EB_3 and T_2EB_3).

For the operator X_6, the energies (in units of a_6) of the singlets of symmetry $\Gamma(D_4) = A_2$, B_1 and B_2 are

$$W_6(3A_2) = \frac{10}{21}f(-12 + 8f - f^2),$$

$$W_6(3B_1) = +(6-f)[5]! + 10\left(264 - \frac{480}{7}f + \frac{92}{21}f^2 - \frac{1}{21}f^3\right),$$

$$W_6(3B_2) = -(6-f)[5]! + 10\left(264 - \frac{480}{7}f + \frac{92}{21}f^2 - \frac{1}{21}f^3\right), \tag{26}$$

while the energies of the doublets of symmetry $\Gamma(D_4) = E$ are

$$W_6(3E)_\pm = \frac{1}{2}\left[\alpha_6 + \beta_6 \pm \sqrt{(\alpha_6 - \beta_6)^2 + 4\gamma_6^2}\right], \tag{27}$$

where the matrix elements α_6, β_6 and γ_6 are given by

$$\alpha_6 = -\frac{1}{4}\sqrt{15}\sqrt{[6]!}\sqrt{f}(17-f) + 10\left(1377 - \frac{1285}{7}f + \frac{134}{21}f^2 - \frac{1}{21}f^3\right),$$
$$\beta_6 = +\frac{1}{4}\sqrt{15}\sqrt{[6]!}\sqrt{f}(17-f) + 10\left(831 - \frac{795}{7}f + \frac{92}{21}f^2 - \frac{1}{21}f^3\right),$$
$$\gamma_6 = +\frac{1}{4}\sqrt{[6]!}\sqrt{f}(17-f) + 10\sqrt{15}(273 - 35f + f^2). \tag{28}$$

The two doublets arise from the interaction via X_6 of some cubical levels of symmetry $\Gamma(O) = T_1$ and T_2.

In the limiting situation where $p = q^{-1} = 1$, Eqs. (23) to (28) lead to the energy levels corresponding to the ordinary cubical potentials of the degrees 4 and 6. In this situation, both the operators X_4 and X_6 yield a singlet of symmetry $\Gamma(O) = A_2$ and two triplets of symmetry $\Gamma(O) = T_1$ and T_2. For arbitrary values of q and p, the energy levels for X_4 and X_6 are characterized by IRC's of the group D_4. As for d electrons, we have an $O \to D_4$ symmetry breaking described here by

$$A_2 \to B_1, \quad T_1 \to A_2 \oplus E, \quad T_2 \to B_2 \oplus E. \tag{29}$$

As a conclusion, the energy levels for f electrons in a qp-quantized cubical potential exhibit the same degeneracies as the ones for f electrons in an ordinary tetragonal potential (involving one invariant of the degree 0, one invariant of the degree 2, two invariants of the degree 4, and two invariants of the degree 6).

5. Conclusions and perspectives

The main point of this paper may be summed up as follows. The q- or qp-quantization of an operator $T(\mathcal{J})$ defined in the enveloping algebra of $u(2)$ and invariant under a subgroup G of $O(3)$ yields an operator $T(J)$ the spectrum of which (on a subspace $\varepsilon(j)$ of constant angular momentum j) exhibits the degeneracy allowed by a subgroup H of G.

We have proved the latter point in the special case where $T(J)$ corresponds to cubical invariants of interest for d and f electrons in crystalline fields. As a net result, we have obtained that a qp-quantization of the cubical invariants of the degrees 4 and 6 is equivalent to a symmetry breaking of the type $G = O \to H = D_4$. Our proof has been concerned with the subspaces $\varepsilon(2)$ and $\varepsilon(3)$ that characterize d and f electrons, respectively, in the absence of the spin–orbit interaction. Actually, it is possible to show that the $O \to D_4$ symmetry breaking manifests itself equally well when the subspaces $\varepsilon(2)$ and $\varepsilon(3)$ are replaced by $\varepsilon(3/2) \oplus \varepsilon(5/2)$ and $\varepsilon(5/2) \oplus \varepsilon(7/2)$, respectively, i.e., when the spin–orbit interaction is taken into consideration.

It would be interesting to examine the conjecture addressed in the present work in more general mathematical terms. In particular, one may ask the question:

what are the possible subgroups H which may arise from a given group G ? The answer to this question is probably not unique. In this respect, should we have taken the potentials of the degrees 4 and 6 written in an $SO(3) \supset O \supset D_3 \supset C_3$ basis, i.e., oriented according to a C_3 axis, we would have obtained probably a symmetry breaking of type $O \to D_3$.

As another perspective, it would be also useful to attack the problem considered in this paper by using a qp-version of the $SU(2)$ unit tensor investigated in Ref. [21].

We hope to return on these matters and to apply the symmetry breaking mechanism discovered here (to the Jahn–Teller effect as well as to electron spin resonance) in forthcoming papers.

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